

1 **Title:** Numerical Modeling of Self-Potential in Subsurface Reservoirs

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3 **Author names and affiliations:**

4 Mutlaq Alarouj^{1,2}

5 Amadi Ijioma¹

6 Malcolm Thomas Graham^{1,3}

7 Donald John MacAllister^{1,4}

8 Matthew David Jackson¹

9 ¹: Novel Reservoir Modelling and Simulation Group, DEPARTMENT OF EARTH SCIENCE AND
10 ENGINEERING, Imperial College London, SW7 2AZ, United Kingdom

11

12 ²: Kuwait Oil Company, 61008 Ahmadi, Kuwait

13 ³: Now at: Atkins, Woodcote Grove, Ashley Road, Epsom, United Kingdom

14 ⁴: Now at: British Geological Survey, Lyell Centre, Research Avenue South, Edinburgh

15 ¹

16 **Corresponding author:**

17 Mutlaq Alarouj

18 Email: m.alarouj17@imperial.ac.uk

19 **Link to the code:** <https://github.com/mutlaqalarouj/SP-SOLVER.git>

20 **Highlights:**

- 21
- Introduce a new tool for numerical simulating self-potential in subsurface reservoirs.
 - Validate the accuracy of the new tool on single- and multiphase test cases.
 - Demonstrate the application of the tool on an oil reservoir supported by water injection.
- 22
- 23

¹ **Authorship Statement:**

Mutlaq Alarouj: Wrote new sections of code handling variable polarity, LGRs, faults. Produced all results. Wrote first draft of paper.

Amadi Ijioma: Wrote early version of code, which this work further develops.

Malcolm Thomas Graham: Modified early version of code, to improve performance and stability.

Donald John MacAllister: Modified early version of code, which this work further develops.

Matthew David Jackson: Guidance on underlying physics, test solutions, case studies. Revised paper and figures.

ABSTRACT

24
25 We report a new, open-source, MATLAB-based 3D code for numerically simulating the self-potential
26 (SP) in subsurface reservoirs. The code works as a post-processor, using outputs from existing
27 reservoir flow and transport simulators at a selected timestep to calculate the SP throughout the
28 reservoir model. The material properties required to calculate the SP are user defined and may be
29 constant or vary in each cell. The code solves the equations governing flow and transport of electrical
30 charge and global charge conservation using a control-volume-finite-difference scheme. Electrical
31 currents associated with the SP may spread beyond the reservoir model domain, and the code allows
32 for the domain to be extended vertically and laterally to account for this. Here, we present the
33 governing equations and the numerical method used and demonstrate application of the code using
34 an example in which we predict the SP signals associated with oil production from a subsurface
35 reservoir supported by water injection.

Keywords

36
37 Self-Potential – Subsurface Reservoirs – Electrokinetic Potential – Exclusion-Diffusion potential –
38 Thermoelectrical potential.

39

1. Introduction

40
41 The self-potential (SP) is a naturally occurring electrical potential that can be measured using
42 electrodes at the Earth surface or in boreholes. Measurement of the SP is one of the oldest
43 geophysical surveying methods with numerous applications (Jackson, 2015). Here, we focus on the
44 use of SP to characterize and monitor water flow and the associated transport of salt species and/or
45 heat in subsurface reservoirs. Numerous studies have investigated the SP associated with water flow
46 in geothermal reservoirs (e.g., Corwin and Hoover, 1979; Revil and Pezard, 1998; Darnet et al., 2004)
47 and during volcanic unrest (e.g., Zlotnicki and Nishida, 2003; Ishido, 2004; Finizola et al., 2004; Mauri
48 et al., 2010); groundwater flow in aquifers (e.g., Fagerlund and Heinson, 2003; Titov et al., 2005; Linde
49 et al., 2011; Jackson et al., 2012a; Hu et al., 2020); water flow in hydraulically active fractures (e.g.,
50 Revil and Pezard, 1998; Wishart et al., 2006, Roubinet et al., 2016, DesRoches et al. 2018; Jougnot et

51 al., 2020); contaminant transport in aquifers (e.g., Naudet et al., 2003, 2004; Minsley et al., 2007; Linde
52 and Revil, 2007; Jougnot et al., 2015); saltwater intrusion in coastal aquifers (MacAllister et al., 2018;
53 Graham et al., 2018), and water flow during hydrocarbon production (Saunders et al., 2008; Gulamali
54 et al., 2011; Jackson et al., 2012b; Ijioma, 2016). The SP method has also been found very useful in
55 mineral exploration (e.g., Caglar, 2000; Murthy et al., 2005; Abdelrahman et al., 2008; Di Maio et al.,
56 2016) and more recently eco-hydrology (Voytek et al. 2019). However, prediction or interpretation of
57 the SP in these subsurface environments is challenging as there may be several source mechanisms;
58 moreover, flow and transport paths may be complicated by geological heterogeneity.

59 The aim of this paper is to report a new, open-source, MATLAB-based 3D code for numerically
60 simulating the self-potential (SP) in subsurface reservoirs. Sources of SP in natural environments are
61 numerous (e.g. Jackson, 2015) and here we restrict ourselves to the SP arising in partially or entirely
62 water-saturated rocks in response to gradients in pressure (above hydrostatic, also termed water
63 potential or head), water composition (salt concentration) and temperature. Numerous studies have
64 described these SP source mechanisms (e.g. Ishido and Mizutani, 1981; Hunter, 1986; Revil et al.,
65 1999a; Revil, 1999; Jackson et al., 2012b) and we provide a summary for the interested reader in
66 Appendix A. A number of codes to simulate SP have been reported in the literature, but are limited
67 to modelling the SP arising from pressure gradients in water saturated rocks (e.g., Soueid Ahmed et
68 al, 2013; Rücker et al., 2017).

69 The new code works as a post-processor, taking outputs from existing reservoir flow and transport
70 simulators at a selected timestep, and calculating the SP throughout the reservoir model using the
71 simulated values of water saturation, pressure, concentration and temperature. The additional
72 material parameters required to calculate the SP are user defined and may be constant or vary in each
73 cell. Earlier versions of the code have been used previously in studies of saline intrusion into
74 freshwater aquifers (MacAllister et al., 2018; Graham et al., 2018), and oil production from
75 hydrocarbon reservoirs (Ijioma, 2016). However, the governing equations and method of solution

76 were not reported in these studies and the code has not hitherto been made available. Additional
 77 functionality included here also allows local grid refinement and simulation of SP in models of faulted
 78 reservoirs.

79 The code solves the equations governing flow and transport of electrical charge and global charge
 80 conservation using a control-volume-finite-difference scheme on the reservoir 3D mesh. Electrical
 81 currents associated with the SP may spread beyond the reservoir model domain, and the code allows
 82 for the domain to be extended vertically and laterally to account for this. The code can be used to
 83 predict the SP in a given reservoir, which is useful for (i) designing and implementing SP monitoring
 84 programmes, (ii) interpreting SP measurements from existing monitoring programmes, and (iii)
 85 understanding SP source mechanisms and the link between source mechanisms and flow and
 86 transport processes in the reservoir. Future applications could include inversion of SP measurements
 87 for reservoir properties of interest. The code can be used in a broad range of subsurface reservoir
 88 types including aquifers, geothermal reservoirs, targets for CO₂ storage, and hydrocarbon reservoirs.
 89 We present the governing equations and the numerical methods used to solve these and show that
 90 the code returns the correct solution for some simple test cases. We demonstrate application of the
 91 code using an example in which we predict the SP signals associated with oil production from a
 92 subsurface reservoir supported by water injection.

93 2. Governing equations

94 Assuming that water is the only charge-carrying fluid in the rock pore space, the general form of the
 95 constitutive equations used to describe the coupled problem can be written as (De Groot and Mazur,
 96 1962)

$$97 \begin{pmatrix} j \\ q_w \\ h \\ v \end{pmatrix} = - \begin{bmatrix} \sigma_{fs}(S_w) & L_{EK} & L_{TE} & L_{ED} \\ L_{EK} & \frac{kk_{rw}(S_w)}{\mu_w} & A_1 & A_2 \\ L_{TE} & A_1 & K(S_w) & A_3 \\ L_{ED} & A_2 & A_3 & D(S_w) \end{bmatrix} \begin{bmatrix} \nabla U \\ \nabla \Phi \\ \nabla T \\ \nabla C_f \end{bmatrix} \quad (1)$$

98 where j is the current density ($A \cdot m^{-2}$), σ_{fs} is the saturated rock electrical conductivity ($S \cdot m^{-1}$), S_w is the
99 water saturation, ∇U is the electrical potential gradient ($V \cdot m^{-1}$), q_w is the water Darcy velocity ($m \cdot s^{-1}$),
100 k is the rock absolute permeability (m^2), k_{rw} is the relative permeability of water (fraction), μ_w is the
101 dynamic viscosity of water ($Pa \cdot s$), $\nabla \Phi$ is the pressure gradient above hydrostatic (or water potential in
102 $Pa \cdot m^{-1}$) where $\Phi = P_w - \rho_w g z$, h is the heat flux ($W \cdot m^{-2}$), K is thermal conductivity ($W \cdot m^{-1} \cdot K^{-1}$), ∇T is
103 the temperature gradient ($K \cdot m^{-1}$), v is the concentration flux ($M \cdot s^{-1} \cdot m^{-2}$), D is the diffusion coefficient
104 ($m^2 \cdot s^{-1}$), and ∇C_f is the concentration gradient ($M \cdot m^{-1}$).

105 The on-diagonal terms in equation (1) appear in the well-known constitutive equations of Ohm's law,
106 Darcy's law, Fourier's law, and Fick's law, respectively. The matrix is symmetric in linear
107 thermodynamic systems in which fluxes are linear functions of thermodynamic forces
108 (∇U , $\nabla \Phi$, ∇T and ∇C_f) (De Groot and Mazur, 1962). The off-diagonal terms L_{EK} , L_{ED} and L_{TE} are the
109 electrokinetic (EK), exclusion-diffusion (ED), and thermoelectrical (TE) cross-coupling terms,
110 respectively. These terms describe the cross-coupling between electrical current and gradients in
111 water potential, concentration, and temperature. The off-diagonal terms A_1 through A_3 represent
112 cross-coupling terms governing the interactions between fluxes and gradients in electrical potential,
113 water potential, temperature, and concentration that are not considered here.

114 The water flux, heat flux, and ion species flux can be calculated using existing commercial and
115 academic reservoir flow and transport simulators such as Eclipse (Schlumberger, 2010), TOUGH2
116 (Pruess et al., 1999), IC-FERST (e.g. Gomes et al., 2016), the Matlab Reservoir Simulation Toolkit
117 (MRST; Lie, 2019), SUTRA3D (Voss and Provost, 2002) and many more. These simulators neglect the
118 cross-coupling terms L because their impact on the calculated fluxes is negligible in the reservoirs of
119 interest (Ishido and Mizutani, 1981; Wurmstich and Morgan, 1994; Revil et al., 1999b; Saunders et al.,
120 2008). Given this, we can solve for the electrical current independently from the flux calculations in a
121 'post-processing' step, given the water potential, temperature, and concentration fields obtained
122 from reservoir simulation.

123 3. Numerical solution

124

125 3.1. Electrodynamic Problem

126 The equation governing transport of charge solved here, which includes the cross-coupling of current
127 flow j with gradients in water potential, concentration and temperature, is extracted from equation
128 (1)

$$129 \quad j = -\sigma_{fs}(S_w)\nabla U - L_{EK}(S_w)\nabla\Phi - L_{ED}(S_w)\nabla C_f - L_{TE}(S_w)\nabla T \quad (2)$$

130 The coupling terms L_x are functions of the electrical conductivity of the fluid saturated rock σ_{fs} and
131 the so-called coupling coefficients c_x (Jackson et al., 2010)

$$132 \quad L_x = \sigma_{fs}c_x \quad (3)$$

133 where subscript x represents EK, ED, or TE. The coupling coefficients (c_x) are petrophysical properties
134 that relate electrical potential to gradients in water potential, concentration and temperature, and
135 have units of $V\cdot Pa^{-1}$, $V\cdot M^{-1}$ and $V\cdot K^{-1}$, respectively.

