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1 **An innovative computationally efficient hydromechanical coupling**
2 **approach for fault reactivation in geological subsurface utilization**

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15 **Keywords**

16 Hydromechanical coupling; Semi-analytical coupling; Multiphase fluid flow; Geological faults;
17 Numerical simulation; Subsurface gas storage

18 **Abstract**

19 Estimating the efficiency and sustainability of geological subsurface utilization, i.e., Carbon Cap-
20 ture and Storage (CCS) requires an integrated risk assessment approach, considering the occurring
21 coupled processes, beside others, the potential reactivation of existing faults. In this context, hy-
22 draulic and mechanical parameter uncertainties as well as different injection rates have to be con-
23 sidered and quantified to elaborate reliable environmental impact assessments. Consequently, the
24 required sensitivity analyses consume significant computational time due to the high number of
25 realizations that have to be carried out. Due to the high computational costs of two-way coupled
26 simulations in large-scale 3D multiphase fluid flow systems, these are not applicable for the pur-
27 pose of uncertainty and risk assessments.

28 Hence, an innovative semi-analytical hydromechanical coupling approach for hydraulic fault re-
29 activation will be introduced. This approach determines the void ratio evolution in representative
30 fault elements using one preliminary base simulation, considering one model geometry and one
31 set of hydromechanical parameters. The void ratio development is then approximated and related
32 to one reference pressure at the base of the fault. The parametrization of the resulting functions is
33 then directly implemented into a multiphase fluid flow simulator to carry out the semi-analytical
34 coupling for the simulation of hydromechanical processes. Hereby, the iterative parameter ex-
35 change between the multiphase and mechanical simulators is omitted, since the update of porosity
36 and permeability is controlled by one reference pore pressure at the fault base. The suggested
37 procedure is capable to reduce the computational time required by coupled hydromechanical sim-
38 ulations of a multitude of injection rates by a factor of up to 15.

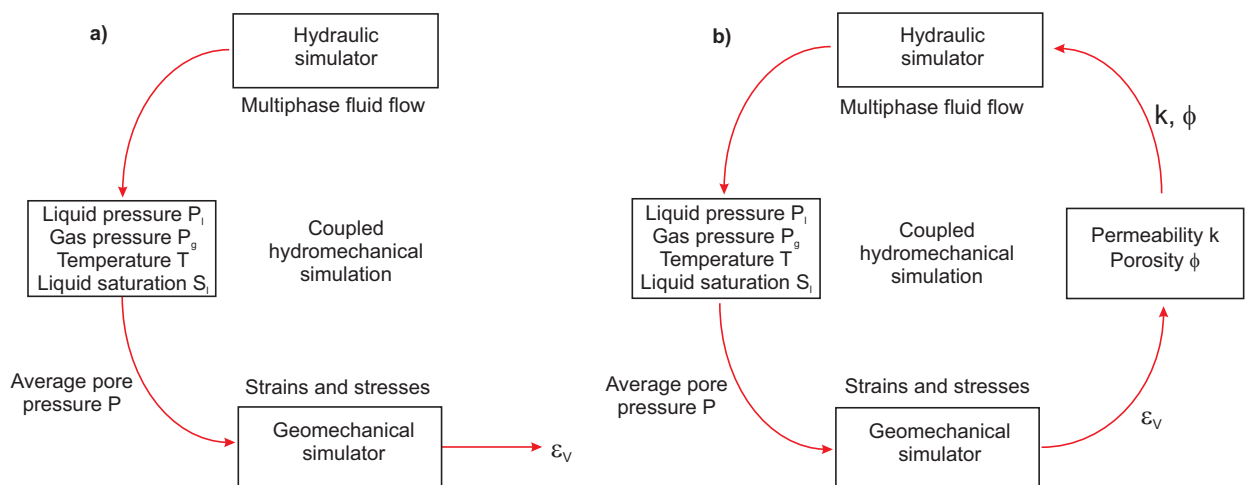
39 **1. Introduction**

40 For the simulation of hydromechanical multiphase fluid flow processes in reservoirs, i.e., Carbon
41 Capture and Storage (CCS), numerical modelling is state of the art (Altmann et al., 2014; Cappa
42 and Rutqvist, 2011; Kempka and Kühn, 2013; Rutqvist and Tsang, 2002; Rutqvist et al., 2007,
43 2008; Rutqvist, 2010). For that purpose, hydraulic multiphase flow and geomechanical simulators
44 are sequentially coupled using one-way or two-way approaches (Settari and Mourits, 1994; Settari
45 et al., 2005; Settari, 2012; Kempka et al., 2014, 2015; Tillner et al., 2014; Walters et al., 2002).

46 For a one-way coupling, parameters like liquid phase pressure P_l , gas phase pressure P_g , and liquid
47 saturation S_l have to be determined using a multiphase flow simulator. After converting these data
48 into an average pore pressure P following Eq. 1

$$49 \quad P = S_l \cdot P_l + (1 - S_l) P_g, \quad (1)$$

50 P is transferred to the geomechanical simulator. An additional coupling parameter for non-isother-
 51 mal studies is the temperature T. If this data transfer is occurring only in one direction (one-way),
 52 the resulting volumetric strain ε_v will not be fed back to the multiphase flow simulator for updating
 53 porosity and permeability (Fig. 1 (a)). In case of large volumetric strains ε_v occurring during the
 54 simulation, a one-way coupling may lead to inaccurate results (Cappa and Rutqvist, 2011; Chabab
 55 and Kempka, 2016; Langhi et al., 2010; Lautenschläger et al., 2013; Righetto et al., 2013; Zhang
 56 et al., 2011). A method to consider large volumetric strains comprises the use of sequentially two-
 57 way coupled simulations, where the coupling parameters P, intrinsic permeability k and porosity
 58 ϕ are transferred in both directions (two-way) between the simulators. Hence, porosity and perme-
 59 ability are updated iteratively during the entire simulation cycle (Fig. 1 (b)) and considered in the
 60 hydraulic simulator.



61
 62 **Fig. 1 Types of sequential coupling: (a) One-way coupling (no update of porosity and permeability) and (b)**
 63 **Two-way coupling (with update of porosity and permeability).**

64 To estimate the efficiency and sustainability of geological subsurface utilization, uncertainty and
 65 risk assessments considering the occurring coupled processes, i.e., the potential reactivation of
 66 existing faults, are mandatory. For reliable environmental impact assessments, hydraulic and me-
 67 chanical parameter uncertainties, with their consideration would extending beyond the scope of

68 the present study, as well as the injection rate of the fluid or gas have to be considered and quan-
69 tified by a representatively high number of computational realizations. Consequently, the required
70 sensitivity analyses consume significant computational time. Due to the high computational de-
71 mand of sequentially two-way coupled simulations in large-scale 3D simulations, these are not
72 applicable for the purpose of risk assessments. Hence, an innovative approach for a hydromechan-
73 ical two-way coupling to assess hydraulic fault reactivation, based on a semi-analytical coupling
74 is introduced in the following.

75 Parameterizing the semi-analytical approach, using the mechanical response of a one-way coupled
76 single-phase fluid flow simulation and implementing it directly into a multiphase fluid flow sim-
77 ulator, enables us to omit the iterative parameter exchange between the hydraulic and the mechan-
78 ical simulators, whereby permeability and porosity updates are controlled analytically. Under va-
79 lidity of the hypothesis that during the CO₂ injection period, the hydromechanical behavior of
80 geological faults is predominantly controlled by the brine properties, we implement and discuss a
81 semi-analytical approach in Section 2.1. For its general validation, we present and discuss the re-
82 sults of three parametric studies of single-phase fluid flow simulations carried out with Abaqus[®]
83 (Abaqus, 2010) in Section 2.2. Finally, a validation of our hypothesis for coupled hydromechanical
84 simulations involving multiphase fluid flow by comparing semi-analytically coupled simulation
85 results against those of our benchmark simulations, carried out as sequentially two-way coupled
86 hydromechanical simulations with multiphase fluid flow, and established by using a coupling be-
87 tween the TOUGH2-MP/ECO₂N and FLAC^{3D} simulators (Cappa and Rutqvist, 2011; Itasca, 2013;
88 Rutqvist et al., 2007; Pruess, 2005; Zhang et al., 2008) is discussed in Section 3.

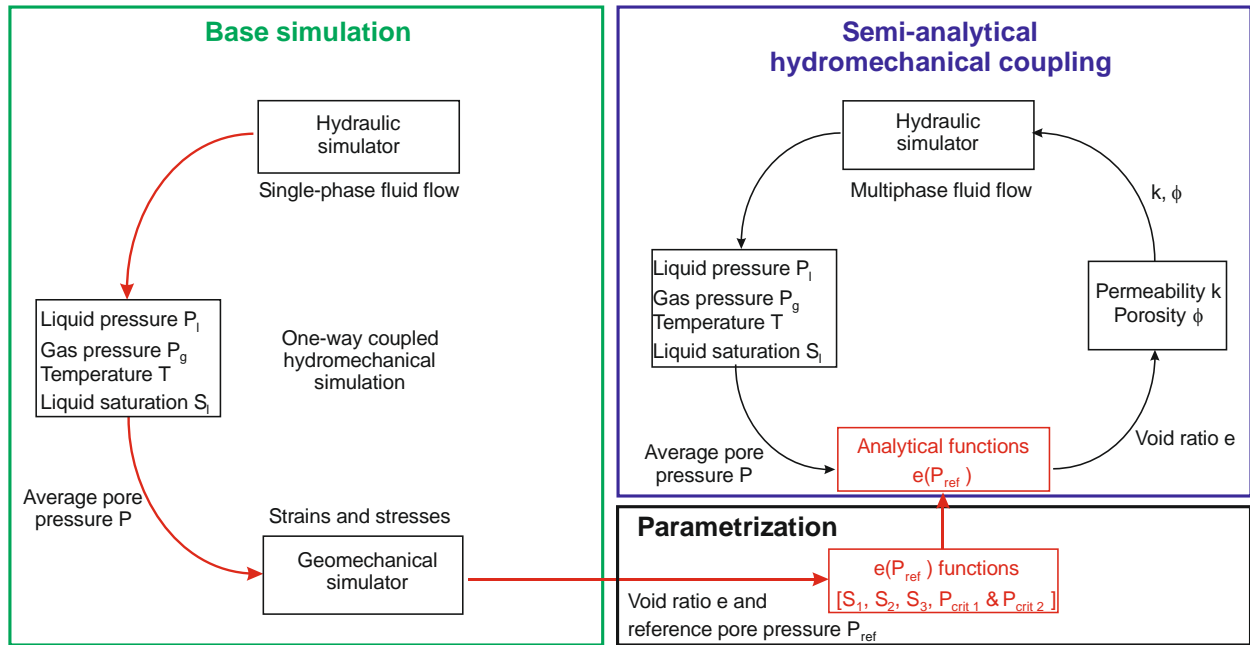
89 **2. Implementation and validation of the semi-analytical coupling ap-** 90 **proach considering single phase fluid flow**

91 To reduce the computational time for two-way coupled simulations a methodology to decouple
92 the hydraulic and geomechanical simulators is introduced in this study.

