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3 **to International Journal of Greenhouse Gas Control for peer-review.**

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11 **Rapid Fault Leakage Modeling for CO₂**
12 **Storage in Saline Aquifers**

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1 **Rapid Fault Leakage Modeling for CO₂ Storage in Saline Aquifers**

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11 **Abstract**

12 Simulating the fluid flow along fault zones at different scales is essential for predicting the CO₂
13 leakage and containment during injection and storage. However, this can be challenging,
14 especially in the early stages of a storage project when knowledge of the reservoir and caprock
15 is limited and the cost of obtaining the relevant data is high. This study proposes a tool for fast
16 screening of fault leakage at the site screening stage. The tool uses a vertically integrated
17 reservoir model coupled with an upscaled fault leakage function based on source/sink relations.
18 The fault is conceptualized as an increased vertical permeability through the caprock due to the
19 presence of a fracture network in the damage zone and a reduced horizontal permeability in the
20 reservoir due to fault throw and presence of a low-permeability fault core. Simulation results
21 of various CO₂ injection scenarios in a reservoir with potential for fault leakage demonstrate
22 that the tool can produce physically consistent leakage predictions. The computationally
23 efficient model presented in this study is a valuable tool for quantifying uncertainties in key
24 fault parameters, and other constitutive relations that affect the behavior of the storage reservoir
25 and potential fault leakage. By incorporating this tool into the site screening stage, stakeholders

1 can quickly screen the risk of CO₂ leakage along faults across a range of possible storage sites
2 and subsequently design targeted data acquisition campaigns to better characterize and model
3 the faults. Overall, the proposed tool is a cost-effective and efficient method for screening fault
4 leakage risk during CO₂ injection and storage, helping to ensure safe and effective carbon
5 storage.

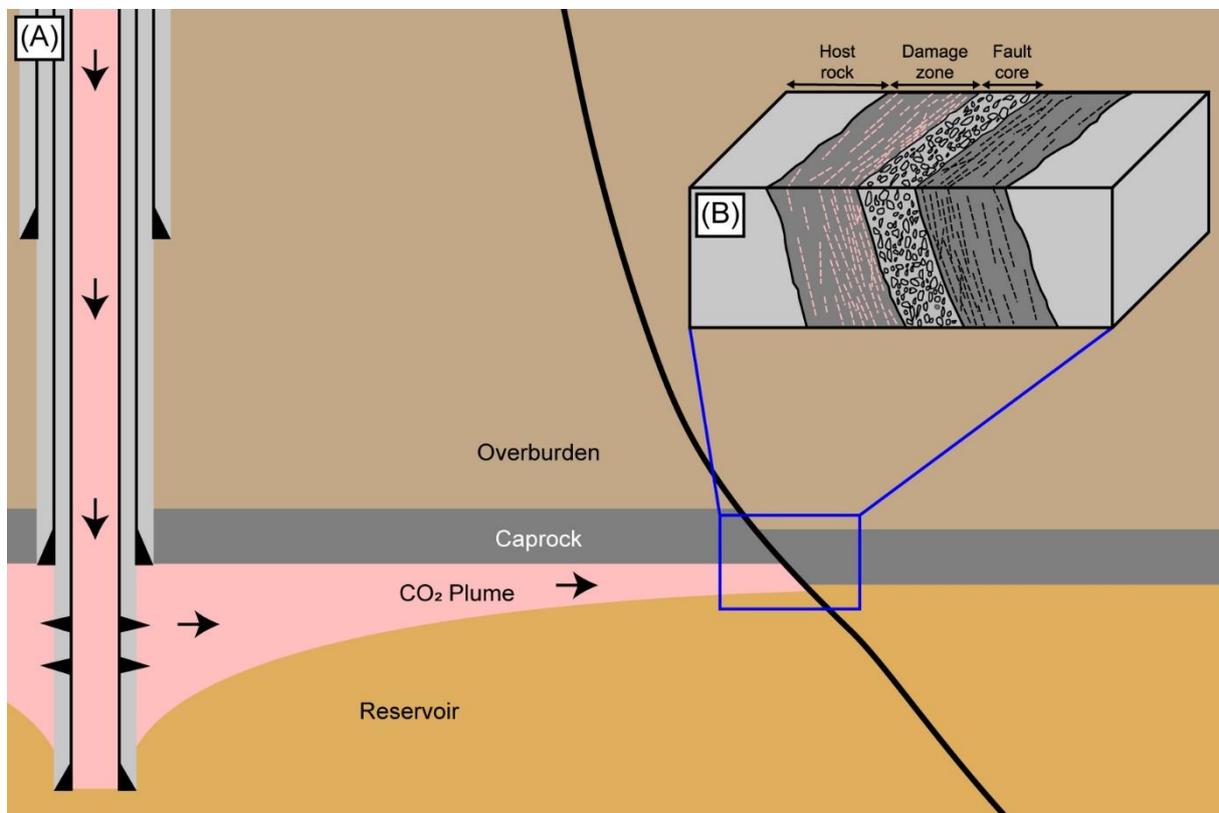
6 **Keywords:** CO₂ Leakage; Faults; CCS; Vertical Equilibrium Modelling; MRST.