136 Given that charge is conserved and assuming no net current flow across the boundaries of the model
137 domain, then

$$138 \quad \nabla \cdot j = 0 \quad (4)$$

139 Combining equations (2) and (4) results in

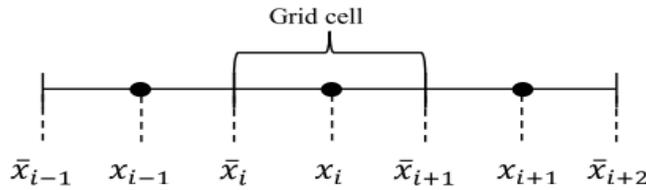
$$140 \quad \nabla \cdot (\sigma_{fs}(S_w)\nabla U) = -\nabla \cdot (L_{EK}(S_w)\nabla\Phi) - \nabla \cdot (L_{ED}(S_w)\nabla C_f) - \nabla \cdot (L_{TE}(S_w)\nabla T) \quad (5)$$

141 In order to solve for the SP (U), equation (5) is discretized and solved for given values of saturation
142 (S_w), water potential (Φ), salt concentration (C_f), and temperature (T), and appropriate values of
143 σ_{fs} , L_{EK} , L_{ED} , and L_{TE} . The S_w , Φ , C , and T data are obtained using any commercial or academic
144 reservoir simulator. The resulting values usually represent discrete properties defined at the center of
145 each grid cell of the model. To be consistent with this, we use a control-volume-finite-difference
146 method to discretize and solve equation (5). We assume the simulator uses either a regular Cartesian

147 grid or a cornerpoint grid. Many commercial and academic reservoir simulation codes are compatible
 148 with these schemes for discretizing space (e.g. Schlumberger, 2010; Voss and Provost, 2002).

149 3.2. Discretization for Numerical Solution

150 A one-dimensional system is used to explain the discretization (Figure 1). The domain is divided into
 151 grid cells with properties of interest defined at the center of each cell.



152

153

Figure 1: An example of a 1-D grid system

154 For simplicity, the numerical solution will be demonstrated considering only the EK potential; the
 155 procedure is the same to obtain the ED and TE potentials, replacing water potential Φ by
 156 concentration C or temperature T , and L_{EK} by L_{ED} or L_{TE} respectively.

157 For a non-boundary cell such as cell i in Figure 1, equation (5) can be written as

$$159 \quad \frac{d}{dx} \left(\sigma_{fs} \frac{dU}{dx} + L_{EK} \frac{d\Phi}{dx} \right) = 0 \quad (6)$$

158

160 Integrating equation (6) over cell i results in

$$161 \quad \int_{\bar{x}_i}^{\bar{x}_{i+1}} \frac{d}{dx} \left(\sigma_{fs} \frac{dU}{dx} + L_{EK} \frac{d\Phi}{dx} \right) dx$$

$$162 \quad = \left[\left(\sigma_{fs} \frac{dU}{dx} \right)_{\bar{x}_{i+1}} - \left(\sigma_{fs} \frac{dU}{dx} \right)_{\bar{x}_i} \right] + \left[\left(L_{EK} \frac{d\Phi}{dx} \right)_{\bar{x}_{i+1}} - \left(L_{EK} \frac{d\Phi}{dx} \right)_{\bar{x}_i} \right] = 0$$

163 (7)

164 Substituting $\frac{dU}{dx}$ and $\frac{d\Phi}{dx}$ with their central difference approximation leads to

165
$$\left[\left(\sigma_{fs\bar{x}_{i+1}} \frac{U_{x_{i+1}} - U_{x_i}}{x_{i+1} - x_i} \right) - \left(\sigma_{fs\bar{x}_i} \frac{U_{x_i} - U_{x_{i-1}}}{x_i - x_{i-1}} \right) \right] + \left[\left(L_{EK\bar{x}_{i+1}} \frac{\Phi_{x_{i+1}} - \Phi_{x_i}}{x_{i+1} - x_i} \right) - \left(L_{EK\bar{x}_i} \frac{\Phi_{x_i} - \Phi_{x_{i-1}}}{x_i - x_{i-1}} \right) \right] = 0$$

166 (8)

167 where variables U_{x_i} and Φ_{x_i} are identified at cell centers and $\sigma_{fs\bar{x}_i}$ and $L_{EK\bar{x}_i}$ are identified at cell
 168 faces. To further simplify equation (8), it can be written as

169
$$a_{\bar{x}_{i+1}} U_{x_{i+1}} + a_p U_{x_i} + a_{\bar{x}_{i-1}} U_{x_{i-1}} = b_{\bar{x}_{i+1}} \Phi_{x_{i+1}} + b_p \Phi_{x_i} + b_{\bar{x}_{i-1}} \Phi_{x_{i-1}}$$
 (9)

170 where

172
$$a_{\bar{x}_{i+1}} = \frac{\sigma_{fs\bar{x}_{i+1}}}{x_{i+1} - x_i} \quad (10a), \quad a_{\bar{x}_{i-1}} = \frac{\sigma_{fs\bar{x}_i}}{x_i - x_{i-1}} \quad (10b)$$

171

173
$$a_p = -\frac{\sigma_{fs\bar{x}_{i+1}}}{x_{i+1} - x_i} - \frac{\sigma_{fs\bar{x}_i}}{x_i - x_{i-1}} = -(a_{\bar{x}_{i+1}} + a_{\bar{x}_{i-1}}) \quad (10c)$$

175
$$b_{\bar{x}_{i+1}} = -\frac{L_{EK\bar{x}_{i+1}}}{x_{i+1} - x_i} \quad (11a), \quad b_{\bar{x}_{i-1}} = -\frac{L_{EK\bar{x}_i}}{x_i - x_{i-1}} \quad (11b)$$

174

176
$$b_p = \frac{L_{EK\bar{x}_{i+1}}}{x_{i+1} - x_i} + \frac{L_{EK\bar{x}_i}}{x_i - x_{i-1}} = -(b_{\bar{x}_{i+1}} + b_{\bar{x}_{i-1}}) \quad (11c)$$

177 Equation (9) can be applied to all non-boundary cells. In boundary cells, we choose to set $\nabla U = 0$
 178 consistent with equation (4) which assumes no current enters or leaves the domain, by assigning
 179 virtual cells outside of the model boundary with the same electrical potential as the boundary cells.

180 3.3. Interface Properties

181 Solution of equations 9 - 11 requires values for the properties at the interface between connected grid
 182 cells ($\sigma_{fs\bar{x}_{i+1}}$ and $L_{EK\bar{x}_i}$). Earlier approaches (Ijioma, 2016; Graham et al., 2018) used a harmonic
 183 average of the cell-center values, which is a reasonable assumption when the polarity of the coupling
 184 terms L for the two connected grid cells are the same. However, coupling terms can have variable

185 polarity, depending on the rock mineralogy, brine composition and mineral surface wettability (e.g.
 186 Leinov and Jackson 2014; Jackson et al. 2016). Thus, there is no guarantee that the coupling terms in
 187 each connected cell have the same polarity. When they have opposing polarity, the harmonic mean
 188 is not the appropriate averaging scheme to calculate the coupling term at the interface.

189 The new averaging scheme proposed in this paper uses conservation of charge to recognize that the
 190 total current (sum of the conduction and streaming currents) must be continuous at the interface to
 191 give

$$192 \quad I_{\bar{x}_{i+1}} = -\sigma_{fs_{\bar{x}_{i+1}}} \nabla U_{\bar{x}_{i+1}} - L_{EK_{\bar{x}_{i+1}}} \nabla \Phi_{\bar{x}_{i+1}} \quad (12a)$$

$$193 \quad I_{x_i} = -\sigma_{fs_{x_i}} \nabla U_{x_i} - L_{EK_{x_i}} \nabla \Phi_{x_i} \quad (12b)$$

$$194 \quad I_{x_{i+1}} = -\sigma_{fs_{x_{i+1}}} \nabla U_{x_{i+1}} - L_{EK_{x_{i+1}}} \nabla \Phi_{x_{i+1}} \quad (12c)$$

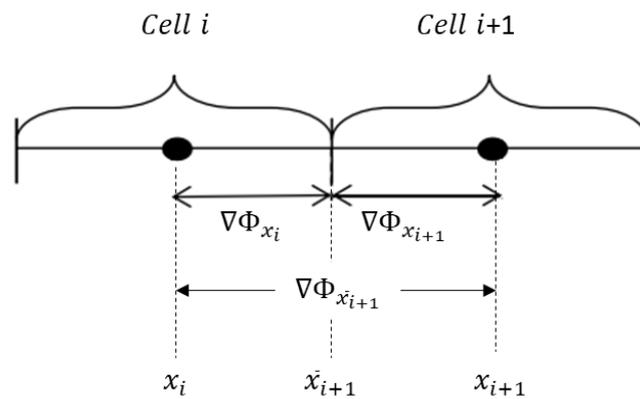
195
 196 where x_i and x_{i+1} are the location of the centers of grid cells i and $i + 1$, while \bar{x}_{i+1} represent the
 197 location of the interface between the two grid cells (Figure 2). The subscripts in equation (12) reflect
 198 the location at which each property (I , σ_{fs} , ∇U or L_{EK}) is calculated. The first term on the right-hand
 199 side of equation (12) describes the conduction current while the second term represents the
 200 streaming current. The interface properties are calculated assuming continuous total current ($I_{\bar{x}_{i+1}} =$
 201 $I_{x_i} = I_{x_{i+1}}$). The final equations for calculating the interface properties are as follows (the derivation
 202 is shown in Appendix B)

$$203 \quad \sigma_{fs_{\bar{x}_{i+1}}} = \frac{\sigma_{fs_{x_i}} \sigma_{fs_{x_{i+1}}} (x_{i+1} - x_i)}{(x_{i+1} - \bar{x}_{i+1}) \sigma_{fs_{x_i}} + (\bar{x}_{i+1} - x_i) \sigma_{fs_{x_{i+1}}}} \quad (13)$$

$$204 \quad L_{EK_{\bar{x}_{i+1}}} = \frac{\sigma_{fs_{x_{i+1}}} L_{EK_{x_i}} (\bar{x}_{i+1} - x_i) + \sigma_{fs_{x_i}} L_{EK_{x_{i+1}}} (x_{i+1} - \bar{x}_{i+1})}{(x_{i+1} - \bar{x}_{i+1}) \sigma_{fs_{x_i}} + (\bar{x}_{i+1} - x_i) \sigma_{fs_{x_{i+1}}}} \quad (14)$$

206 The same formulations are used for the EC and TE potentials, replacing L_{EK} and $\nabla\Phi$ by L_{EC} and ∇C or
 207 L_{TE} and ∇T , respectively.

208



209

210 Figure 2: Variation in grid properties at the interface between two connected grid cells i and $i + 1$.

211

212 3.4. Fault Modeling

213 Faults represent planar discontinuities in the rock mass across which rock units are offset. These
 214 discontinuities may modify fluid flow, and component and heat transport, depending on the
 215 properties of the fault (Cherubini et al., 2013; Knipe et al., 1998; Nurafiqah et al., 2019). Thus, they
 216 may modify charge transport in response to gradients in water potential, concentration and
 217 temperature. Faults may also modify the conduction currents that maintain overall electroneutrality.
 218 Hence, it is important to include them in reservoir models.

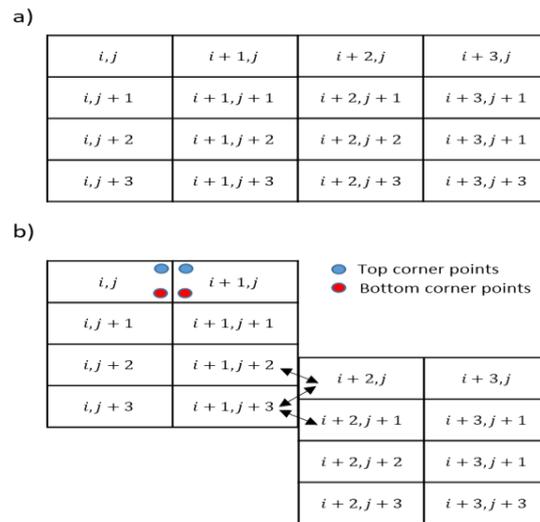
219 In many numerical models, the (cornerpoint) grid follows the geometry of the rock layers and the grid-
 220 cells are offset across fault planes in similar manner to the way in which the rocks are offset (e.g. Qu
 221 et al., 2015; Figure 4). Thus, cells juxtaposed across the fault are not logically neighbors and must be
 222 connected using so-called 'non-neighbor' connections (NNCs; e.g. Schlumberger, 2010).

223 In our example faulted grid (Figure 3b), grid cells $(i + 1, j + 2)$ and $(i + 2, j)$ are juxtaposed across
 224 the fault and NNCs must be defined between these cells to model charge transport across the fault.
 225 We also need to identify new boundary cells resulting from the offset of the grid across the fault. In

226 our example faulted grid (Figure 3b), grid cell $(i + 1, j + 1)$ is a boundary cell. The SP solver is
227 equipped with built-in functions to specify NNCs and boundary cells in order to correctly model charge
228 transport. Modeling the charge flux into/out of each grid cell requires knowledge of all the grid cells
229 connected to that cell. In our 2D example faulted grid (Figure 3b), grid cell $(i + 1, j + 2)$ has three
230 neighbor connections with cells $(i + 1, j + 1)$, $(i, j + 2)$ and $(i + 1, j + 3)$ and one NNC with cell
231 $(i + 2, j)$.