93 **2.1 Description of the approach and derivation of its parametrization**

94 In one-way and two-way coupled simulations, the presence of a gaseous phase is only indirectly
95 considered by updating P at each time step (Equation 1), as the average pore pressure P is the
96 hydraulic coupling parameter between the multiphase flow and the geomechanical simulations.
97 Generally, the presence or absence of a gas phase, i.e., CO_2 influences the average pore pressure
98 P determined in the multiphase fluid flow simulator due to gas compressibility, viscosity and the
99 occurrence of capillary pressures. Conceptually, CO_2 storage reservoirs are generally located in
100 geological anticline structures to benefit from structural and stratigraphic trapping mechanisms.
101 Furthermore, average fluid flow velocities of brine and gaseous CO_2 amount to only a few meters
102 per year (Holloway 2005; IPCC 2005). Hence, the migration of the CO_2 -rich phase in a reservoir
103 proceeds over a relatively long time period. Both mechanisms are suitable to avoid uncontrolled
104 CO_2 migration towards known geological faults in the injection well near- and far-field. Anyhow,
105 before CO_2 can flow through hydraulically reactivated faults, it has to displace the brine in the
106 reservoir and in a present hydraulically conductive fault. This is accompanied by a pore pressure
107 increase, and hence decreasing effective stresses. Until leaking CO_2 reaches the upper fault region
108 and possibly enters a shallower aquifer, the pore pressure increase inside the fault is predominantly
109 controlled by the fluid properties of brine (Cappa and Rutqvist, 2011; Birkholzer et al., 2009;
110 Tillner et al., 2013). Hence, in our approach we make the assumption that during this process, the
111 analytical functions for updating the fault's permeability and porosity can be sufficiently calibrated
112 and parametrized by a single phase fluid flow base simulation, as discussed in Section 3.

113 Fig. 2 shows the general workflow of the semi-analytical coupling approach. In a first step, a single
 114 one-way coupled base simulation, indicated by the green box is carried out for one model geometry
 115 and one set of hydromechanical parameters to estimate the void ratio evolution in representative
 116 fault elements and the pore pressure distribution of one reference element.



117
 118 **Fig. 2 General workflow of the semi-analytical hydromechanical coupling scheme. Based on a one-way coupled**
 119 **single-phase fluid flow base simulation, $e(P_{ref})$ functions (void ratio e over reference pore pressure P_{ref} are**
 120 **generated (red box). These functions are directly implemented into a multiphase fluid flow simulator to control**
 121 **the update of porosity and permeability of the fault zone, since the geomechanical simulator is omitted in the**
 122 **suggested approach.**

123 Changing stress states of shallower fault elements, potentially resulting in fault reactivation, can
 124 result from pore pressure increases within these elements as well as from a stress relocation from
 125 deeper located and already plastified elements. Hence, we relate the void ratio evolutions e of all
 126 observation points to a single reference pressure P_{ref} , to address both cases. While the observation
 127 points representing the mechanical behavior of adjacent element groups are located in the fault
 128 damage zone (Points 1 to 6 in Fig. 4), P_{ref} is located at the intersection between the fault and the
 129 storage reservoir.

130 Within our studies, we recognized that elements experiencing a similar amount of void ratio in-
131 crease during fault reactivation are distributed over a large fault region. As a consequence, the
132 distance between two observation points can be set in maximum to 200 m to partition the homo-
133 geneous fault in our study. In case of a heterogeneous hydraulic parameter distribution on the fault
134 plane, additional observation points are required.

135 The analytical $e(P_{ref})$ functions (red box in Fig. 2) are generated and parametrized (black box in
136 Fig. 2) on the basis of the results of a single fluid flow base simulation. As the pore pressure
137 distribution is driven by the Darcy velocity and a pressure gradient, the constant hydraulic con-
138 ductivity in one-way coupled simulations leads to linear void ratio-to-pore pressure relations,
139 while we recognize nonlinear behavior in two-way coupled simulations. Thus, the $e(P_{ref})$ functions
140 of one-way coupled simulations can be sufficiently linearized, which will be demonstrated in Sec-
141 tion 2.2.2 on the basis of the simulation results of parametric studies 1 and 2 presented in Table 1,
142 providing an overview of the simulations discussed in the scope of this study.

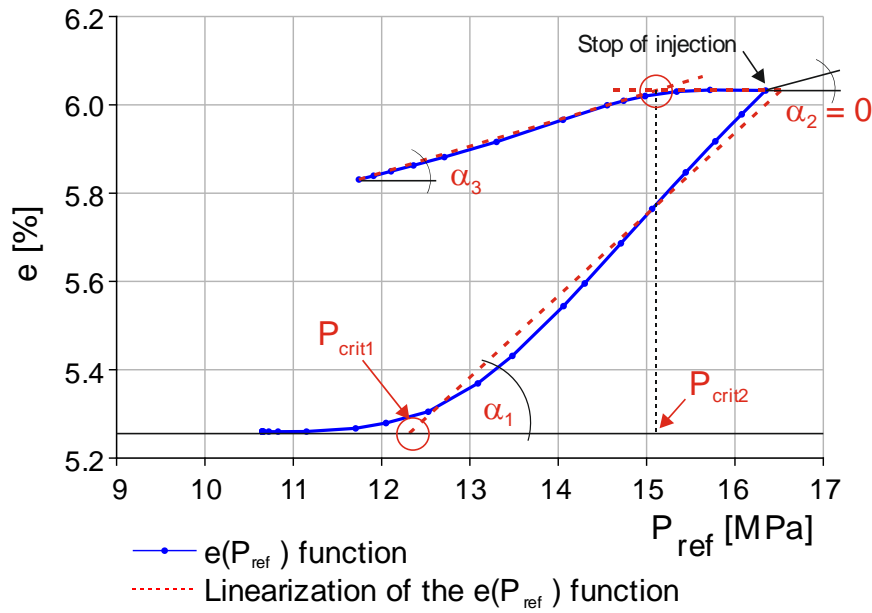
143 These 35 simulations are organized in three parametric studies, where studies 1 and 2 aim at in-
144 vestigation of the hydromechanical behavior of fault zones in one-way coupled simulations, con-
145 sidering varying injection regimes and initial fault permeabilities. Study 3 considers one-way, two-
146 way and semi-analytically coupled simulations to validate the new coupling approach.

147

148 **Table 1 Studies undertaken to show that $e(P_{ref})$ functions show an invariant behavior towards the injection rate**
 149 **(study 1), that α_1 , α_2 and α_3 are invariant towards the initial fault permeability (study 2) and to validate the**
 150 **semi-analytical hydromechanical coupling approach (study 3).**

Study 1: Invariant behavior of $e(P_{ref})$ towards the injection rate				Study 3: Validation of the semi-analytical coupling approach			
Scenario	Permeability k [m ²]	Injection rate [kg/s/m]	H-M cou- pling method	Scenario	Permeability k [m ²]	Injection rate [kg/s/m]	H-M coupling method
S1	5 x 10 ⁻¹⁶	0.0018	one-way	S18	5 x 10 ⁻¹⁶	0.0027	one-way
S2	5 x 10 ⁻¹⁶	0.0023	one-way	S19	1 x 10 ⁻¹⁶	0.0018	two-way
S3	5 x 10 ⁻¹⁶	0.0027	one-way	S20	1 x 10 ⁻¹⁶	0.0023	two-way
S4	5 x 10 ⁻¹⁶	0.0032	one-way	S21	1 x 10 ⁻¹⁶	0.0027	two-way
S5	5 x 10 ⁻¹⁵	0.0018	one-way	S22	1 x 10 ⁻¹⁶	0.0032	two-way
S6	5 x 10 ⁻¹⁵	0.0023	one-way	S23	1 x 10 ⁻¹⁶	0.0018	semi-analytical
S7	5 x 10 ⁻¹⁵	0.0027	one-way	S24	1 x 10 ⁻¹⁶	0.0023	semi-analytical
S8	5 x 10 ⁻¹⁵	0.0032	one-way	S25	1 x 10 ⁻¹⁶	0.0027	semi-analytical
Study 2: Invariant behavior of α_1, α_2 and α_3 towards the initial fault permeability				S26	1 x 10 ⁻¹⁶	0.0032	semi-analytical
S9	2.5 x 10 ⁻¹⁶	0.0027	one-way	S27	5 x 10 ⁻¹⁵	0.0027	one-way
S10	5 x 10 ⁻¹⁶	0.0027	one-way	S28	1 x 10 ⁻¹⁵	0.0018	two-way
S11	7.5 x 10 ⁻¹⁶	0.0027	one-way	S29	1 x 10 ⁻¹⁵	0.0023	two-way
S12	1 x 10 ⁻¹⁵	0.0027	one-way	S30	1 x 10 ⁻¹⁵	0.0027	two-way
S13	2.5 x 10 ⁻¹⁵	0.0027	one-way	S31	1 x 10 ⁻¹⁵	0.0032	two-way
S14	5 x 10 ⁻¹⁵	0.0027	one-way	S32	1 x 10 ⁻¹⁵	0.0018	semi-analytical
S15	7.5 x 10 ⁻¹⁵	0.0027	one-way	S33	1 x 10 ⁻¹⁵	0.0023	semi-analytical
S16	1 x 10 ⁻¹⁴	0.0027	one-way	S34	1 x 10 ⁻¹⁵	0.0027	semi-analytical
S17	2.5 x 10 ⁻¹⁴	0.0027	one-way	S35	1 x 10 ⁻¹⁵	0.0032	semi-analytical

151 Exemplarily for all others, Fig. 3 shows the $e(P_{ref})$ function (blue solid line) for Point 3 of Scenario
 152 S18 to introduce the linearization (red dashed line) and parametrization of the one-way coupled
 153 single-phase fluid flow base simulations, used to determine the analytical functions applied for the
 154 semi-analytical coupling approach. For the determination of these parameters, the length of one
 155 percent void ratio evolution has to be scaled to 1 MPa P_{ref} in general.