7 1 Introduction

8 Storing carbon dioxide (CO₂) in geological formations is a crucial method for mitigating
9 climate change and will be an essential component of a Net Zero Carbon Emission energy
10 landscape in the coming decades (Hepple & Benson, 2004; Krevor et al., 2023). Among the
11 most attractive storage options are saline aquifers, which are widely distributed and possess
12 substantial total storage capacities exceeding gigatons of CO₂ globally (Kumar et al., 2004;
13 Herzog, 2011; Celia et al., 2015). However, successful implementation hinges on the long-term
14 secure containment of CO₂ within these aquifers. Leakage undermines mitigation efforts, poses
15 environmental/health risks, and can erode public trust in Carbon Capture and Storage (CCS)
16 (Bielicki et al., 2014; Ashworth et al., 2015; Jones et al., 2015). Regulatory bodies emphasize
17 the importance of comprehensive geological characterization and storage site assessment to
18 identify significant leakage risk (Dixon et al., 2015; Anderson, 2017; Climate Change
19 Committee, 2021; Romanak & Dixon, 2022). In this context, faults play a crucial role as they
20 can either increase or reduce trapping potential trapping storage, depending on host and fault
21 rock properties. In some cases, by juxtaposing impermeable rock layers, they can function as
22 structural traps, confining the injected CO₂ (Knipe et al., 1998). Conversely, faults also possess
23 the potential to act as leakage pathways that connect the storage reservoir through the overlying
24 caprock to shallower geological layers (Bachu, 2008; Rutqvist, 2012; Snippe et al., 2021).
25 While several successful CCS operations have not encountered significant challenges posed by

1 faults, the In Salah CCS project exemplifies this risk. CO₂ injection in this project induced
2 seismic activity along a fault, demonstrating the potential for faults to act as pathways for CO₂
3 leakage (Morris et al., 2011; Ringrose et al., 2013; White et al., 2014; Krevor et al., 2023). As
4 the scale of CCS deployment increases, we will inevitably encounter storage formations
5 containing faults, many of which may be sub-seismic. To expedite the storage site screening,
6 rapid assessment tools are needed to screen for fault-related leakage risks during the early stages
7 of project development.

8



9

10 Figure 1 – An illustrative representation of CO₂ storage in a faulted reservoir-caprock system.
11 CO₂ is injected into permeable rock layers spanning hundreds of meters in thickness, with a
12 low-permeability regional seal acting as the primary caprock. The presence of faults can either
13 result in enhanced entrapment, or vertical leakage, depending on fault properties (a). Schematic
14 illustration of fault zone properties, including the fault core and adjacent damage zone (b).
15 Figure adapted from Gasda et al. (2022).

16

17 Faults are complex zones of deformation characterized by a central zone of intensely

18 sheared rock, referred to as the fault core, surrounded by a fractured damage zone with a

1 progressively decreasing fracture density with increasing distance from the fault core (Figure
2 1) (Sibson, 1977; Gillespie et al., 1993; Walsh et al., 1998; Childs et al., 2009; Faulkner et al.,
3 2010; Phillips et al., 2020). The fault core typically exhibits relatively low permeability because
4 of cataclasis or clay smear (Tueckmantel et al., 2012; Ballas et al., 2015; Dewhurst et al., 2018),
5 while the associated damage zones, dominated by fractures, can exhibit permeabilities several
6 orders of magnitude greater, which can increase their leakage potential (Caine et al., 1996;
7 Childs et al., 2009; Seebeck et al., 2014). The critical factors controlling leakage through faulted
8 zones include fault geometry, architecture, stress regime, rock properties, and fracture density,
9 among others (Rutqvist et al., 2012). Additionally, fault reactivation due to injection-induced
10 changes in pore pressure and stress conditions can potentially generate new leakage
11 pathways/fractures or alter existing ones (Tewari et al., 2023). The sub-seismic nature of these
12 fractures within the damage zone introduces significant uncertainties in CCS operations, as their
13 presence, properties, and ability to form interconnected networks at larger scales remain poorly
14 understood (Rizzo et al., 2024). Furthermore, sub-seismic faults can impede fluid flow and
15 cause unwanted pressure increases within the reservoir or aquifer, potentially compromising
16 the injectivity and containment of CO₂ within geological formations. This limited knowledge,
17 particularly during the early stages of a CCS project when reservoir data is scarce and data
18 acquisition expensive, can significantly hinder informed decision-making (Oladyskin et al.,
19 2011; Pawar et al., 2015; Pawar et al., 2016). Moreover, in the early phase of CCS project
20 development, operators typically have multiple potential storage sites in their portfolio,
21 necessitating efficient screening methods to identify the most geologically suitable candidates.
22 Therefore, the development of fast and efficient modeling tools for fault leakage assessment is
23 crucial for CCS projects, guiding site selection, risk mitigation strategies, and long-term
24 monitoring plans.