232 Reservoir simulators that use this approach to represent faults typically generate a list of NNCs across
233 fault surfaces. However, this list may be modified based on a cutoff transmissibility value (default or
234 user defined) below which a NNC is deleted (Schlumberger, 2010). It is assumed that no fluid flow
235 occurs across the deleted NNCs. However, there may be charge transport across these connections
236 depending on the coupling terms and rock conductivity in the cells on each side. Hence, the NNC list
237 calculated for fluid flow in a reservoir simulator may not be suitable for charge transport in the SP
238 solver presented here. Hence, we have developed a bespoke function to generate the NNC list for the
239 SP solver. The NNC list is generated based on the coordinates of the corner points of each cell,
240 identifying any deviation in the grid geometry from the non-faulted case and generating NNC's across
241 the boundaries of all juxtaposed cells (Figure 3). For the non-faulted case, the depths of the corner
242 points at the interface between each two neighboring cells are the same, while in the presence of
243 fault, layers offset across the fault interface, and hence, the depths of the corner points are not the
244 same. The NNC list is generated by comparing the vertical offset in the depths of the corner points
245 between all the cells across the fault interface. The layers offset may not be uniform resulting in
246 multiple NNCs for one cell (figure 3b, grid Cell $(i + 1, j + 3)$). In this case, the interface properties
247 calculated according equations (13) and (14) need to be corrected by multiplying by the ratio of the
248 cross-sectional area in contact with each non-logical neighbor to the total cross-section area. The
249 modeling approach described in this section deals with sealing faults only. However, faults could be
250 hydraulically active; in this case, the SP may behave differently across the fault interface (e.g., Revil

251 and Pezard, 1998; Wishart et al., 2006, Roubinet et al., 2016, DesRoches et al. 2018; Jougnot et al.,
 252 2020). Modelling of the SP arising from flow in faults remains an area of active research.



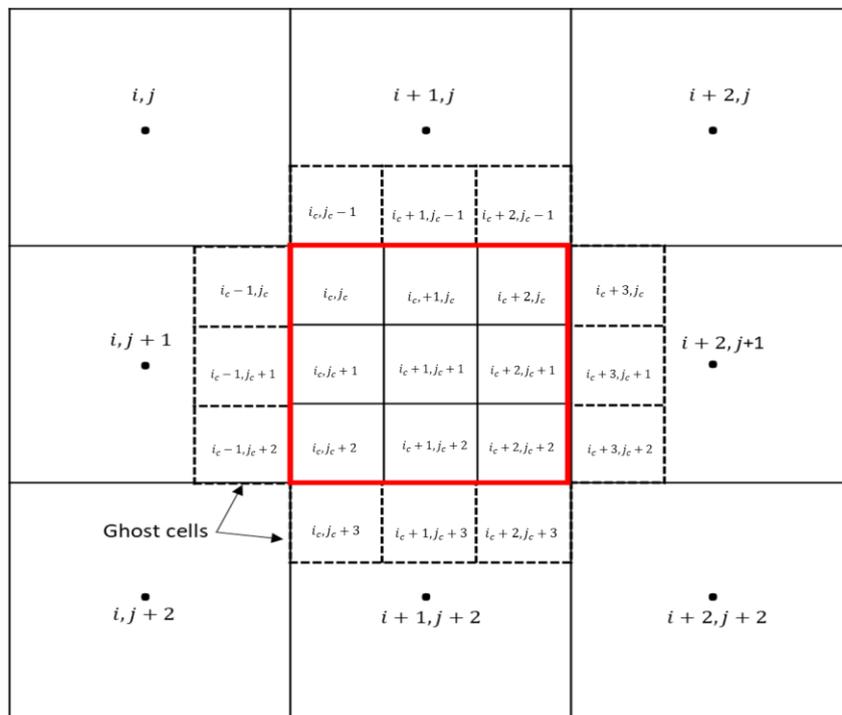
253
 254 Figure 3: a) Example of an unfaulted 2D mesh. b) Example of a 2D mesh offset across a simple
 255 vertical fault. Arrows represent the non-neighbor connections that allow flow and transport
 256 between cells on opposite sides of the fault.

257
 258 **3.5. Local Grid Refinement**

259 In many models used to simulate SP monitoring scenarios, the grid resolution that provides a
 260 reasonable approximation of fluid flow and heat and mass transport is too coarse for accurate
 261 prediction of the SP, especially in the vicinity of SP monitoring locations where it may be necessary to
 262 capture changes in the hydrodynamic properties (e.g. water saturation, potential, concentration and
 263 temperature) at higher resolution. However, refining the grid across the entire model domain may be
 264 excessively computationally expensive. Instead, it may be sufficient to locally refine the grid (termed
 265 here ‘Local Grid Refinement’ (LGR) or ‘child’ model) around SP monitoring locations within the coarse
 266 (‘parent’) model (Ijioma, 2016; Figure 4). Many commercial and academic reservoir simulation codes
 267 allow LGR and we include functionality to allow these LGRs to be included in the SP solver.

268 We use a ‘ghost-node’ model-linking method (James et al. 2006) to couple the parent model with the
 269 LGR with appropriate LGR boundary conditions. The SP is simulated on the parent model, and the

270 electrical (SP, rock conductivity, coupling terms) and dynamic water saturation, potential,
 271 concentration and temperature) properties in each parent grid cell bordering the LGR are used to
 272 determine boundary conditions for simulating SP within the LGR. At the boundaries of the LGR, ghost
 273 cells similar in dimension to the LGR cells are placed in the parent cells (e.g. cells: $i_c - 1, j_c$ in Figure
 274 4). Properties for these ghost cells are calculated by linearly interpolating values between the parent
 275 cells. For example, pressure and SP for ghost cell $i_c - 1, j_c$ (Figure 4) are interpolated between the
 276 parent cell hosting that ghost cell ($i, j + 1$ in Figure 4) and the parent cell hosting the LGR ($i + 1, j + 1$
 277 in Figure 4). The electrodynamic model is then solved within the LGR subjected to the boundary
 278 conditions identified in the ghost cells.



279
 280 Figure 4: Example LGR within the parent grid (denoted by the red boundary). Cells outlined by dashed
 281 lines are the ghost cells introduced at the boundaries of the LGR. Subscript c (e.g., i_c, j_c) denotes cells
 282 within the LGR or ghost cells at the LGR boundaries.

283
 284 **3.6. Electrical Properties**

285 In order to solve equation (2), the concentration and temperature dependent material properties
 286 (rock conductivity (σ_{fs}) and coupling terms (L_{EK}, L_{ED}, L_{TE})) must be specified. The operation of the

287 SP solver is independent of the models used to describe these material properties and the user can
288 modify the code to implement their own preferred descriptions. We outline in Appendix C the
289 approach we use in the code at present, and that was used to obtain the results presented.

290 3.7. Numerical Solution of the Linear System of Discretized Equations

291 Equations 9-11 were used to write the formulation in matrix form considering all the grid cells in the
292 system

$$293 \quad Ax = By \quad (15)$$

294 where A and B are $n \times n$ sparse matrices (n is the total number of grid cells) comprising the a and b
295 terms in equation (9), respectively. x and y are $n \times 1$ vectors representing the unknown EK, ED or TE
296 potential and the known water potential, concentration, or temperature from the reservoir
297 simulation, respectively.

298 MacAllister et al. (2018) and Graham et al. (2018) found that the solution obtained for x using an
299 iterative solver was unstable and highly sensitive to changes in the iterative solver tolerance, and
300 Graham et al. (2018) recommended using a direct solver to obtain a stable solution. Therefore, we
301 typically use a direct solver using the `mldivide` function in MATLAB (APPENDIX D) to solve for x in
302 equation (15). Although slower than the various iterative methods implemented in MATLAB, speed is
303 not essential as we do not need to solve for the SP at numerous timesteps. We solve equation (15)
304 for each of the EK, EC and TE potentials using the appropriate material properties and water potential,
305 concentration or temperature as required. The total SP is obtained by summing over the EK, ED and
306 TE potentials thus obtained.

307 As the SP signal is a potential difference between two points, the modelled SP is the difference in
308 potential between a given location and that of a reference location, which is usually chosen at some
309 distance above the reservoir layer.

310

311 4. Results

312

313 4.1. Model Validation

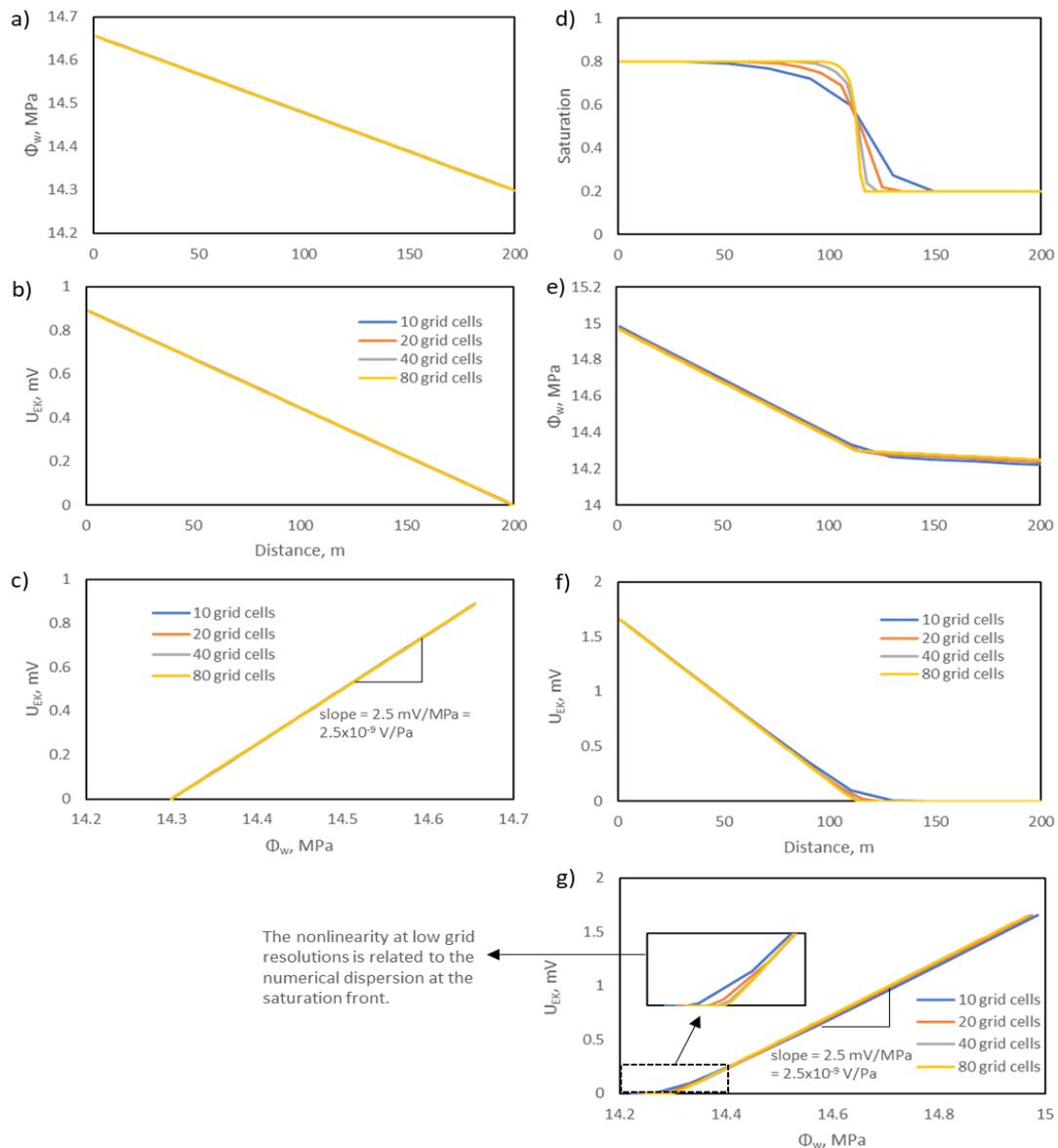
314 A simple 1-D case was used to confirm that the code works correctly. The test case represents a
315 sandstone reservoir measuring 200x100x50m with one oil/water production well and one water
316 injection well. The ECLIPSE reservoir simulator was used to model two scenarios: first, water displacing
317 water to represent single-phase flow and second, water displacing oil to represent two-phase flow.

318 First, we test the EK potential solver. Salinity and temperature were assumed to be constant across
319 the reservoir (0.5 M/L and 80C°), so that EK potential is the only contributor to overall SP. We used a
320 constant value of the EK coupling coefficient for the flow of water at fully water saturated conditions
321 and at the residual non-wetting (oil) phase saturation ($C_{ek}(S_w = 1) = C_{ek}(S_w = 1 - S_{nwr}) = 2.5 \times$
322 10^{-9} VPa^{-1}) (see Appendix C). For the two phase scenarios, we used fluid viscosities and relative
323 permeability curves that yield a piston-like displacement such that oil is flowing at the irreducible
324 water saturation ahead of the displacement front ($S_w = S_{wirr}$) and water is flowing at residual oil
325 saturation behind the front ($S_w = 1 - S_{nwr}$). These material properties were used in the SP solver
326 along with the outputs of the ECLIPSE reservoir simulator (S_w, Φ_w) to predict the EK potential.