156
 157 **Fig. 3 Linearization and parametrization of the semi-analytical hydromechanical coupling approach, applying**
 158 **the $e(P_{ref})$ function of a one-way coupled simulation, using a five times higher initial fault permeability and**
 159 **introducing the inclinations α_1 , α_2 and α_3 and two pore pressure control points P_{crit1} and P_{crit2} . Note that the**
 160 **lengths of 0.2 percent void ratio evolution are scaled to 1 MPa P_{ref} to improve visibility.**

161 We identify a first control pore pressure P_{crit1} at the intersection of the red-dashed line inclined at
 162 the angle α_1 and the parallel to the x-axis at the level of the initial void ratio (5.263 %), indicating
 163 the occurrence of increasing volumetric strain/void ratio prevalently induced by shear failure ac-
 164 companied with plastic deformation in the corresponding fault group. Hence, the update of per-
 165 meability and porosity starts, when P_{ref} in the reference element exceeds the P_{crit1} value, and is
 166 controlled by the three inclinations α_1 , α_2 and α_3 , which operate as a stiffness to control the void
 167 ratio evolution. In this context, α_1 represents the void ratio evolution during the injection period
 168 predominantly induced by plastic deformations, while α_2 and α_3 apply for the post-injection period
 169 characterized by elastic deformations only. Furthermore, a second control pore pressure P_{crit2} is
 170 introduced at the intersection of the lines inclined at α_2 and α_3 , which acts as transition parameter
 171 between the two straight lines. The sectionalized linearization of α_1 is approximated by the method
 172 of least squares, α_2 and α_3 by tangents touching the two parts of the curves representing the post-

173 injection period. The transition point between α_1 and α_2 is variable and represents the maximum
 174 pore pressure depending on the fluid injection history of the reservoir.

175 The semi-analytical parametrization (α_1 , α_2 , α_3 , $P_{\text{crit 1}}$ and $P_{\text{crit 2}}$) used for the semi-analytical sim-
 176 ulations, considering initial fault permeabilities of $k = 10^{-16} \text{ m}^2$ and $k = 10^{-15} \text{ m}^2$ (Section 2.2.2) to
 177 validate the new approach is given in Table 2 and Table 3. Furthermore, the average depth at each
 178 observation point (Points 1 to 6) is provided.

179 **Table 2 Parametrization used for the semi-analytically coupled simulation runs with $k_{\text{ini}} = 10^{-16} \text{ m}^2$.**

Point	Depth [m]	Linearized inclinations of $e(P_{\text{ref}})$ functions			Pore pressure control points in the reference cell (P_{ref}) [MPa]	
		α_1 [°]	α_2 [°]	α_3 [°]	$P_{\text{crit 1}}$	$P_{\text{crit 2}}$
1	570.3	7.2	0.0	1.2	13.3	14.8
2	695.3	10.2	0.0	2.5	13.1	14.9
3	820.3	11.9	0.0	3.4	12.6	15.3
4	945.3	12.5	1.1	3.7	12.3	15.6
5	1012.5	12.2	2.0	3.7	12.2	15.7
6	1160.0	13.0	0.0	4.6	12.4	15.5

180
 181 **Table 3 Parametrization used for the semi-analytically coupled simulation runs with $k_{\text{ini}} = 10^{-15} \text{ m}^2$.**

Point	Depth [m]	Linearized inclinations of $e(P_{\text{ref}})$ functions			Pore pressure control points in the reference cell (P_{ref}) [MPa]	
		α_1 [°]	α_2 [°]	α_3 [°]	$P_{\text{crit 1}}$	$P_{\text{crit 2}}$
1	570.3	6.1	0.2	1.1	11.9	14.0
2	695.3	8.4	0.5	2.1	11.7	14.0
3	820.3	10.5	1.4	3.1	11.5	14.0
4	945.3	10.9	3.7	3.7	11.4	14.0
5	1012.5	10.7	3.6	3.6	11.3	14.1
6	1160.0	10.8	2.1	4.2	11.4	14.1

182 As one base simulation can be employed to investigate the impact of a multitude of different in-
183 jection rates, the invariant behavior of the semi-analytical parametrization related to the injection
184 rates is required and is validated by the results of parametric study 1 (Table 1). In addition, the
185 results of study 2 are used to demonstrate that the parameters α_1 , α_2 and α_3 show invariant behavior
186 related to the initial fault permeability. This allows us to demonstrate that the nonlinear shape of
187 the $e(P_{ref})$ functions, generated with two-way coupled simulations can be sufficiently approxi-
188 mated by one-way coupled simulations. Therefore, $p_{crit 1}$ has to be shifted to a lower value, which
189 is realized by generally employing a fault permeability multiplier of 5 in the base simulation to
190 estimate the $e(P_{ref})$ function used for the parameterization of the semi-analytically coupled simu-
191 lations. This permeability multiplier is only applied in the base simulation, while the semi-analyt-
192 ically coupled simulations of course consider the initial fault permeability. A detailed explanation
193 of this general permeability multiplier is given in Section 2.2.2.

194 Finally, these functions are implemented into the semi-analytical coupling approach as shown in
195 the blue box in Fig. 2. The coupling approach operates in a semi-analytical manner, whereby the
196 averaged pore pressures P are determined numerically by the multiphase flow simulator during the
197 simulation run, whereas permeability k and porosity ϕ updates are directly managed by a set of
198 functions representing the void ratio evolution determined at observation points. Hence, the itera-
199 tive parameter exchange between both simulators is omitted.

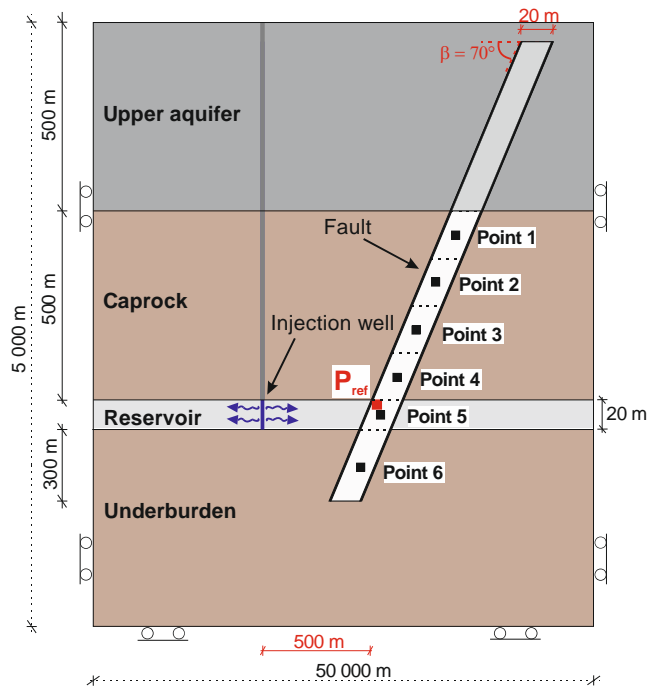
200 Further, permeability and porosity updates are undertaken for the geological fault only, implying
201 that reservoir and caprock integrity are not compromised by the induced pore pressure increase.
202 To overcome this restriction into our approach, we suggest to assign elasto-plastic material behav-
203 ior for the surrounding rocks to parametrize the base simulation. In consequence, only the results
204 of the base simulations are suitable for parameterization, exhibiting that pore pressure increase
205 does not compromise the integrity of the surrounding rocks. Considering the limitation of one base

206 simulation being valid for a specific model geometry and one set of hydromechanical parameters,
207 the suggested procedure is capable to significantly reduce the computational time required by cou-
208 pled hydromechanical simulations of a multitude of injection rates.

209 **2.2 Validation of the semi-analytical coupling approach**

210 **2.2.1 Setup of the synthetic model**

211 To validate the semi-analytical coupling approach for single phase fluid flow, 35 simulation runs
212 organized in three parametric studies shown in Table 1, considering a synthetic 2D model plotted
213 in Fig. 4 were undertaken as described in Adams et al., 2015 and are discussed in detail in Sec-
214 tion 2.2.2. The top of the 20-m thick reservoir formation is located at 1,000 m depth and an aquifer
215 with a thickness of 500 m is implemented at the model top. Caprock formations are present above
216 and below the reservoir, cut by a fault dipping by 70° in 500 m distance from the injection well
217 (injection rates are given in Table 1). As it is not possible to differentiate between fault cores and
218 damage zones within large-scale models, we apply a lumped fault permeability as previously in-
219 troduced by Cappa and Rutqvist (2011). The fault is partitioned into six element groups, with one
220 element representing each group (Points 1 to 6, black squares in Fig. 4). Additionally, one single
221 element is defined as reference element at the transition between the fault and reservoir to derive
222 the reference pore pressure P_{ref} for the parametrization of the semi-analytical hydromechanical
223 coupling (red square in Fig. 4). We simulated a 20-year injection and a 30-year post-injection pe-
224 riod of brine (salinity of 20 % NaCl by weight) to maintain a simulation setup not potentially
225 compromised by multiphase flow effects. In Section 3, this generalization is validated for multi-
226 phase fluid flow, and we demonstrate that our coupling approach is capable to handle multiphase
227 flow effects in the presence of a gas phase.



228
 229 **Fig. 4 Schematic overview of the synthetic model considering a 20 m wide fault with a dip of $\beta = 70^\circ$ as applied**
 230 **for the implementation of the semi-analytical coupling methodology, based on single-phase fluid flow simula-**
 231 **tions.**

232 The finite element program Abaqus[®] is used, assuming a 50 km wide and 5 km thick model, plane-
 233 strain conditions and an extensional stress regime with $\sigma_h / \sigma_v = 0.7$ (total horizontal to vertical
 234 stresses). Considering a hydrostatic pressure gradient, atmospheric pressure at the ground surface
 235 and salinity in all formations according to the information given in Table 4, the initial fluid pres-
 236 sure at the top of the reservoir amounts to 10.62 MPa. Temperature distribution is calculated using
 237 a geothermal gradient of 30 °C/km, resulting in an average temperature of 40 °C in the reservoir.
 238 Isothermal conditions are assumed for all simulation runs. Reservoir rock behavior is considered
 239 to be elastic for simplicity, whereas the fault zone follows a linear and ideal elastoplastic constitu-
 240 tive behavior based on the Mohr-Coulomb failure criterion (Altmann et al., 2014; Langhi et al.,
 241 2010; Mandl, 1988; Nguyen et al., 2016; Orlic, 2016; Pan et al., 2016; Rutqvist et al., 2016; Verdon
 242 and Stork, 2016; Vilarrasa et al, 2016; Zhang et al., 2009, 2010, 2011, 2013, 2015). The initial
 243 permeability of the fault is varied between $k = 1 \times 10^{-16} \text{ m}^2$ and $k = 2.5 \times 10^{-14} \text{ m}^2$. All further ma-
 244 terial properties, e.g., dry specific weight γ_d , Young's modulus E , Poisson's ratio ν , friction angle

245 φ , cohesion c , dilation angle ψ , porosity ϕ , permeability k for each formation used in the simula-
246 tions are given in Table 4. Besides the initial permeability and porosity, the given material prop-
247 erties are valid for the entire fault zone. Hereby, porosity and permeability of the upper part of the
248 fault (50 m to 500 m depth) are equal to those of the upper aquifer.

249 In all simulations presented here, porosity and permeability are updated according to
250 Chin et al., 2000 using Equations (2) and (3)

$$251 \quad \phi = 1 - (1 - \phi_i)e^{-\varepsilon_v} \quad (2)$$

$$252 \quad k = k_i \left(\frac{\phi}{\phi_i} \right)^n \quad (3)$$

253 Here, ϕ is the porosity at a given volumetric strain, ϕ_i the initial porosity, ε_v the volumetric strain
254 increment, k the permeability at a given strain, k_i the initial permeability, and n a porosity sensi-
255 tivity exponent. In the present study, n is set to 10 to achieve a fault permeability increase by about
256 one magnitude (Cappa and Rutqvist, 2011) for a maximum volumetric strain of 1.5 %. Brine and
257 CO₂ fluid data are derived from Battistelli et al., 1997 and Spycher et al., 2003.

258

259 **Table 4 Material properties used to simulate single-phase fluid flow in the reservoir-caprock system with one**
 260 **fault.**

Parameters	Reference	Reservoir	Caprock	Underburden	Upper aquifer	Fault
Young's modulus, E (GPa)	Cappa and Rutqvist, 2011	10	10	10	10	1
Poisson's ratio, ν (-)	Cappa and Rutqvist, 2011	0.25	0.25	0.25	0.25	0.25
Rock density, ρ_s (kg/m ³)	Cappa and Rutqvist, 2011	2 260	2 260	2 260	2 260	2 260
Biot's coefficient, α (-)	Cappa and Rutqvist, 2011	1	1	1	1	1
Friction angle, φ (°)	Cappa and Rutqvist, 2011	-	-	-	-	25
Dilation angle, ψ (°)	Cappa and Rutqvist, 2011	-	-	-	-	20
Porosity, ϕ (-)	Cappa and Rutqvist, 2011	0.1	0.01	0.01	0.1	0.05
Permeability, k (m ²)	Cappa and Rutqvist, 2011	10 ⁻¹³	10 ⁻¹⁹	10 ⁻¹⁹	10 ⁻¹⁴	-
Salinity (% NaCl by weight)	Assumed	20	15	20	10	15

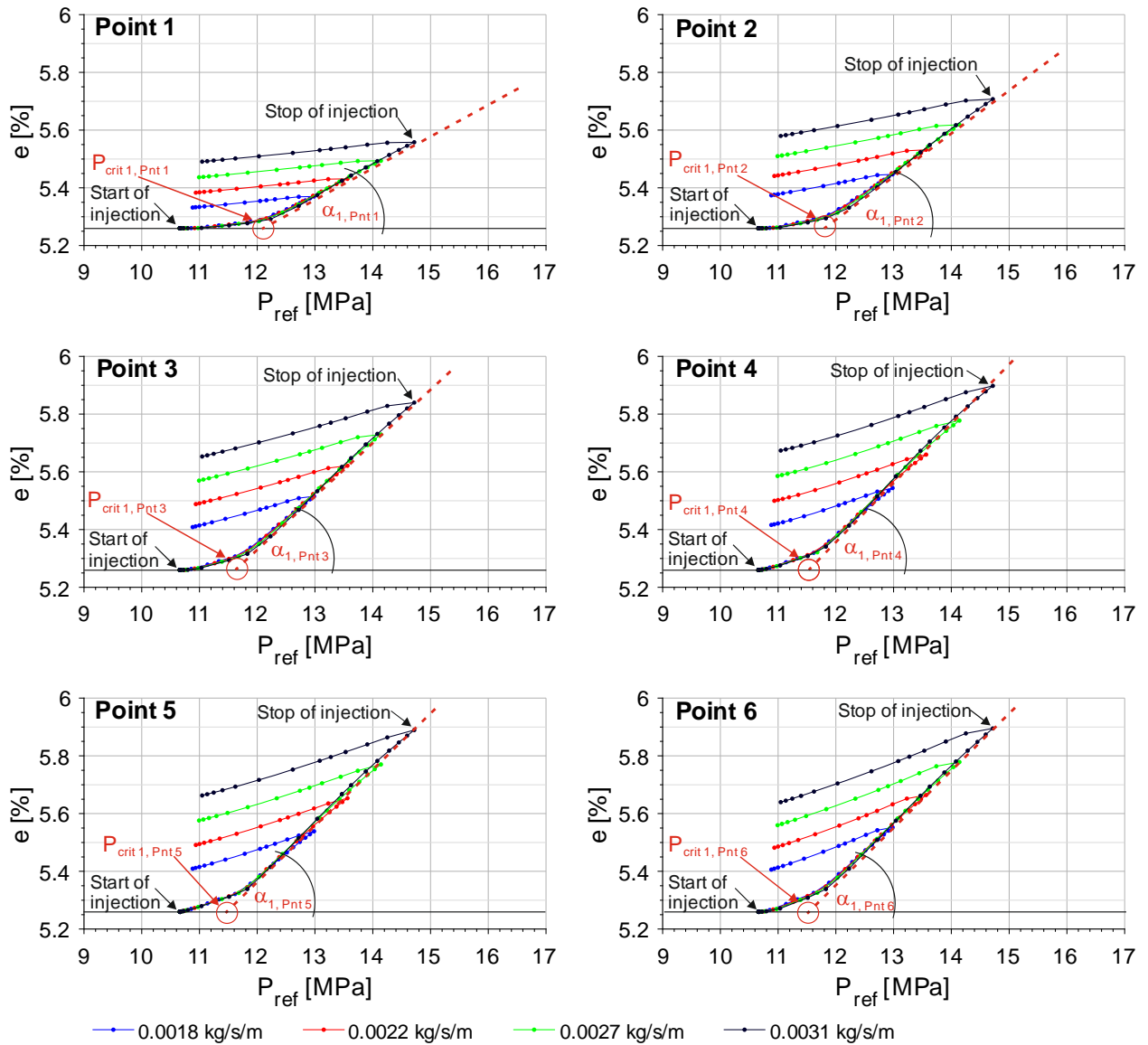
261 **2.2.2 Results and discussion**

262 The influence of varying initial intrinsic fault permeability and injection rate on the fault's void
 263 ratio evolution was investigated in three parametric studies (S1 – S8, S9 – S17 and S18 – S35)
 264 given in Table 1. The first and the second study were run in an one-way coupled manner, while
 265 the third one was employed to validate the coupling approach by a comparison of the pore pressure
 266 distribution determined by the two-way and semi-analytically coupled simulations.

267 Fig. 5 shows the $e(P_{ref})$ functions of all six observation points determined in one-way coupled
 268 simulations, considering four different injection rates (S5 – S8) and an initial fault permeability of
 269 5×10^{-15} m². As all void ratio evolutions of one simulation run are related to one reference pore

270 pressure, all six curves show the same maximum pore pressure, i.e., 13 MPa for the lowest (blue
271 curve) and 14.8 MPa for the highest injection rate (black curve). Linearizing and parametrizing
272 these curves according to Fig. 3, we observe decreasing maximum void ratio evolutions for shal-
273 lower observation points, which lead to six different parameter sets describing the semi-analytical
274 coupling, i.e, $\alpha_{1, \text{Pnt 1}}$ to $\alpha_{1, \text{Pnt 6}}$ and $P_{\text{crit 1, Pnt 1}}$ to $P_{\text{crit 1, Pnt 6}}$ in Fig. 5.