327 Results are shown in Figure 5 for both single- and multiphase flow scenarios. For the single-phase
328 scenario, the correct solution yields a linear variation in EK potential from the inlet to the outlet
329 boundary, with the most positive value adjacent to the inlet boundary where the water potential has
330 the largest positive value. Moreover, a cross-plot of EK potential against water potential yields a linear
331 relationship, with the gradient giving the EK coupling coefficient. We find that the SP solver predictions
332 confirm the expected behavior irrespective of the grid resolution tested (Figure 5b), and the coupling
333 coefficient obtained from the numerical solution is identical to the input value to high precision (Figure
334 5c).

335 For the multi-phase scenario, the correct solution yields constant EK potential ahead of the
336 displacement front where there is no water flow, and a linear variation in EK potential from the inlet

337 to the location of the displacement front (see, for example, Figure 14 in Jackson, 2015). Moreover, a
338 cross-plot of EK potential against water potential in the region behind the displacement front yields a
339 linear relationship, with the gradient giving the EK coupling coefficient. As is well known (e.g. Aziz and
340 Settari, 1979), numerical solutions of the multiphase displacement problem are highly dependent on
341 grid resolution. However, as the grid is refined, the Eclipse simulator results converge to capture the
342 correct sharp displacement front across which the water saturation changes sharply and the water
343 phase potential changes gradient (Figure 5d,e). The SP solver results also converge to give the correct
344 solution for the EK potential (Figure 5f); note that the rate of convergence is dominated by
345 convergence of the Eclipse simulation results, not the SP solver itself. Behind the displacement front,
346 the coupling coefficient obtained from the numerical solution approaches the input value as the grid
347 is refined to high precision for the most refined case tested (Figure 5g). Thus, we have confidence
348 that the SP solver returns correct solutions for the EK potential for both single and multiphase flow.



349

350 Figure 5: Numerical solutions from a single timestep of the EK validation model as a function of
 351 distance from the inlet to the outlet boundary. A) Water potential for the single-phase problem. b) EK
 352 potential for the single-phase problem. c) Cross-plots of EK potential against water potential for the
 353 single-phase problem. d) Water saturation for the multiphase problem. e) Water potential for the
 354 multiphase problem. f) EK potential for the multiphase problem. g) Cross-plots of EK potential against
 355 water potential for the multiphase problem. Lines in each plot correspond to different grid resolutions
 356 used in the model between the inlet and outlet boundaries.

357

358 To validate the ED potential solver, we modelled injection of lower salinity (ionic strength) brine
 359 ($C_{inj} = 0.5\text{M/L}$) into a reservoir containing higher salinity brine ($C_{res} = 1\text{M/L}$) using the ECLIPSE
 360 reservoir simulator. We assumed constant reservoir temperature of $80\text{ }^\circ\text{C}$. For the single-phase
 361 scenario, we assumed an exclusion efficiency of zero for the reservoir rock (similar to sandstone; see

362 Appendix C) and described the saturation dependence using equation (C.13) in the multi-phase
363 scenario. These material properties together with the outputs of the ECLIPSE reservoir simulator
364 (S_w, C) were used in the SP solver to predict the ED potential.

365 Results are shown in Figure 6 for both single- and multiphase flow scenarios. The correct solution
366 yields constant ED potential behind the trailing edge of the salinity front and ahead of the leading
367 edge of the salinity front (representing maximum and minimum values). Across the salinity front, the
368 ED potential varies between these two values. We find that the SP solver predictions confirm the
369 expected behavior. However, the grid resolution used significantly affects the modelled variation of
370 the ED potential across salinity front, especially for the multiphase scenario (Figures 6b,f). This is
371 primarily due to the grid-resolution-dependence of the solutions for salinity (and water saturation for
372 the multiphase case) in the ECLIPSE simulator (Fig. 6a,d,e), rather than the solution for ED in our SP
373 solver. As the grid is refined the solutions converge as expected, although high resolution is required
374 for the multiphase case.

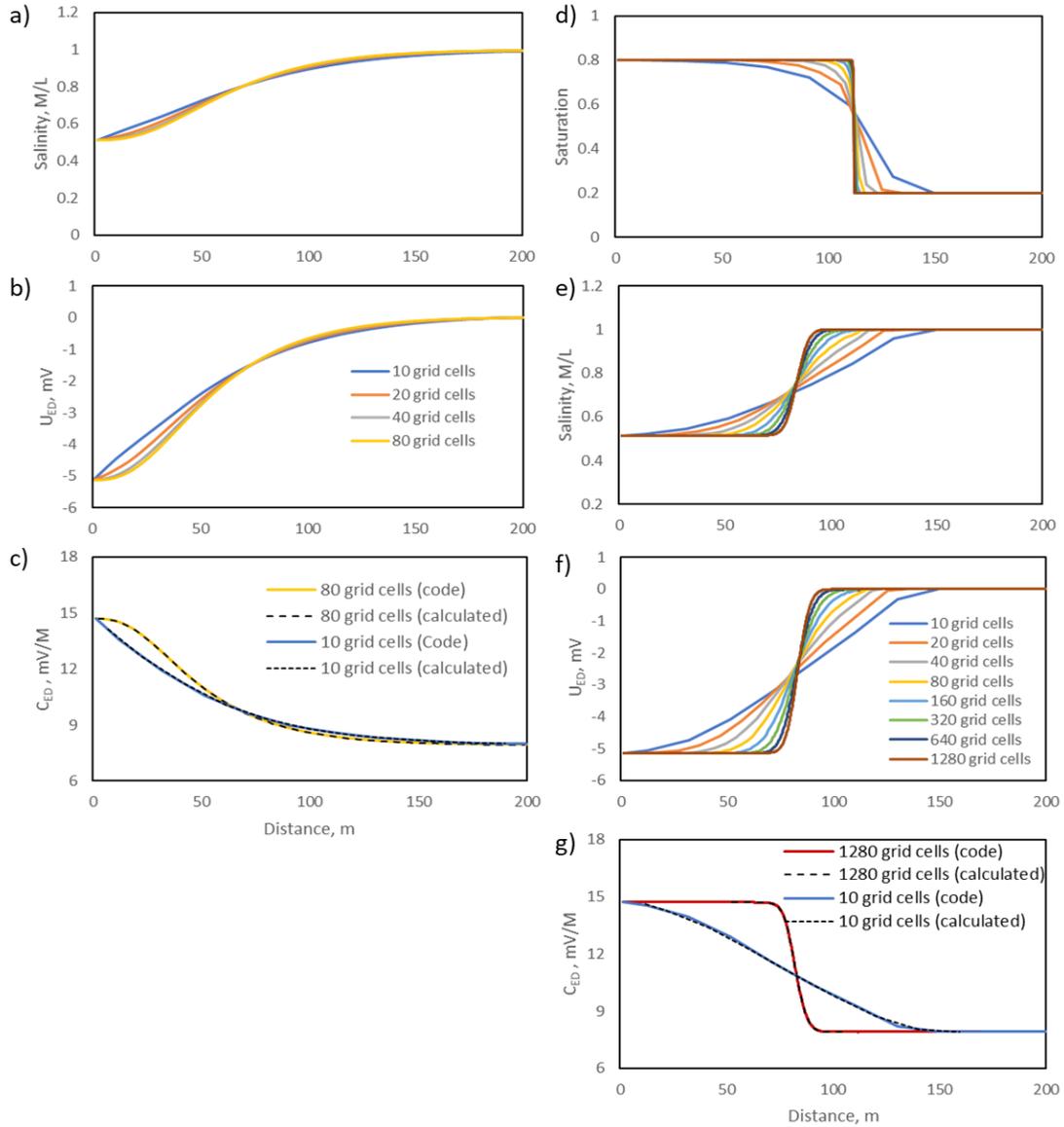
375 We confirm the validity of the SP solver solution by plotting the ED coupling coefficient values used as
376 input to the SP code together with the simulated coefficients, determined using the ED potential
377 determined by the solver and associated salinity (recalling $C_{ED} = \Delta U_{ED} / \Delta C_f$) for each neighboring
378 cells as a function of distance from the inlet to the outlet boundary (Figure 6c,g). The coupling
379 coefficient obtained from the numerical solution is the same as the input value to high precision.
380 Therefore, we have confidence that the SP solver returns correct solutions for the ED potential for
381 both single and multiphase flow.

382 Finally, to validate the TE potential solver, we modelled injection of cooler water ($T_{inj} = 20^\circ\text{C}$) into
383 a hotter reservoir ($T_{res} = 80^\circ\text{C}$) using the ECLIPSE reservoir simulator. Salinity was assumed to be
384 constant ($C_{res} = C_{inj} = 0.5\text{M}$). We again assumed an exclusion efficiency of zero for the reservoir
385 rock for the single-phase scenario and described the saturation dependence of the exclusion efficiency
386 using equation (C.13) in the multi-phase scenario (Appendix C). These material properties together

387 with the outputs of the ECLIPSE reservoir simulator (S_w, T) were used in the SP solver to predict the
388 TE potential.

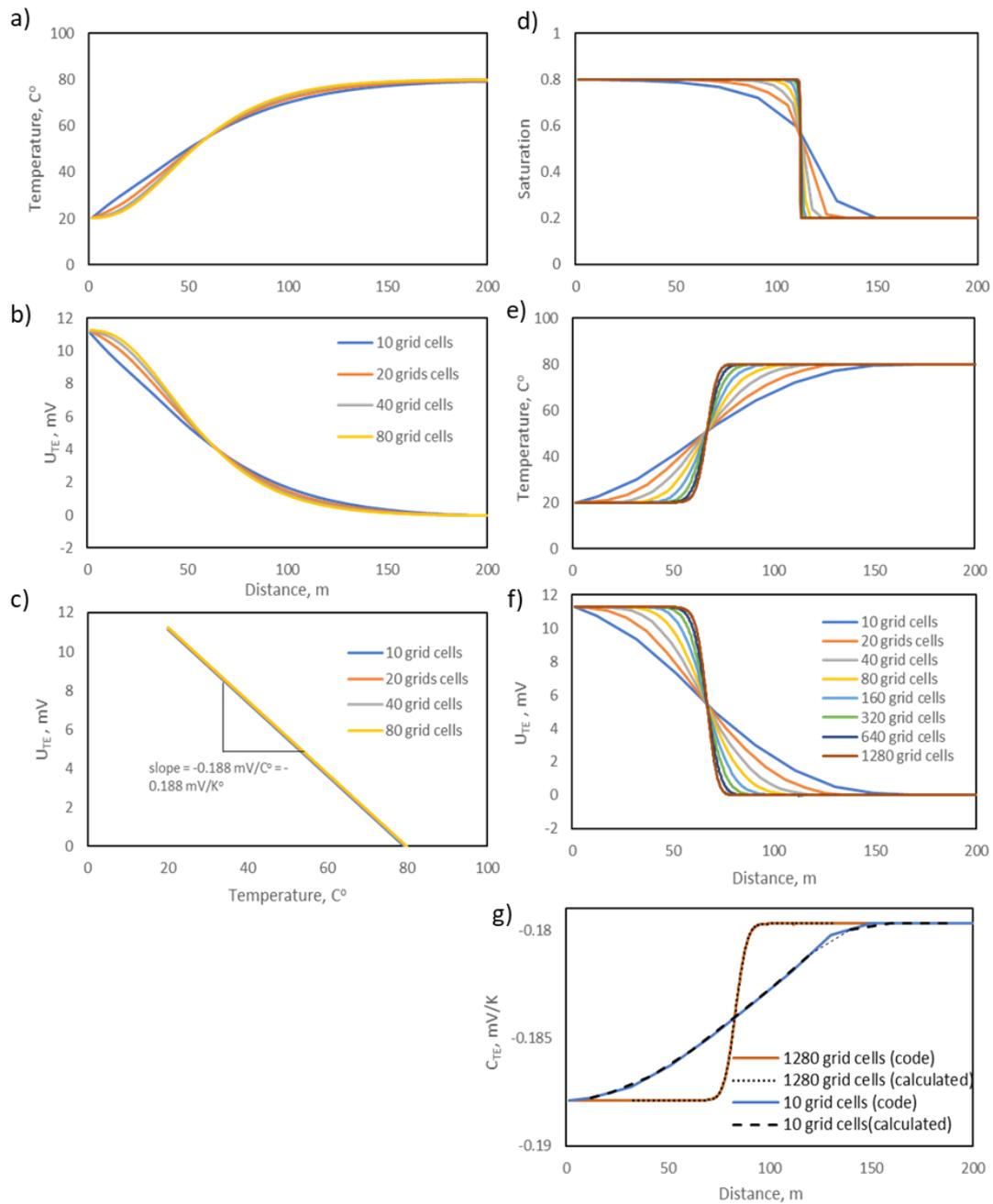
389 Results are shown in Figure 7 for both single- and multiphase flow scenarios. The correct solution
390 yields constant TE potential behind the trailing edge of the temperature front and ahead of the leading
391 edge of the temperature front (representing maximum and minimum values). The TE potential varies
392 between these two values across the temperature front. The SP solver predictions are consistent with
393 the expected behavior. However, the variation of the TE potential across the temperature front is
394 highly affected by the grid resolution, especially for the multiphase scenario (Figures 7b,f). This is
395 mainly due to the grid-resolution-dependence of the solutions for temperature (and water saturation
396 for the multiphase case) in the ECLIPSE simulator (Figure 7a,d,e), rather than the solution for TE in our
397 SP solver. As expected, we find that the TE solutions converge as the grid is refined.