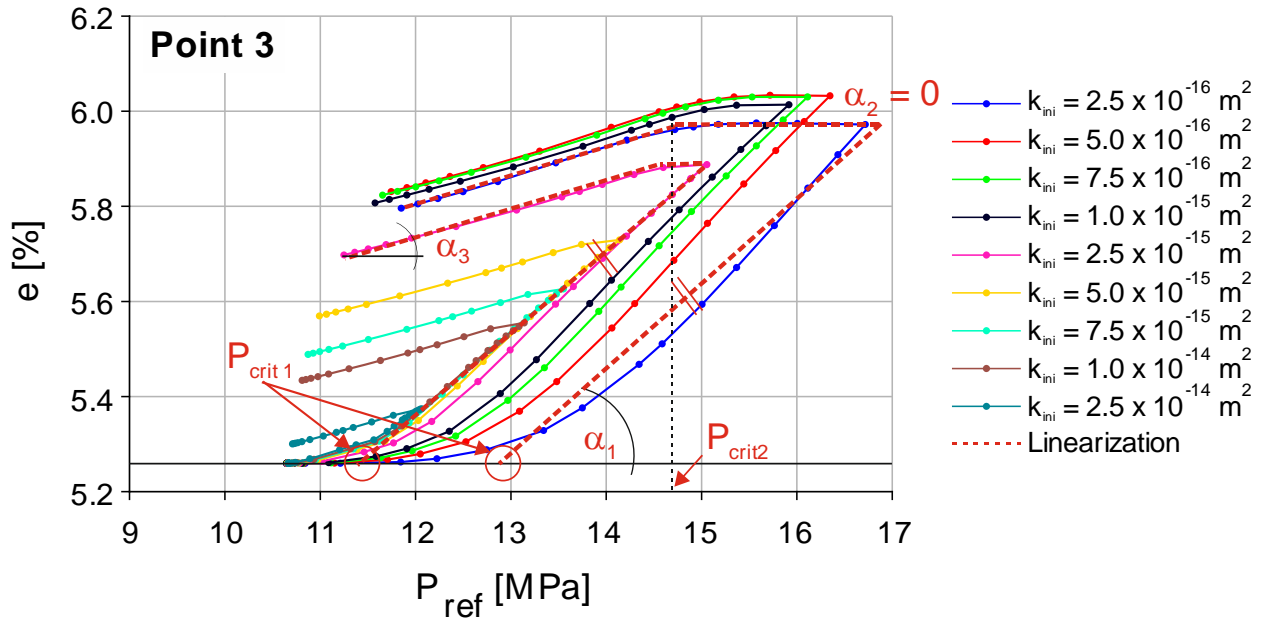
275 As we recognize for each injection rate identical values for α_1 , α_2 , α_3 and P_{crit1} in each observation
276 point, we emphasize that the calibration and parametrization of the semi-analytical coupling is
277 injection rate-independent. Opposite to this, Fig. 5 shows an injection rate-dependent behavior for
278 P_{crit2} : the higher the injection rate, the higher P_{crit2} . In hydromechanically coupled simulations,
279 porosity and permeability updates are undertaken based on the results calculated in the prior sim-
280 ulation step and remain constant during the subsequent one. As a consequence, a constant void
281 ratio is automatically considered by the semi-analytical coupling approach. Furthermore, we rec-
282 ognize a fast pore pressure decrease by more than 1 MPa within the first days in the reservoir and
283 the fault after the injection stop, what emphasizes the short time period for which the inclination
284 α_2 is valid. Hence, we consider the non-invariant behavior of $p_{\text{crit 2}}$ related to different injection
285 rates to have negligible influence on the results of the semi-analytical coupling only.



286
 287 **Fig. 5** Diagrams of $e(P_{ref})$ functions of one-way coupled simulations, considering the same initial permeability
 288 and four different injection rates (scenarios S5 – S8) occurring at all observation points (Points 1-6). These
 289 functions show the same inclinations α_1 , α_2 and α_3 and P_{crit1} for each injection rate. Hence, the calibration and
 290 parametrization of the semi-analytical coupling approach is independent from the injection rate used in the
 291 base simulation.

292 Representative for all other curves, the $e(P_{ref})$ curves at Point 3, considering one-way coupling, a
 293 constant injection rate of 0.0027 kg/s/m and varying initial fault permeabilities between 2.5×10^{-16}
 294 and $2.5 \times 10^{-14} \text{ m}^2$ are shown in Fig. 6. Linearizing these $e(P_{ref})$ functions (red dashed lines) illus-
 295 trates that also this parameter setup leads to identical inclinations α_1 , α_2 and α_3 as for Point 3 in
 296 Fig. 5. Furthermore, we identify decreasing P_{crit1} values accompanied by increasing initial fault
 297 permeabilities, converging against 11.4 MPa for permeabilities smaller/equal than $2.5 \times 10^{-15} \text{ m}^2$.

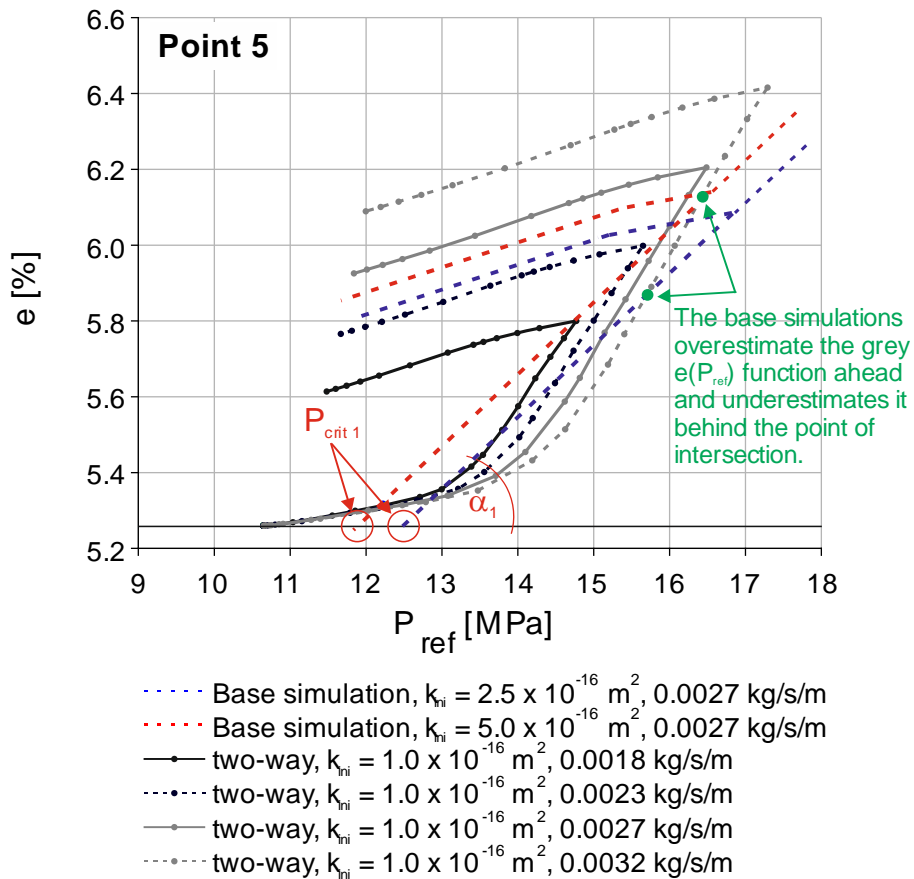
298 The residual initial permeabilities result in P_{crit1} values between 11.4 MPa and 12.9 MPa. Hence,
 299 varying initial permeabilities only shift the $e(P_{ref})$ functions controlled by P_{crit1} , but do not affect
 300 the inclinations α_1 to α_3 .



301
 302 **Fig. 6** Nine $e(P_{ref})$ functions determined by one-way coupled base simulations, considering an injection rate of
 303 **0.0027 kg/s/m** and varying initial fault permeabilities between 2.5×10^{-16} and $2.5 \times 10^{-14} \text{ m}^2$ show equal inclina-
 304 tions α_1 to α_3 and a shift of the linearized functions controlled by P_{crit1} .

305 Due to the update of porosity and permeability, the results of two-way coupled simulations, con-
 306 sidering four different injection rates and an initial fault permeability of $k = 10^{-16} \text{ m}^2$ (Fig. 7, black
 307 and grey shaded lines) show a nonlinear relationship between void ratio evolution and P_{ref} , increas-
 308 ing with higher injection rates. Additionally, the linearized run of one-way coupled $e(P_{ref})$ func-
 309 tions (dashed blue and red lines in Fig. 7), considering initial fault permeabilities specifically
 310 higher ($k = 2.5$ and $5.0 \times 10^{-16} \text{ m}^2$) show that the nonlinear behavior of two-way coupled simula-
 311 tions can be approximated by the one-way coupled base simulations. At the intersection between
 312 the linearized $e(P_{ref})$ functions and the two-way coupled $e(P_{ref})$ functions (green points in Fig. 7),
 313 a boundary between two different sections is introduced.

314 Hence, that approximation method generally overestimates the void ratio evolution at the begin-
 315 ning of the update and underestimates it at the end of the injection period (section right to the green
 316 points in Fig. 7). This goes along with a better fit of the one-way coupled base simulation using a
 317 permeability multiplier of 2.5 (blue line) in the section left of the point of intersection with the
 318 grey $e(P_{ref})$ function (green point in Fig. 7), while the use of a permeability multiplier of 5.0 (red
 319 line) provides an improved approximation of the section right to the intersection. However, as the
 320 permeability update used in this paper (Chin et al., 2000) is driven by a power law exponent (see
 321 Equations (2) and (3)), a good approximation of the section right to the intersection is more rele-
 322 vant.



324 **Fig. 7** $e(P_{ref})$ functions show the nonlinear behavior of four two-way coupled simulations. The nonlinearity
 325 increases with increasing injection rates. The linearized run of two base simulations (blue and red dashed lines),
 326 considering $k_{ini} = 2.5 \times 10^{-16}$ and $k_{ini} = 5 \times 10^{-16} \text{ m}^2$ can sufficiently approximate the $e(P_{ref})$ functions of two-way
 327 coupled simulations.

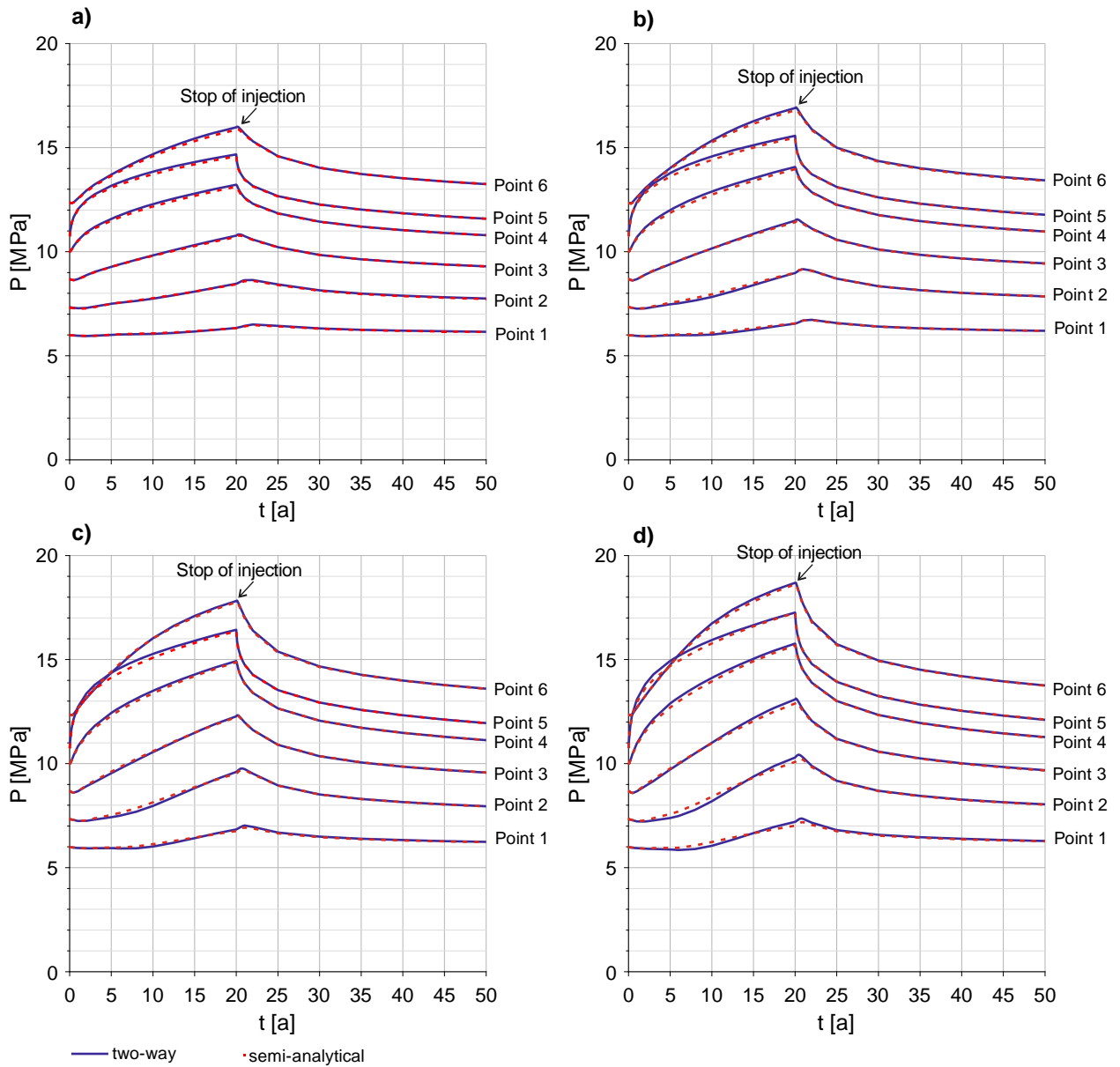
328 Additionally, the approximation of the $e(P_{ref})$ curves by the semi-analytical parametrization con-
329 sidering a permeability multiplier of 5.0 shows higher coefficients of approximation compared to
330 the parametrization considering a multiplier of 2.5.

331 In an additional parametric study which is not discussed in detail in here, we investigated the
332 influence of different sensitivity exponents n for deriving permeability from porosity (Equation 3)
333 in two-way coupled simulations. Considering n values between 10 and 20 as well as an injection
334 rate of 0.0027 kg/s/m, we identified flattening pore pressure increases in the fault and reservoir
335 elements with increasing sensitivity exponents, accompanied by lower void ratio increases. In ad-
336 dition, we recognized that the parameters α_1 , α_2 , α_3 and $P_{crit 1}$ are identical for all exponent varia-
337 tions. Since higher exponents result in higher permeabilities for the same porosity increase, this
338 corresponds with higher hydraulic conductivities resulting in lower pore pressure increases.
339 Hence, we state that an upper limit for pore pressure increases exists, while the parametrization of
340 the semi-analytical approach is invariant with respect to the rate of fault permeability increase.

341 In combination with the results of the aforementioned studies, i.e., convergence of $P_{crit 1}$ against a
342 fix value for initial permeabilities less than or equal to $2.5 \times 10^{-15} \text{ m}^2$ (Fig. 6) and the discussion of
343 the results shown in Fig. 7, we generally recommend to use an initial fault permeability five times
344 higher than that in the two-way coupled simulations to parameterize the semi-analytical approach
345 by one base simulation. Furthermore, these general perceptions, i.e., injection rate-independent
346 parametrization and linear void ratio-over-reference pore pressure behavior for one-way coupled
347 simulations point out the general validity of the suggested approach.

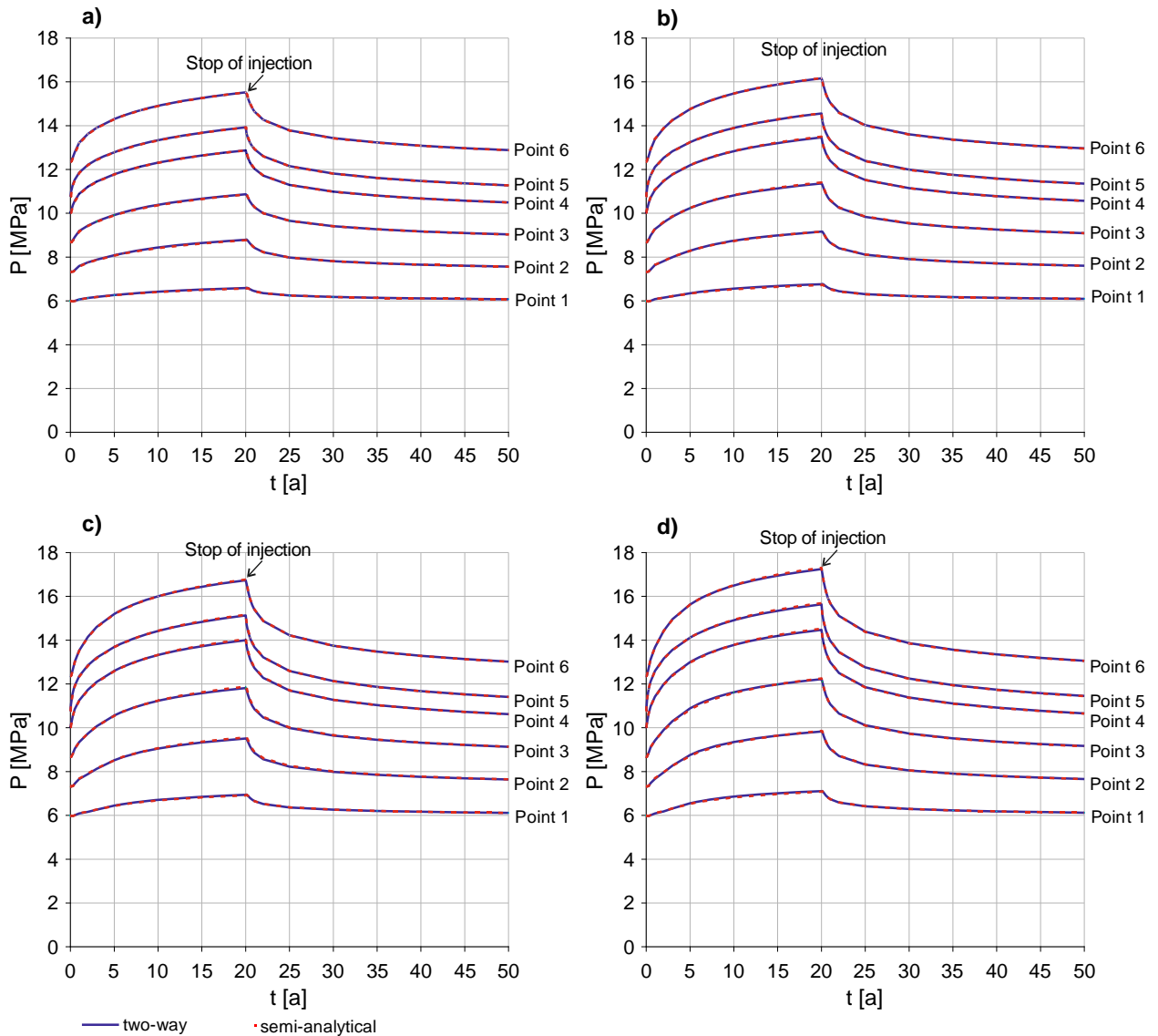
348 Finally, the semi-analytical coupling approach is validated by a comparison of pore pressure dis-
349 tributions over time, resulting from four different brine injection rates given in Table 1. Based on
350 two single base simulations (S18 and S27) considering an initial permeability five times higher

351 than that applied in the benchmark simulations (10^{-15} and 10^{-16} m²), the parametrization for the
 352 semi-analytical coupling method is given in Table 2 and Table 3. A comparison of pore pressure
 353 distributions over time between the semi-analytically (red dashed lines) and two-way coupled
 354 (blue solid lines) simulations is given in Fig. 8 and Fig. 9 for all observation points. Maximum
 355 reference pore pressure P_{ref} increases by 4.12 MPa for the lowest and by 6.64 MPa for the highest
 356 injection rate are observed. For all investigated scenarios, we achieve a remarkably good agree-
 357 ment between the validation (semi-analytical) and benchmark simulation (two-way) results.



358

359 **Fig. 8** Pore pressure distribution over time at selected fault depths with $k_{ini}=10^{-16} \text{ m}^2$ and four brine injection
 360 rates of a) 0.0018 kg/s/m, b) 0.0023kg/s/m, c) 0.0027 kg/s/m and d) 0.0032 kg/s/m show a very good agreement
 361 between the two-way (blue solid line) and semi-analytical coupling schemes (red dashed line).