398 For the single-phase scenario, a cross-plot of TE potential against temperature should yield a linear
399 relationship, with the gradient giving the TE coupling coefficient. We find that the coupling coefficient
400 obtained from the numerical solution (0.188 mV/K; gradient from figure 7c) is identical to the input
401 value (0.188 mV/K, according to equation (C.9); Appendix C) regardless of the grid resolution. This
402 confirms the validity of the SP solver for TE solutions in the single-phase scenario. For the multi-phase
403 scenario, the validity of the TE solution is confirmed by plotting the TE coupling coefficient values used
404 as input to the SP code, together with the simulated coefficients determined using the TE potential
405 determined by the solver and associated temperature (recalling $C_{TE} = \Delta U_{TE} / \Delta T$) for each pair of
406 neighboring cells, as a function of distance from the inlet to the outlet boundary (Figure 7g). The
407 coupling coefficient obtained from the numerical solution is the same as the input value to high
408 precision. Thus, we also have confidence that the SP solver returns correct solutions for the TE
409 potential in multiphase flow.



410

411 Figure 6: Numerical solutions from a single timestep of the ED validation model as a function of
 412 distance from the inlet to the outlet boundary. A) Water salinity for the single-phase problem. b) ED
 413 potential for the single-phase problem. c) ED coupling coefficient for the single-phase problem. d)
 414 Water saturation for the multiphase problem. e) Water salinity for the multiphase problem. f) ED
 415 potential for the multiphase problem. g) ED coupling coefficient for the multiphase problem. Lines in
 416 each plot correspond to different grid resolutions used in the model between the inlet and outlet
 417 boundaries.



418

419 Figure 7: Numerical solutions from a single timestep of the TE validation model as a function of
 420 distance from the inlet to the outlet boundary. A) Temperature for the single-phase problem. b) TE
 421 potential for the single-phase problem. c) Cross-plots of TE potential against temperature for the
 422 single-phase problem. d) Water saturation for the multiphase problem. e) Temperature for the
 423 multiphase problem. f) TE potential for the multiphase problem. g) Cross-plots of TE potential against
 424 temperature for the multiphase problem. Lines in each plot correspond to different grid resolutions
 425 used in the model between the inlet and outlet boundaries.

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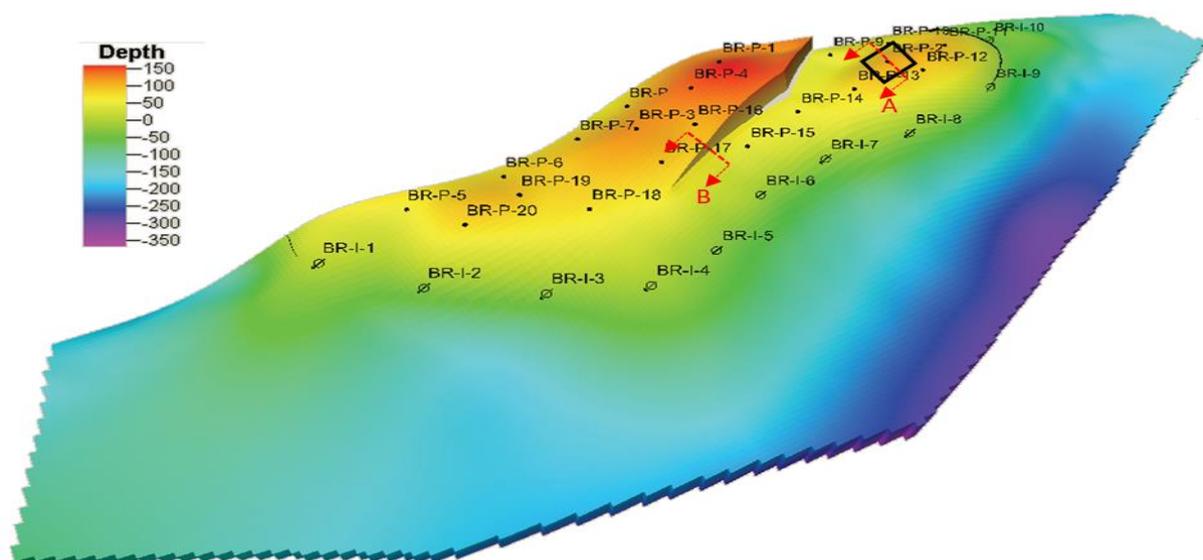
430 4.2. Self-Potential in a Hydrocarbon Reservoir: Brugge Field Model

431

432 The Brugge field case is a synthetic oil reservoir model comprising four stratigraphic layers: Schelde,
 433 Maas, Waal and Schie, from top to bottom (Figure 8; Table 1; Peters et al., 2010). The reservoir is
 434 initially saturated with oil and formation brine and overlies a water saturated aquifer (Figure 8; Table
 435 2).

436 The production scenario considered here comprises 20 oil producers and 10 water injectors. The initial
 437 reservoir temperature and formation brine salinity were assumed to be 80 C° and 1 M/L, respectively.

438 The injected brine was assumed to have lower temperature (30 C°) and salinity (0.5 M/L).



439

440 Figure 8: Structure of the Brugge field model showing the depth above and below the oil/water
 441 contact (in m) and the 30 wells (BR-P: production wells and BR-I: injection wells; Peters et al., 2010).

442

443 Table 1: Stratigraphy in the Brugge field model with main petrophysical properties (Peters et al., 2010).

Reservoir formation	Average thickness, m	Average porosity, %	Average permeability, md	Average NTG, fraction
Schelde	10	20.7	1105	0.6
Maas	20	19	90	0.88
Waal	26	24.1	814	0.97
Schie	5	19.4	36	0.77

444

Table 2: Rock and fluid used in the Brugge model.

Properties	Water	Oil	Rock
Density, (lbm/ft ³)	62.2	56	-
Compressibility, (1/psi)	3x10 ⁻⁶	9.26x10 ⁻⁶	3.5x10 ⁻⁶
Viscosity, (cp)	1	1.294	-
Irreducible water saturation	0.252	-	-
Critical water saturation	0.29	-	-
Residual oil saturation	0.15	-	-
Endpoint water relative permeability	0.3	-	-
Endpoint oil relative permeability	0.8	-	-

445

446 The average grid size in the model is 120 × 120 × 10 m in the i,j,k directions respectively, which is too
447 coarse to accurately simulate the SP in the vicinity of a well (Jackson et al. 2012a). Therefore, we
448 placed LGRs of resolution 4 × 4 × 0.5 m around selected production wells to improve the predictions
449 of the SP solver. Refining the grid to this level across the whole model would be computationally
450 infeasible as the number of grid blocks required would be in excess of 1 billion. Hence, the LGR
451 functionality in the SP solver is essential to obtain high resolution solutions around the wells of
452 interest. A sensitivity study of the LGR resolution confirmed that the resolution used is sufficient to
453 capture the SP solution. The refinement strategy that we follow is to refine in x,y and z until we
454 observe convergence in the SP profile at the monitoring well of interest. The SP solver was used to here
455 to predict the signals that might be recorded at a production well equipped with permanently installed
456 downhole electrodes (Gulamali et al., 2011).

457 After running the dynamic simulation in ECLIPSE, the results were used as inputs for the SP solver. The
458 model was modified in the solver to include electrically conductive, water saturated shale layers of
459 thickness 70m above and below the reservoir. These shale layers represent the under- and over-
460 burden and are required for the SP modelling as electrical currents may spread beyond the reservoir.
461 The EK coupling coefficients in the reservoir were calculated according to Appendix C, but were zero
462 in the shale layers as there is no flow. The ED and TE coupling coefficients were calculated following

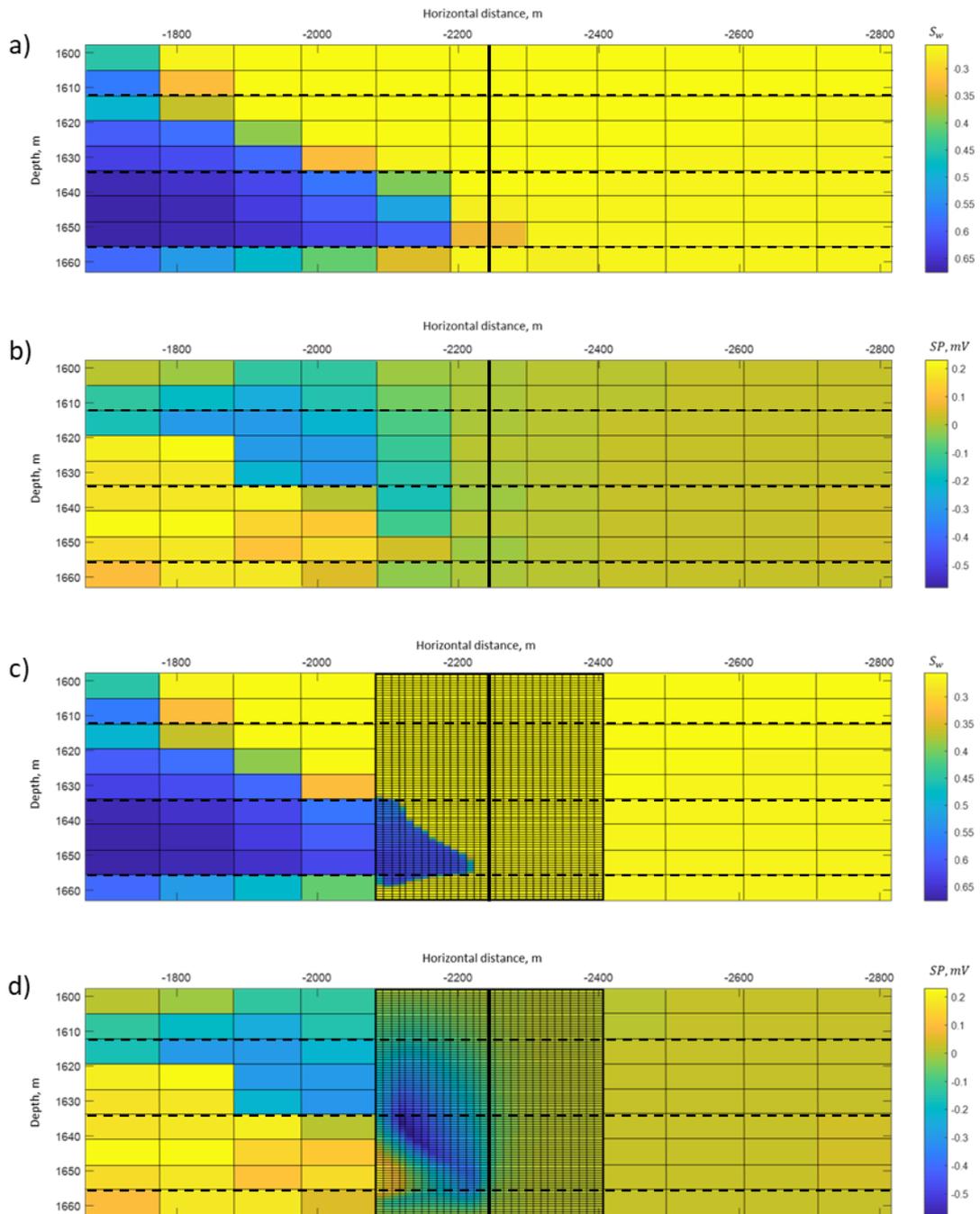
463 the approach in Appendix C. The exclusion efficiency in the reservoir was assumed to vary between 0
464 to 1 as a function of saturation, while a constant value of 0.4 was used in the shale layers. The SP
465 solver was used to simulate the EK, ED and TE contributions to the overall SP.

466 The results presented here focus on the new functionality of our SP solver. We begin by considering
467 the benefits of the LGR functionality. The effect of increased grid resolution on the solution obtained
468 is clearly observed (Figure 9). The LGR solutions yields a sharper saturation front as there is less
469 numerical diffusion (compare Figure 9a, 9c), which significantly affects the simulated SP (compare
470 Figure 9b, 9d). The higher resolution solution delivered by the LGR shows that the SP signal extends
471 to the production well, ahead of the moving waterfront. Consequently, monitoring of the SP recorded
472 at the well would provide useful information about the location of the waterfront as it approached
473 the well (e.g. Gulamali et al., 2011; Saunders et al., 2012). In contrast, the coarse grid solution suggests
474 that the SP would be featureless at the well (Figure 10). These results demonstrate the utility of the
475 LGR modelling capability in our SP solver.

476 We next consider the modelling of faults. Figure 11 shows an example on the behavior of SP across
477 fault (at cross-section B; figure 8). The fault shown in figure 11a is a sealing fault so there is no flow
478 across the fault. In the simulation model grid, there are therefore no NNCs across the fault. However,
479 the fault is electrically conductive so electrical current can flow across the fault. Consequently, the
480 SP generated by flow on one side of the fault penetrates into the reservoir and bounding shales on
481 the other side of the fault. These current fluxes are modelled using the NNCs generated by our SP
482 solver. The results demonstrate the utility of the fault modelling capability in our SP solver.

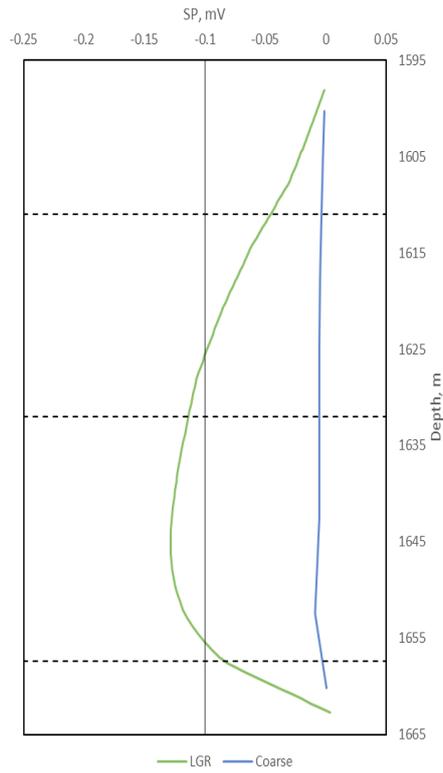
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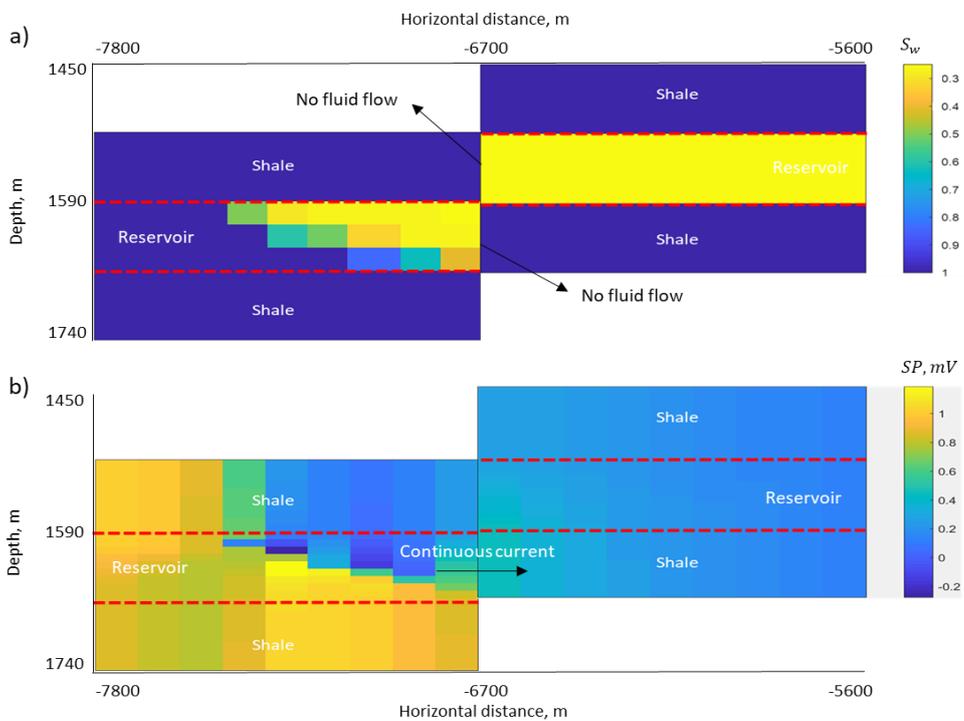
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486 Figure 9: Vertical cross-sections along the plane A in Figure 10, showing a snapshot in time of (a)
 487 water saturation in the coarse model; (b) SP in the coarse model; (c) water saturation in the LGR
 488 model, and (d) SP in the LGR model. The dashed lines denote the 4 reservoir layers and the solid line
 489 represents the production well BR-P-2.



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Figure 10: Predicted SP that would be measured along the well from the coarse and LGR models. The dashed lines denote the 4 reservoir layers and the solid line represents an assumed noise level of 0.1 mV.



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498 Figure 11: Vertical cross-sections along the plane B in Figure 10, showing a snapshot in time of (a)
499 water saturation and (b) SP across the fault. The dashed lines denote the reservoir layers. There is
500 no fluid flow across the fault, but there is current flow, so the SP generated by flow on one side of
501 the fault penetrates into the reservoir and bounding shales on the other side of the fault.

502

503 **5. Conclusions**

504 We report a new, open-source, MATLAB-based code for numerically simulating the self-potential (SP)
505 in subsurface reservoirs. The code works as a post-processor, using outputs from existing reservoir
506 flow and transport simulators at a selected timestep to calculate the SP throughout the reservoir
507 model. The material properties required to calculate the SP are user defined and may be constant or
508 vary in each cell. The code solves the equations governing flow and transport of electrical charge and
509 global charge conservation using a control-volume-finite-difference scheme.

510 We implement a new approach to calculate the current fluxes across grid-cell boundaries that can
511 account for changes in polarity of the SP coupling coefficients. Electrical currents associated with the
512 SP may spread beyond the reservoir model domain, and the code allows for the domain to be
513 extended vertically and laterally to account for this. Accurate modelling of the SP may require locally
514 fine grid resolution, and the code allows the use of local grid refinement in the reservoir flow or
515 transport simulator and in the modelling of SP. Many subsurface reservoirs include faults, and the
516 code allows the use of faulted grid, generating non-neighbor connections as necessary to model
517 current flow across the fault. These non-neighbor connections may differ from those created in the
518 reservoir flow or transport simulator, because the fault may act as a barrier to fluid flow or salt
519 transport, but not as a barrier to electrical current.

520 We demonstrate that the SP solver produces accurate SP solutions for both single and multiphase flow
521 in a series of test case, and then demonstrate its utility in predicting the SP signal that would be
522 measured at a production well during oil production from a faulted sandstone reservoir bounded
523 above and below by shales. Accurate simulation of the SP requires local grid refinement around the

524 production well, and must capture the flow of electrical current across the fault. The results suggest
525 that downhole SP monitoring could be useful to identify and locate moving waterfronts in the
526 reservoir.

527

528 **Computer code availability**

529 The code presented in this paper was developed in MATLAB. In order to run the code, the Parallel
530 Computing toolbox should be installed. The code along with a detailed user manual can be
531 downloaded from <https://github.com/mutlaqalarouj/SP-SOLVER.git>. Please cite this paper if you use
532 the code. Test data for a simple hydrocarbon reservoir are also available in the same repository. The
533 developers can be contacted via: m.alarouj17@imperial.ac.uk or m.d.jackson@imperial.ac.uk. Kuwait
534 Oil Company are thanked for financial support. We thank TNO for making the Brugge Field dataset
535 available.

536

537

538 **Appendix A**

539 **Origin of the self-potential**

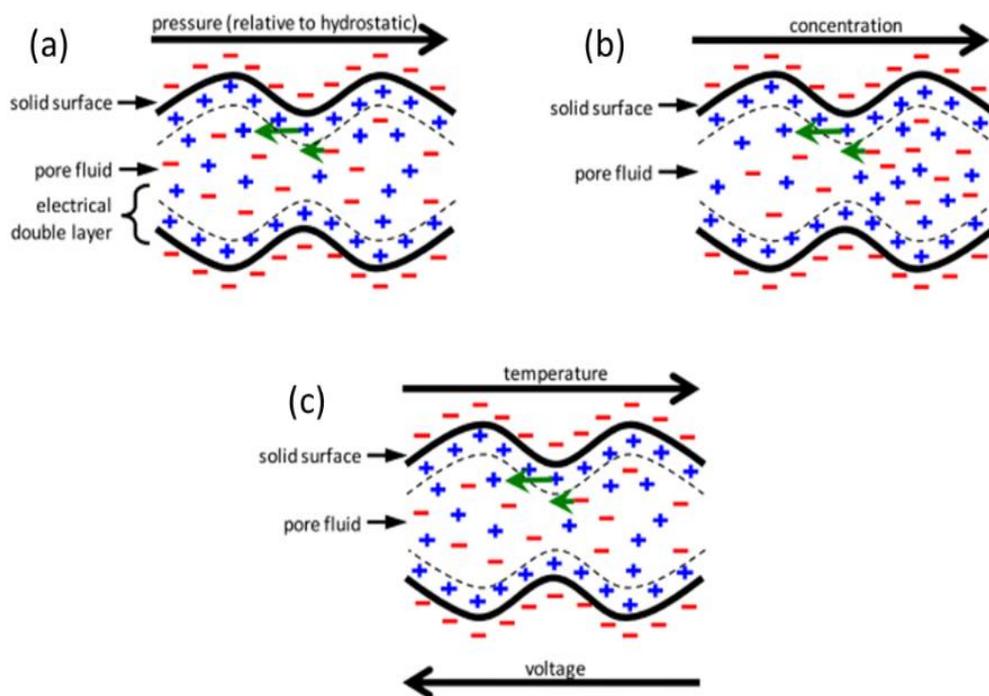
540 Sources of SP in natural environments are numerous (e.g. Jackson, 2015). Here we restrict ourselves
541 to the SP arising in partially or entirely water-saturated rocks in response to gradients in pressure
542 (above hydrostatic, also termed water potential or head), water composition (salt concentration) and
543 temperature.

544 Gradients in water potential cause water and other fluids to flow through the rock. The water drags
545 with it an excess of electrical charge in the so-called 'electrical double layer' adjacent to the mineral
546 surfaces, establishing a current termed the 'streaming current' (Hunter, 1986; Jackson et al., 2012b;
547 Figure A.1a). However, the water is electrically conductive, so the charge dragged along by the flow
548 cannot accumulate. Instead, a conduction current is established that *globally* balances the streaming
549 current to ensure overall electroneutrality. The streaming current may not follow the same pathways
550 as the conduction current, so *locally* they may not balance. From Ohm's Law, it is well known that a
551 conduction current must be driven by an electrical potential difference; this potential difference is
552 termed the 'electrokinetic' (EK) or 'streaming' potential and is the part of the SP that arises from
553 gradients in water potential (Ishido and Mizutani, 1981; Revil et al., 1999a).

554 The water (brine) found in subsurface reservoirs contains dissolved, dissociated salt species.
555 Gradients in salt species concentration cause ion transport by diffusion. However, the salt ions do not
556 migrate at the same rate, causing an electrical charge separation that is countered by an electrical
557 potential termed the 'diffusion potential'. The effect of the diffusion potential is to cause salt ions to
558 migrate down the concentration gradient at the same rate irrespective of their mobility (Revil et al.,
559 1999). If there is a concentration gradient across a rock with very small pore-size, then the electrical
560 charge on the mineral surfaces may prevent ions of the same polarity from entering the pores; only
561 ions with the opposing polarity can migrate down the concentration gradient, giving rise to an
562 electrical potential termed the 'exclusion potential'. Together, these two sources of SP are termed

563 the 'exclusion-diffusion' (ED) or 'electrochemical' (EC) potential; this is the part of the SP that arises
 564 from concentration gradients (Revil, 1999; Jackson et al., 2012b; Figure A.1b).

565 Gradients in temperature also cause ion transport by diffusion, and the resulting electrical charge
 566 separation is countered by an electrical potential termed the 'thermoelectric' (TE) potential; this is the
 567 part of the SP that arises from temperature gradients (Jackson et al., 2012b). Hence, the overall SP
 568 modelled here comprises three components which sum to give the total SP: the electrokinetic (EK)
 569 potential, the exclusion-diffusion (ED) potential and the thermoelectrical (TE) potential, which arise in
 570 response to gradients in pressure, concentration and temperature, respectively.



571
 572 Figure A.1: Representation of charge separation due to (a) pressure, (b) concentration and (c)
 573 temperature gradients. The electrical double layer is denoted simply by the dashed line and here
 574 contains an excess of positive charge that balances the negative charge on the mineral surfaces
 575 (Jackson et al., 2012b). Ion transport is denoted by arrows.