362
 363 **Fig. 9** Pore pressure distribution over time at selected fault depths for $k_{ini}=10^{-15} \text{ m}^2$ and four brine injection
 364 rates of a) 0.0018 kg/s/m, b) 0.0023kg/s/m, c) 0.0027 kg/s/m and d) 0.0032 kg/s/m show a very good agreement
 365 between the two-way (blue solid line) and semi-analytical coupling schemes (red dashed line).

366 In the aforementioned simulations, we observe a maximum fault slip of 15.5 cm (simulation S22),
 367 accompanied by a maximum pore pressure increase of 7 MPa in the reservoir. These results com-
 368 pletely qualitatively with the findings of Cappa and Rutqvist (2011). Their investigations of a synthetic
 369 model consisting of one single fault zone dipping with 80° show a maximum fault slip of 11.5 cm
 370 achieved for a maximum pore pressure increase of approximately 9 MPa. As both investigations

371 use identical material parameters (see Table 4), the results of both studies are comparable and the
 372 difference of 4 cm can be explained by the deviation of the dipping angle by 10°.

373 In Section 3, multiphase fluid flow simulations are used to verify the hypothesis that one set of
 374 functions, determined by one base simulation is suitable to significantly reduce the computational
 375 time for simulating a multitude of different injection rate scenarios.

376 **3. Application example for fault reactivation due to CO₂ injection con-** 377 **sidering multiphase fluid flow**

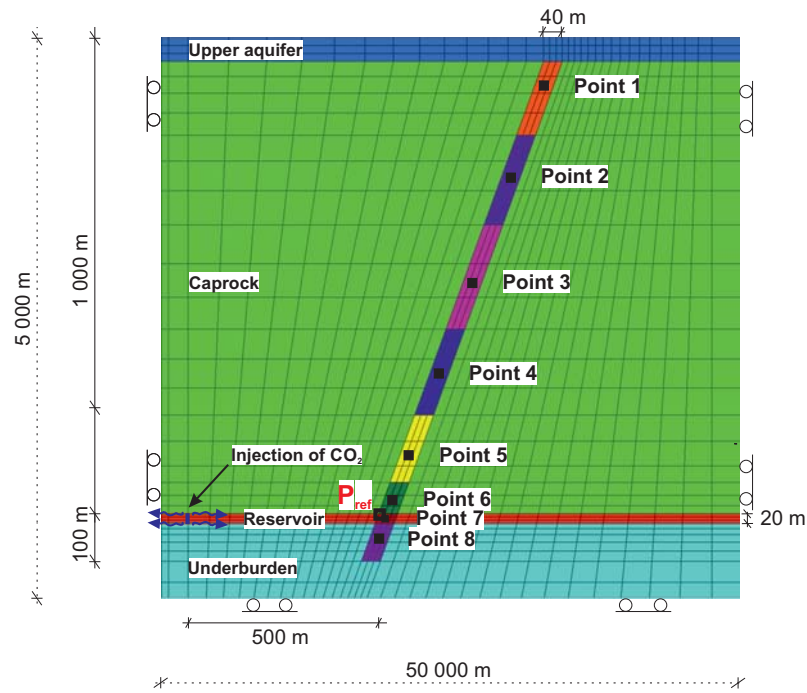
378 The isothermal simulations discussed in the following consider 20-year injection and 30-year post-
 379 injection periods. We use the previously discussed one- and two-way hydromechanical coupling
 380 approaches by combining the TOUGH2-MP and FLAC^{3D} simulators (Cappa and Rutqvist, 2011;
 381 Itasca, 2013; Kempka and Kühn, 2013; Pruess, 2005; Zhang et al., 2008). The applied model par-
 382 ametrization is given in Table 5.

383 **Table 5 Material properties used to simulate CO₂ injection in a reservoir-caprock system with one fault.**

Parameters	Reference	Reservoir	Caprock	Underbur- den	Upper aquifer	Fault
Young's modulus, E (GPa)	Cappa and Rutqvist, 2011	10	10	10	10	1
Poisson's ratio, ν (-)	Cappa and Rutqvist, 2011	0.25	0.25	0.25	0.25	0.25
Rock density, ρ_s (kg/m ³)	Cappa and Rutqvist, 2011	2 260	2 260	2 260	2 260	2 260
Biot's coefficient, α (-)	Cappa and Rutqvist, 2011	1	1	1	1	1
Friction angle, φ (°)	Cappa and Rutqvist, 2011	-	-	-	-	25
Dilation angle, ψ (°)	Cappa and Rutqvist, 2011	-	-	-	-	20

Porosity, ϕ (-)	Cappa and Rutqvist, 2011	0.1	-	-	0.1	0.05
Permeability, k (m^2)	Cappa and Rutqvist, 2011	10^{-13}	-	-	10^{-14}	10^{-16}
Residual non-wetting phase (CO_2) saturation (-)	Cappa and Rutqvist, 2011	0.05	-	-	0.05	0.05
Residual wetting phase (water) saturation (-)	assumed	0.15	-	-	0.15	0.15
Capillary entry pressure (van Genuchten 1980)	assumed	12.6	-	-	12.6	12.6
Parameter m (-) (van Genuchten 1980)	assumed	0.65	-	-	0.65	0.65

384 Beside a reduction of the upper aquifer thickness down to 50 m and an increase of the caprock
385 thickness up to 950 m, a fault width of 40 m as shown in Fig. 10 as well as impermeable caprock
386 and underburden, the model and parameter setup is equal to the one given in Section 2. This adap-
387 tion was done, as we aim at validating the new approach under extreme conditions, i.e., a doubling
388 of the flow path length through the low permeable part of the fault by increasing the caprock
389 thickness. Considering a hydrostatic pressure gradient and an atmospheric pressure of
390 0.101325 MPa at the ground surface, the initial fluid pressure at the top of the reservoir equates to
391 9.91 MPa. The applied injection rates are given in Table 6 and the fault is partitioned into eight
392 element areas here (Points 1 to 8 in Fig. 10) due to the increase of the caprock thickness.



393
 394 **Fig. 10** Close-view of injection elements and fault zone in the synthetic model used for the implementation and
 395 validation of the semi-analytical hydromechanical coupling. The black-filled rectangles (Points 1–8) are repre-
 396 sentative elements and incorporate the hydraulic behavior of the corresponding element group of the fault. The
 397 black rectangle at the intersection of the reservoir and the fault is the reference element for the pore pressure
 398 P_{Ref} .

399 To validate the semi-analytical coupling approach for multiphase fluid flow, seven simulations
 400 listed in Table 6 are carried out. A one-way coupled single-phase fluid flow base simulation with
 401 an initial fault permeability of $5 \times 10^{-16} \text{ m}^2$ (five times higher than in the previously introduced
 402 benchmark simulation) and a brine injection rate of 0.0018 kg/s/m determine the base case.

403 **Table 6** Simulations undertaken for validation of the semi-analytical hydromechanical coupling approach by
 404 two-way coupled simulations.

Simulation type	Flow phases	Initial fault zone permeability [m^2]	Injection rate [kg/s/m]	H-M coupling method
Base case	single	5×10^{-16}	0.0018	one-way
Benchmark	multi	1×10^{-16}	0.00153	two-way
Benchmark	multi	1×10^{-16}	0.0019	two-way
Benchmark	multi	1×10^{-16}	0.0023	two-way
Validation	multi	1×10^{-16}	0.00153	semi-analytical
Validation	multi	1×10^{-16}	0.0019	semi-analytical
Validation	multi	1×10^{-16}	0.0023	semi-analytical

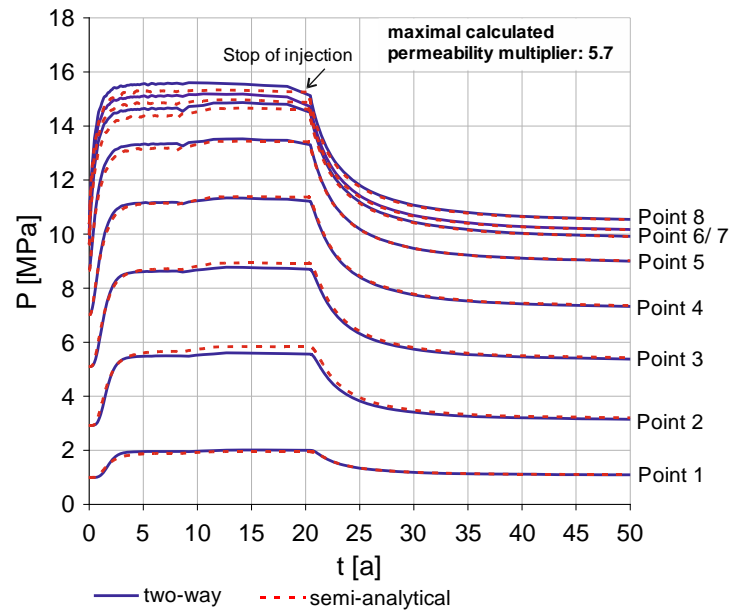
405 Based on this single simulation, the parametrization for the semi-analytical coupling method (see
 406 Table 7) used for validation (see Table 6) is determined as previously discussed in Section 2. To
 407 assess the obtained results of the innovative coupling, benchmark simulations are undertaken using
 408 a sequentially two-way coupled approach according to Table 6.