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581 **Appendix B**

582 The procedures used to derive the formulas for the saturated rock conductivity and coupling terms
 583 at the interface between two grid cells are presented here. We consider only the electrokinetic
 584 potential (EK). The same steps were followed to derive the formulas for the electrochemical and
 585 thermoelectrical potentials. Referring to Figure 2, the total current at the interface is continuous.

$$586 \quad I_{\bar{x}_{i+1}} = -\sigma_{fs_{\bar{x}_{i+1}}} \nabla U_{\bar{x}_{i+1}} - L_{EK_{\bar{x}_{i+1}}} \nabla \Phi_{\bar{x}_{i+1}} \quad (B.1)$$

587 $\nabla U_{\bar{x}_{i+1}}$ can be approximated as

$$588 \quad \nabla U_{\bar{x}_{i+1}} = \frac{U_{x_{i+1}} - U_{x_i}}{x_{i+1} - x_i} = \frac{(U_{x_{i+1}} - U_{\bar{x}_{i+1}}) + (U_{\bar{x}_{i+1}} - U_{x_i})}{x_{i+1} - x_i} = \frac{(U_{x_{i+1}} - U_{\bar{x}_{i+1}})}{x_{i+1} - x_i} + \frac{(U_{\bar{x}_{i+1}} - U_{x_i})}{x_{i+1} - x_i}$$

589 (B.2)

590 Knowing that

$$591 \quad \frac{x_{i+1} - x_i}{x_{i+1} - x_i} = \frac{x_{i+1} - \bar{x}_{i+1}}{x_{i+1} - x_i} + \frac{\bar{x}_{i+1} - x_i}{x_{i+1} - x_i} = m + n = 1 \quad (B.3)$$

592 then $x_{i+1} - x_i$ can be written as

$$593 \quad x_{i+1} - x_i = \frac{x_{i+1} - \bar{x}_{i+1}}{m} = \frac{\bar{x}_{i+1} - x_i}{n} \quad (B.4)$$

594 Substituting equation (B.4) in equation (B.2)

$$595 \quad \nabla U_{\bar{x}_{i+1}} = m \nabla U_{x_{i+1}} + n \nabla U_{x_i} \quad (B.5)$$

596 Now, we apply equation (B.1) for cells i and $i + 1$ as follows

$$597 \quad I_{x_i} = -\sigma_{fs_{x_i}} \nabla U_{x_i} - L_{EK_{x_i}} \nabla \Phi_{x_i} \quad (B.6)$$

$$598 \quad I_{x_{i+1}} = -\sigma_{fs_{x_{i+1}}} \nabla U_{x_{i+1}} - L_{EK_{x_{i+1}}} \nabla \Phi_{x_{i+1}} \quad (B.7)$$

599 Next, we rearrange equations (B.6) and (B.7) for ∇U_{x_i} & $\nabla U_{x_{i+1}}$

600
$$\nabla U_{x_i} = -\frac{I_{x_i}}{\sigma_{fs_{x_i}}} - \frac{L_{EK_{x_i}} \nabla \Phi_{x_i}}{\sigma_{fs_{x_i}}} \quad (B.8)$$

601
$$\nabla U_{x_{i+1}} = -\frac{I_{x_{i+1}}}{\sigma_{fs_{x_{i+1}}}} - \frac{L_{EK_{x_{i+1}}} \nabla \Phi_{x_{i+1}}}{\sigma_{fs_{x_{i+1}}}} \quad (B.9)$$

602 After that, we substitute equation (B.8) and equation (B.9) in equation (B.5)

603
$$\nabla U_{\bar{x}_{i+1}} = m \left(-\frac{I_{x_{i+1}}}{\sigma_{fs_{x_{i+1}}}} - \frac{L_{EK_{x_{i+1}}} \nabla \Phi_{x_{i+1}}}{\sigma_{fs_{x_{i+1}}}} \right) + n \left(-\frac{I_{x_i}}{\sigma_{fs_{x_i}}} - \frac{L_{EK_{x_i}} \nabla \Phi_{x_i}}{\sigma_{fs_{x_i}}} \right) \quad (B.10)$$

604 Rearranging equation (B.10) results in

605
$$\nabla U_{\bar{x}_{i+1}} = -\left(\frac{nI_{x_i}}{\sigma_{fs_{x_i}}} + \frac{mI_{x_{i+1}}}{\sigma_{fs_{x_{i+1}}}} \right) - \left(\frac{nL_{EK_{x_i}} \nabla \Phi_{x_i}}{\sigma_{fs_{x_i}}} + \frac{mL_{EK_{x_{i+1}}} \nabla \Phi_{x_{i+1}}}{\sigma_{fs_{x_{i+1}}}} \right) \quad (B.11)$$

606 Assuming the total current is continuous ($I_{x_i} = I_{x_{i+1}} = I_{\bar{x}_{i+1}}$), we can write equation (B.11) as

607
$$\nabla U_{\bar{x}_{i+1}} = -I_{\bar{x}_{i+1}} \left(\frac{n}{\sigma_{fs_{x_i}}} + \frac{m}{\sigma_{fs_{x_{i+1}}}} \right) - \left(\frac{nL_{EK_{x_i}} \nabla \Phi_{x_i}}{\sigma_{fs_{x_i}}} + \frac{mL_{EK_{x_{i+1}}} \nabla \Phi_{x_{i+1}}}{\sigma_{fs_{x_{i+1}}}} \right) \quad (B.12)$$

608 $I_{\bar{x}_{i+1}}$ can be calculated by arranging equation (B.12) as follows

609
$$I_{\bar{x}_{i+1}} = -\frac{\nabla U_{\bar{x}_{i+1}}}{\frac{n}{\sigma_{fs_{x_i}}} + \frac{m}{\sigma_{fs_{x_{i+1}}}}} - \frac{\frac{nL_{EK_{x_i}} \nabla \Phi_{x_i}}{\sigma_{fs_{x_i}}} + \frac{mL_{EK_{x_{i+1}}} \nabla \Phi_{x_{i+1}}}{\sigma_{fs_{x_{i+1}}}}}{\frac{n}{\sigma_{fs_{x_i}}} + \frac{m}{\sigma_{fs_{x_{i+1}}}}} \quad (B.13)$$

610 The first component of equation (B.11) is the conduction current related to the naturally occurring
 611 SP (∇U), while the second component is the streaming current related to the pressure gradient
 612 ($\nabla \Phi$).

613 The saturated rock conductivity ($\sigma_{fs_{\bar{x}_{i+1}}}$) at the interface between grid cells i and $i + 1$ can be

614 calculated by equating the first term of equation (B.1) and (B.13) as follows

615
$$\sigma_{fs_{\bar{x}_{i+1}}} = \frac{1}{\frac{n}{\sigma_{fs_{x_i}}} + \frac{m}{\sigma_{fs_{x_{i+1}}}}} = \frac{\sigma_{fs_{x_i}} \sigma_{fs_{x_{i+1}}} (x_{i+1} - x_i)}{(x_{i+1} - \bar{x}_{i+1}) \sigma_{fs_{x_i}} + (\bar{x}_{i+1} - x_i) \sigma_{fs_{x_{i+1}}}} \quad (B.14)$$

616 For the coupling term at the interface ($L_{EK_{\bar{x}_{i+1}}}$), we need to equate the second terms of equations

617 (B.1) and (B.13) as

618
$$L_{EK_{\bar{x}_{i+1}}} \nabla \Phi_{\bar{x}_{i+1}} = \frac{\frac{n L_{EK_{x_i}} \nabla \Phi_{x_i}}{\sigma_{fs_{x_i}}} + \frac{m L_{EK_{x_{i+1}}} \nabla \Phi_{x_{i+1}}}{\sigma_{fs_{x_{i+1}}}}{\frac{n}{\sigma_{fs_{x_i}}} + \frac{m}{\sigma_{fs_{x_{i+1}}}}} \quad (B.15)$$

619 Rearranging equation (B.14) considering the numerical approximation of $\nabla \Phi_{x_i}$, $\nabla \Phi_{x_{i+1}}$, and $\nabla \Phi_{\bar{x}_{i+1}}$,

620 and considering the definition of m and n for equation (B.3), equation (B.15) can be written as

621
$$L_{EK_{\bar{x}_{i+1}}} (\Phi_{x_{i+1}} - \Phi_{x_i}) = \frac{\sigma_{fs_{x_{i+1}}} L_{EK_{x_i}} (\Phi_{\bar{x}_{i+1}} - \Phi_{x_i}) + \sigma_{fs_{x_i}} L_{EK_{x_{i+1}}} (\Phi_{x_{i+1}} - \Phi_{\bar{x}_{i+1}})}{m \sigma_{fs_{x_i}} + n \sigma_{fs_{x_{i+1}}}} \quad (B.16)$$

622 The only unknown value in equation (B.16) is $\Phi_{\bar{x}_{i+1}}$, which is the water potential at the interface

623 between cells i and $i + 1$. This value can be approximated by linear interpolation. The final formula

624 of $L_{EK_{\bar{x}_{i+1}}}$ can be written as

625
$$L_{EK_{\bar{x}_{i+1}}} = \frac{\sigma_{fs_{x_{i+1}}} L_{EK_{x_i}} (\bar{x}_{i+1} - x_i) + \sigma_{fs_{x_i}} L_{EK_{x_{i+1}}} (x_{i+1} - \bar{x}_{i+1})}{(x_{i+1} - \bar{x}_{i+1}) \sigma_{fs_{x_i}} + (\bar{x}_{i+1} - x_i) \sigma_{fs_{x_{i+1}}}} \quad (B.17)$$

626 which is the same as equation (14) presented in the main text.

627

628 **Appendix C**

629 In order to solve equation (2), the concentration and temperature dependent material properties
630 (rock conductivity (σ_{fs}) and coupling terms (L_{EK}, L_{ED}, L_{TE})) must be specified. The operation of the
631 SP solver is independent of the models used to describe these material properties and the user can
632 modify the code to implement their own preferred descriptions. Here we outline the approach we
633 use in the code at present, and that was used to obtain the results presented.

634 The saturated rock conductivity is calculated using the well-known Archie's equation (Glover et al.,
635 2000)

$$636 \quad \sigma_{fs} = \emptyset^m \sigma_w S_w^n \quad (C.1)$$

637 where \emptyset is the porosity, m is the cementation exponent, S_w is the water saturation, n is the saturation
638 exponent, and σ_w is the water conductivity (S/m). The water conductivity is calculated as a function
639 of the salt concentration (C , M/L) and temperature (T , °C) using (Sen and Goode, 1992; Figure 6a)

$$640 \quad \sigma_w = (5.6 + 0.27T - 1.5 \times 10^{-4}T^2)C_f - \frac{2.36 + 0.099T}{1 + 0.214C_f^{0.5}} C_f^{1.5} \quad (C.2)$$

641 The coupling terms (L_{EK}, L_{ED}, L_{TE}) are functions of the rock conductivity and the associated coupling
642 coefficients (C_{EK}, C_{ED}, C_{TE}). First, we will consider the electrokinetic coupling coefficient (C_{EK}). A
643 number of experimental and theoretical studies have characterized the electrokinetic coupling
644 coefficients for sandstones (e.g. Revil and Cerepi, 2004; Jaafar et al., 2009; Vinogradov et al., 2010;
645 Glover et al., 2012; Walker et al., 2014; Vinogradov and Jackson, 2015; Esmaeili et al., 2016;
646 Vinogradov et al., 2018; Walker and Glover, 2018; Glover, 2018; Li et al., 2018) and carbonates (e.g.
647 Jackson and Vinogradov, 2012; Chen et al., 2014; Alroudhan et al., 2016; Jackson et al., 2016; Al
648 Mahrouqi et al., 2017; Ghommem et al., 2018; Collini et al., 2020). Here, we focus on sandstones
649 although, as mentioned above, the C_{EK} model used here can easily be modified or changed for other
650 rock types.

651 Most of the published EK coupling coefficient data for sandstones were obtained for fully saturated
652 ($S_w = 1$) conditions at laboratory temperature. We describe the observed trend with brine
653 concentration (ionic strength) using (Vinogradov et al., 2010)

$$654 \quad C_{EK}(S_w = 1) = -1.36C_f^{-0.9123} \times 10^{-9} \quad (C.3)$$

655 Equation (C.3) fits data measured in sandstone samples saturated with simple monovalent NaCl brines
656 (Figure C.1b). Alternative expressions can easily be implemented in the code. We note that the
657 limited data available suggest that the EK coupling coefficient for complex natural brines is smaller in
658 magnitude for a given ionic strength compared to the values in monovalent brines shown in Figure
659 C.1b (Vinogradov et al., 2018; Li et al., 2018). We neglect any temperature dependence of the EK
660 coupling coefficient, consistent with the findings of previous studies that show it is approximately
661 independent of temperature over the range of 20-120°C in brines of moderate to high ionic strength
662 (Reppert and Morgan, 2003a, 2003b; Vinogradov and Jackson, 2015; Vinogradov et al., 2018).