409 **Table 7 Parametrization of the semi-analytically coupled simulation runs.**

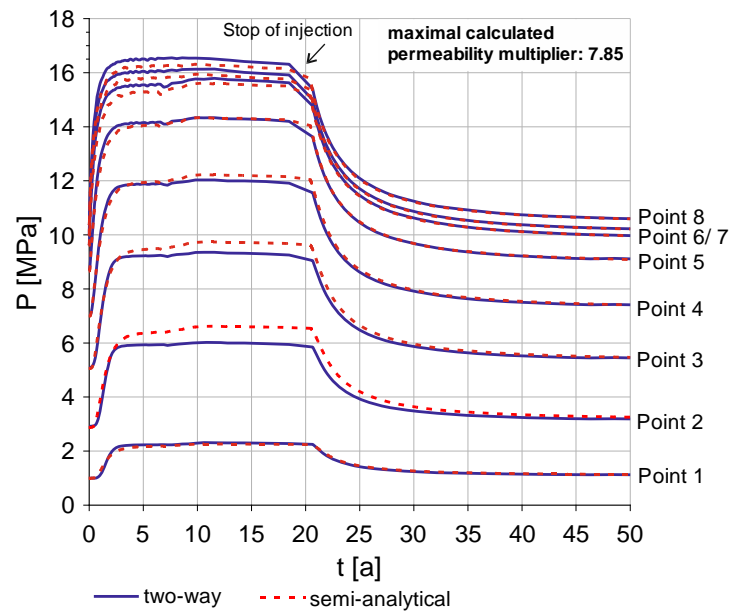
Point	Depth [m]	Linearized inclinations of $e(P_{ref})$ functions			Pore pressure control points in the reference cell (P_{ref}) [MPa]	
		α_1 [°]	α_2 [°]	α_3 [°]	$P_{crit 1}$	$P_{crit 2}$
1	98.9	3.9	0.0	1.0	12.3	12.83
2	290.1	11.7	0.0	2.6	12.44	13.07
3	510.0	15.1	0.0	3.6	12.3	13.34
4	705.2	15.6	0.0	4.1	12.06	13.74
5	873.9	13.8	0.0	4.1	11.77	14.14
6	971.8	11.2	0.4	3.6	11.61	14.38
7	1010.0	9.6	1.9	3.3	11.53	13.97
8	1051.8	7.2	0.4	2.9	11.62	14.52

410 **3.1 Results and discussion**

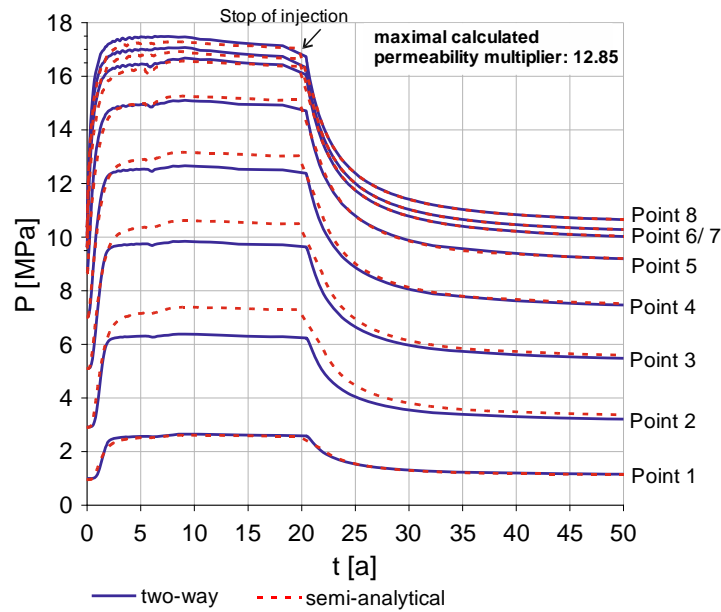
411 A comparison of pore pressure distributions over time, resulting from three different CO₂ injection
 412 rates (see Table 6) using the semi-analytical coupling (red dashed lines) and a two-way coupling
 413 (blue solid line) is given in Figures 11 to 13. For the lowest injection rate, the maximum reservoir
 414 pore pressure increase is equal to 5.25 MPa, 6.17 MPa for the average one and 7.06 MPa for the
 415 highest one. At Point 4, the maximum calculated permeability multipliers (Equations 2 and 3) are
 416 5.7, 7.85 and 12.85, respectively, increasing with the applied injection rate. For all investigated
 417 scenarios, we achieve a remarkably good agreement between the validation and benchmark simu-
 418 lation results.



419
 420 **Fig. 11** Pore pressure evolution over time at selected fault depths for $k_{ini}=10^{-16} \text{ m}^2$ and a CO_2 injection rate of
 421 **0.00153 kg/s/m** shows a very good agreement between the two-way (blue solid line) and semi-analytical coupling
 422 (red dashed line). A maximum pore pressure deviation between both coupling methods of 5 % is observed at
 423 **Point 2.**



424
 425 **Fig. 12** Pore pressure evolution over time at selected fault depths for $k_{ini}=10^{-16} \text{ m}^2$ and a CO_2 injection rate of
 426 **0.0019 kg/s/m** shows a very good agreement between the two-way (blue solid line) and semi-analytical coupling
 427 (red dashed line). A maximum pore pressure deviation between both coupling methods of 10 % is observed at
 428 **Point 2.**



429
 430 **Fig. 13** Pore pressure evolution over time at selected fault depths for $k_{ini}=10^{-16} \text{ m}^2$ and a CO_2 injection rate of
 431 **0.0023 kg/s/m** shows a good agreement for the two-way (blue solid line) and semi-analytical coupling (red
 432 dashed line). A maximum pore pressure deviation between both coupling methods of 20 % is observed at Point
 433 2.

434 Even under this extreme model setup, considering a caprock thickness of 950 m not intersected by
 435 aquifers draining the fault, only minor deviations between both coupling approaches are observed
 436 at Points 2, 3 and 4. In Fig. 11, representing the pore pressure distributions for the lowest injection
 437 rate, we observe a deviation of approximately 5 %, in Fig. 12 one of 10 % and in Fig. 13 one of
 438 20 % for the highest injection rate. Anyhow, compared to the results given in Section 2, we observe
 439 higher deviations in pore pressure distribution over time between both coupling approaches. This
 440 can be explained by an increase in nonlinearity of the void ratio evolution, induced by the increased
 441 flow path length of the fault zone.

442 The required computational time of the semi-analytical coupling approach is significantly lower
 443 than that of the sequential two-way coupling, what emphasizes the actual benefit of using this
 444 innovative coupling method. While the semi-analytical coupling needs between 1.5 and 2.5 hours
 445 CPU time using a parallel calculation on four AMD Opteron 6320 processors (TOUGH2-MP), the
 446 two-way coupled computation consumes between 21.5 and 38.0 hours on one Intel E5-2687W

447 CPU (FLAC^{3D}) and four AMD Opteron 6320 processors (TOUGH2-MP). Savings in computa-
448 tional time by a factor of up to 15 enable carrying out a multitude of time-consuming multiphase
449 fluid flow simulations coupled with mechanics as applied in probabilistic assessments such as
450 uncertainty and risk analyses.

451 **4. Conclusions**

452 The comparative study discussed at the beginning of this manuscript introduces a new computa-
453 tionally-efficient semi-analytical hydromechanical coupling approach for fault reactivation and
454 demonstrates its theoretical validity. In this context, fault reactivation is determined by the Mohr-
455 Coulomb failure criterion and ideal-elastic material behavior, controlled by the fault's friction and
456 dilatancy. Even though this approach may not accurately represent the complex geological reality,
457 it allows to carry out coupled numerical assessments on fault reactivation at reservoir to regional
458 scale. For that purpose, we assumed relatively simple material behaviour, avoiding potential su-
459 perposition effects that could have limited the portability of the numerical findings into semi-ana-
460 lytical transfer functions.

461 Based on linearized $e(P_{ref})$ functions at representative fault depths, derived by a one-way coupled
462 single phase fluid flow base simulation, we defined analytical functions which are directly imple-
463 mented into a hydraulic simulator to update the fault's porosity and permeability. As a one-way
464 coupling shows a linear relation between the void ratio and a reference pore pressure P_{ref} , we
465 demonstrated how these functions can be easily parametrized by three inclinations α_1 , α_2 and α_3
466 and two control pore pressures $P_{crit 1}$ and $P_{crit 2}$. Furthermore, we demonstrated that aside from $P_{crit 2}$
467 this parametrization is injection rate-independent and different initial fault permeabilities result in
468 a shift of the analytical functions controlled by $P_{crit 1}$, only.

469 Subsequently, we presented that a sufficient approximation of the nonlinear void ratio-over-refer-
470 ence pore pressure behavior, obtained by two-way coupled simulations can be achieved by the
471 semi-analytical approach considering a parametrization based on the $e(P_{ref})$ function of a single
472 one-way coupled base simulation. For that purpose, we demonstrated that using a fault permeabil-
473 ity multiplier of five is appropriate in the base case simulation, while, the semi-analytically coupled
474 simulations do not consider a specific multiplier, and thus the initial fault permeability.

475 Finally, we validated the semi-analytical hydromechanical coupling approach for hydraulic reac-
476 tivation of fault zones for multiphase fluid flow simulations. Using a multiphase fluid flow simu-
477 lator coupled to a geomechanical simulator at 2D plane-strain conditions, the hydraulic reactiva-
478 tion of a fault zone induced by CO₂ injection into a saline aquifer was simulated. Our approach
479 was then validated by comparison against sequentially two-way coupled simulation results. In this
480 context, the semi-analytical coupling scheme exhibits a remarkably good agreement with pore
481 pressure distributions even under extreme conditions, i.e., low initial permeabilities and relatively
482 long flow path lengths along the fault due to the 950-m caprock thickness not intersected by inter-
483 mediate aquifers in our synthetic model, resulting in a significant reduction of the required com-
484 putational time by a factor of up to 15.

485 This gain in computational time allows for the application of two-way coupled hydromechanical
486 simulations, incorporating multiphase fluid flow in a more efficient way and contributes to the
487 implementation of probabilistic assessments as required for uncertainty and risk analyses. Conse-
488 quently, a high number of realizations to assess all relevant parameter uncertainties can be under-
489 taken with the support of this innovative coupling approach.

490 To avoid exceeding the purpose of the present study as well as for the sake of comprehensibility,
491 the determination of the new semi-analytical coupling approach has been undertaken assuming

492 exclusively the Mohr-Coulomb failure criterion. As this failure criterion is only one besides many
493 others, our further research will specifically test our coupling approach against other fault failure
494 modes, i.e., a stick-slip mode or a ubiquitous joint model. Therefore, different constitutive models
495 have to be applied in the geomechanical simulator and the parametrization of our semi-analytical
496 coupling approach has to be adapted in an appropriate manner. In the next step, we aim to validate
497 our semi-analytical coupling approach in 3D.

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503

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