663 In reservoirs partially saturated with water, such as oil and gas reservoirs and unconfined aquifers, the
664 EK coupling coefficient is a function of water saturation. A number of studies have measured and/or
665 modelled the relationship between coupling coefficient and water saturation in sandstone and
666 carbonate rocks (Wurmstich and Morgan, 1994; Perrier and Morat, 2000; Guichet et al., 2003; Revil
667 and Cerepi, 2004; Linde et al., 2007; Revil et al., 2007; Jackson, 2010; Vinogradov and Jackson, 2011;
668 Gulamali, et al., 2012; Allègre et al., 2012; Jougnot et al., 2012; Jackson et al. 2012a; Zhang et al., 2017;
669 Soldi et al., 2019). Here, we assume water is the wetting phase and follow the approach of Jackson et
670 al. (2012b) to describe the saturation dependence of the coupling coefficient, noting that it is trivial
671 to replace this model in the code with other published or new models. We assume that the coupling
672 coefficient at the residual non-wetting phase saturation is the same as that at fully water saturated
673 conditions, and define a saturation-dependent relative coupling coefficient (C_{rEK})

$$674 \quad C_{rEK} = S_{wn}^{0.6} \quad (C.4)$$

675
$$S_{wn} = \frac{S_w - S_{wirr}}{1 - S_{wirr} - S_{nwr}} \quad (C.5)$$

676
$$C_{EK}(S_w) = C_{EK}|_{S_w=1} C_{rEK}(S_w) \quad (C.6)$$

677 where S_{wn} is the normalized water saturation, S_{wirr} is the irreducible water saturation and S_{nwr} is
 678 the residual non-wetting phase saturation. Equation (C.4) was chosen to match the results of a bundle
 679 capillary tube model presented by Jackson (2010) and experimental data obtained by Revil and Cerepi
 680 (2004).

681 Next, we consider the ED and TE coupling coefficients. ED and TE potentials have two end-member
 682 cases: pure exclusion and pure diffusion (Figure C.1c,d). The salinity and temperature dependence of
 683 the ED and TE coupling coefficients for pure exclusion and pure diffusion cases are given by (Revil,
 684 1999; Jackson et al., 2012a; Leinov and Jackson, 2014; Jackson, 2015)

685
$$C_{ED}|_{ed} = -8.61 \times 10^{-2} \frac{(2t_{Na} - 1)T}{C_f} \text{ mV} \cdot \text{M}^{-1} \quad (C.7)$$

686
$$C_{ED}|_{ee} = -8.61 \times 10^{-2} \frac{T}{C_f} \text{ mV} \cdot \text{M}^{-1} \quad (C.8)$$

687
$$C_{TE}|_{ed} = -1.984 \times 10^{-1} (2t_{Na} - 1) (\log C_f) + 1.059 t_{Na} - 5.673 \times 10^{-1} \text{ mV} \cdot \text{K}^{-1} \quad (C.9)$$

688
$$C_{TE}|_{ee} = -1.984 \times 10^{-1} (\log C_f) + 5.953 \times 10^{-1} \text{ mV} \cdot \text{K}^{-1} \quad (C.10)$$

689
$$t_{Na} = \begin{cases} 0.39 & C < 0.09 \text{ M} \\ 3.66 \times 10^{-1} - 2.12 \times 10^{-2} (\log_{10} C_f) & C > 0.09 \text{ M} \end{cases} \quad (C.11)$$

690 where subscripts *ed* and *ee* refers to pure diffusion and pure exclusion cases, respectively. t_{Na} is the
 691 macroscopic Hittorf transport number for the Na ions, noting that this approach assumes charge
 692 transport is dominated by Na^+ and Cl^- ions arising from the dissociation of NaCl, which is a reasonable
 693 assumption for subsurface reservoirs (Numbere et al., 1977; Angelis, 2005). Experimentally measured
 694 data on shales, sandstones and carbonate rock samples lie between the pure exclusion and diffusion
 695 limits for both the ED and TE potentials (Figure C.1c,d). Note that the effect of temperature on the TE

696 coupling coefficient is neglected in equations (C.9) and (C.10) because of the small variation of the TE
697 coefficient (<8%) over the temperature range 20 - 120 C° (Jackson et al., 2012b).

698 The relative contribution of the exclusion and diffusion components of the EC and TE potentials can
699 be defined by a dimensionless number termed the 'exclusion efficiency' (ε). An exclusion efficiency of
700 unity corresponds to an exclusion-dominated ED or TE potential, while an efficiency of zero
701 corresponds to a diffusion-dominated ED or TE potential (Leinov and Jackson, 2014). The ED and TE
702 coupling coefficients are modelled as a function of exclusion efficiency as (Graham et al., 2018)

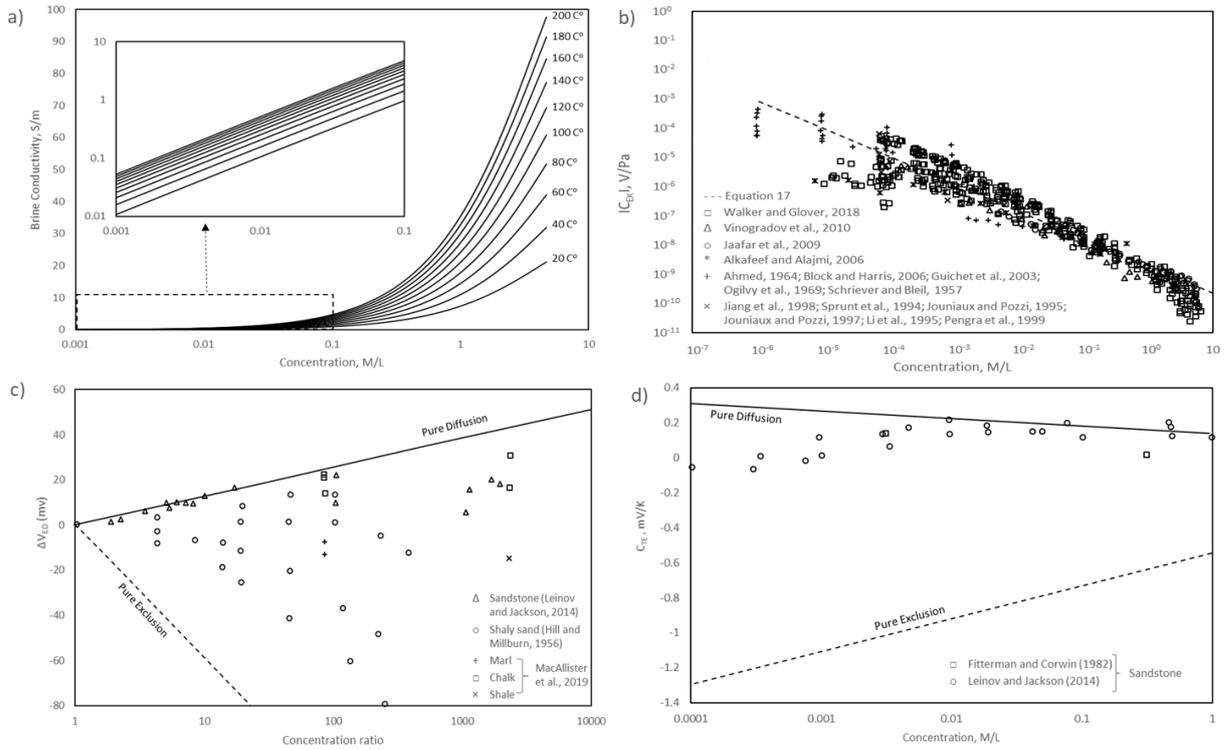
$$703 \quad C_x = \varepsilon_x \cdot (C_x|_{ee} - C_x|_{ed}) + C_x|_{ed} \quad (C.12)$$

704 where subscript x refers to either ED or TC. Unlike EK potential, ED and TE potentials can be generated
705 across impermeable layers if there is a concentration or temperature gradient, even though there is
706 no water flow. The exclusion efficiency in fully saturated rocks varies with the rock pore-size (see
707 REFS) so an appropriate value of exclusion efficiency value must be assigned to each rock type; for
708 example, MacAllister et al. (2019) measured values of $\varepsilon=0-0.1$ and $\varepsilon=0.3-0.4$ for sandstones and
709 shales, respectively.

710 In reservoirs partially saturated with water, the exclusion efficiency also varies with water saturation
711 (Ortiz et al., 1973). We use here the approach described by Ortiz et al. (1973) to model the behavior
712 of the exclusion efficiency at the saturation endpoints ($S_w = S_{wirr}$ and $S_w = 1 - S_{nwr}$). At low water
713 saturation, Ortiz et al. (1973) suggested that the excess charge is confined to thin water films and
714 small, water-occupied pores from which co-charge is efficiently excluded. Thus, the EC and TE
715 potentials are dominated by exclusion ($\varepsilon = 1$ and $C_x(S_{wirr}) = C_x|_{ee}$). Conversely, at high water
716 saturation, the water occupies most of the pores and the EC and TE potentials are dominated by
717 diffusion (ε is the minimum for the rock type of interest). At intermediate saturations, we model the
718 saturation-dependence of the exclusion efficiency as (Jackson et al., 2012b)

$$719 \quad \varepsilon_x = (1 - S_{wn})^3 \quad (C.13)$$

720 where ε_x is the ED or TE exclusion efficiency at intermediate saturation. Equation (C.13) was fitted to
 721 match the data presented in Ortiz et al. (1973) for the ED coupling coefficient, and we assume the
 722 same behavior for the TE relative coupling coefficient.



723

724 Figure C.1: a) Water conductivity versus brine concentration (ionic strength) at different
 725 temperatures. b) EK coupling coefficient versus brine concentration. c) ED coupling coefficient versus
 726 brine concentration ratio. d) TE coupling coefficient versus brine concentration.

727

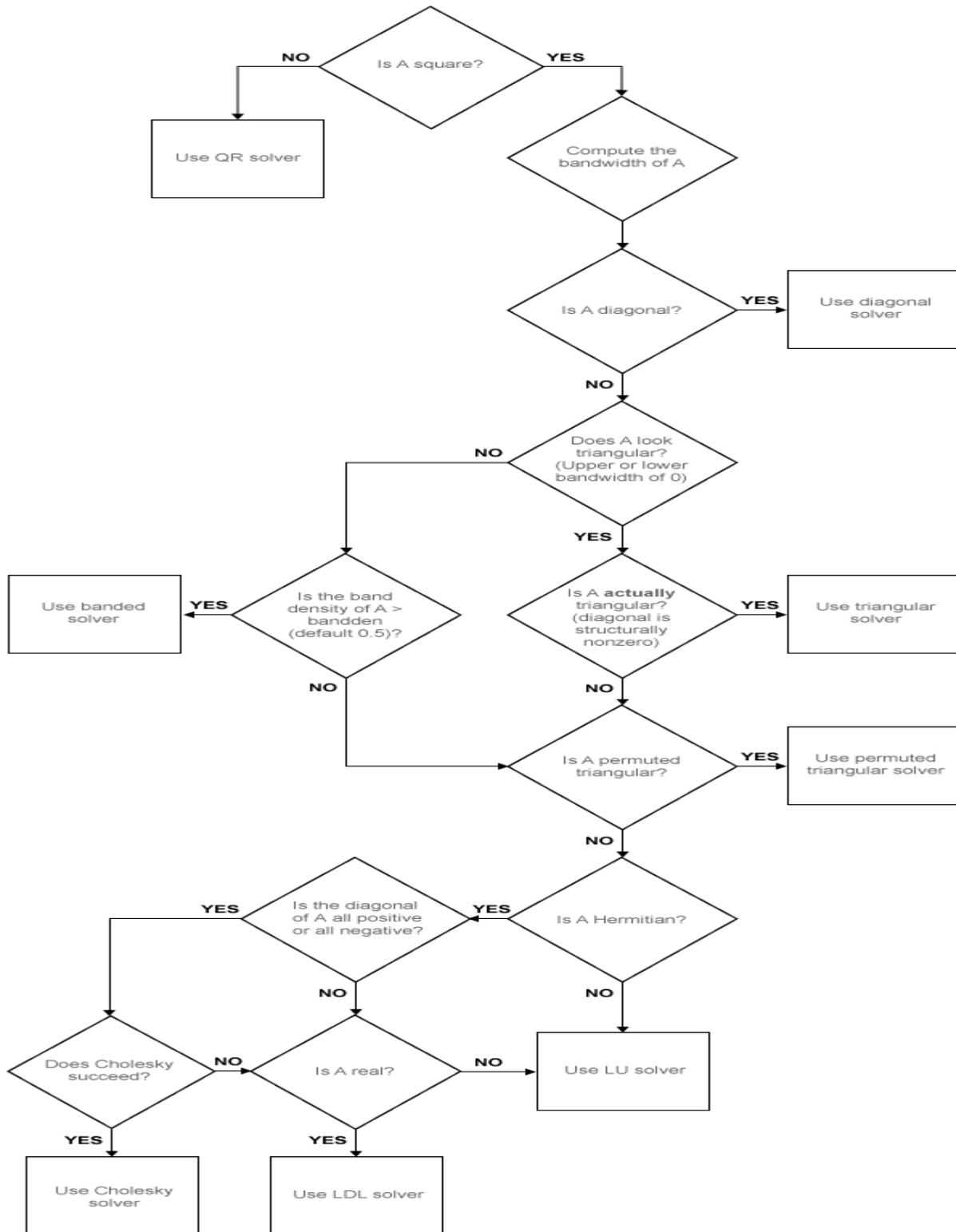
728

729

730 **Appendix D**

731 The algorithm path for the mldivide function for sparse matrices is given in figure D.1

732



733

734

Figure D.1: algorithm path for the mldivide function (MathWorks, 2020)

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