1 Reservoir simulation plays a vital role in quantifying potential fault leakage rates for
2 large-scale CO₂ storage modeling. However, faults and damage zones are significantly smaller
3 than the grid cells employed in typical field-scale simulations. While detailed models that
4 incorporate complex fault geometries, rock properties, and multiphase flow dynamics can
5 capture the interplay between CO₂ migration, leakage, and pressure changes, the computational
6 demands associated with such models can be prohibitive (Jha and Juanes, 2014; Gasda et al.,
7 2022; Snippe et al., 2022; Silva et al., 2023). This is especially true when considering
8 uncertainties in subsurface data and the need for multiple simulations (scenario analyses)
9 (Ringrose and Bentley, 2021). Sub-seismic faults, in particular, pose significant uncertainty
10 due to the lack of detailed data and the computational burden of multiphysics forward modeling,
11 which typically require weeks to run. To address these challenges, researchers have developed
12 well-established simplification strategies that leverage two key characteristics of CO₂ storage
13 systems: the strong buoyancy of CO₂ relative to brine and the significantly larger horizontal
14 dimensions compared to the vertical dimension of the reservoir (Huppert and Woods, 1995;
15 Yortsos, 1995; Nordbotten and Celia, 2011). These characteristics promote rapid CO₂
16 separation and vertical equilibrium within the reservoir. Vertical equilibrium (VE) flow models
17 exploit this phenomenon by enabling the representation of the 3D reservoir system using a set
18 of 2D governing equations, thereby significantly reducing computational costs.

19 Several CO₂ storage studies have demonstrated that VE simulations yield results
20 comparable to those obtained from 3D simulations for benchmark and field-scale problems
21 (Class et al., 2009; Nilsen et al., 2014; Bandilla et al., 2014; Nilsen et al., 2015; Nilsen et al.,
22 2016; Moyner & Nilsen, 2019). The basic formulation of VE models assumes a sharp interface
23 between CO₂ and brine and keeps the mathematical structure of the standard multi-phase Darcy
24 equation. Hence, conventional simulators can be used. This very characteristic allows for their
25 expansion to encompass a wider range of complex phenomena. Recent research has

1 successfully incorporated and evaluated various physical effects within VE models, including:
2 1) capillarity – the presence of non-negligible capillary pressure leads to the formation of a
3 capillary fringe, a transition zone between the CO₂ and brine phases, rather than a sharp
4 interface (Nordbotten & Dahle, 2011, Nilsen 2015); 2) residual trapping and hysteresis – these
5 intrinsic properties of the rock can significantly influence the distribution and flow of fluids
6 within the reservoir (Nordbotten & Celia, 2011; Doster et al., 2012; Doster et al., 2013; Du
7 Plessis et al., 2013 Nilsen et al., 2016); 3) dissolution of CO₂ into reservoir brine (Gasda et al.,
8 2011; Nilsen et al., 2016); 4) compressibility of CO₂ in the vertical extent (Anderson et al.,
9 2015); 5) thermal effects (Gasda et al., 2013); 6) simplified geomechanics (Bjornara et al., 2016;
10 Anderson et al., 2016, 2017); 7) Hybrid-VE – using a coupled approach of mixing 3D and VE
11 models which can help with simulating near-wellbore effects and multilayer reservoir modeling
12 (Moyner & Nilsen., 2019; Becker et al., 2017, 2018, 2022).

13 The objective of this paper is to couple a fault leakage function, which incorporates the
14 fault properties and the vertical flow effects, with a VE reservoir model to facilitate
15 computationally efficient CO₂ storage simulations. We employ a VE flow model implemented
16 within the open-source software package MRST-co2lab, which is a module within the
17 MATLAB Reservoir Simulation Toolkit (MRST) (Anderson, 2017; Lie, 2019). The fault is
18 conceptualized as an increased vertical permeability through the caprock (due to the fracture
19 network in the damage zone) while the horizontal permeability is reduced (due to throw and the
20 presence of the fault core). Leakage rates are estimated using Darcy’s law, considering the
21 pressure differential across the layers connected by the fault. The flow is modelled as vertical
22 single-phase flow along the fault. This simplification allows for a one-dimensional leakage
23 system which lowers the cost of computation. The mathematical formulation of the proposed
24 model is presented in section 2 and the results are discussed in section 3. This approach offers
25 a cost-effective and efficient method for screening fault leakage risk during CO₂ injection and

1 storage, thereby contributing to ensuring safe and effective carbon storage. Furthermore, this
2 methodology facilitates a more robust evaluation of storage potential while accounting for the
3 inherent complexities and uncertainties associated with faulted geological settings.

4

5 2 Methods

6 This study examines the potential for carbon dioxide (CO₂) storage within a faulted
7 reservoir (Figure 1). We employ a vertically integrated numerical model for reservoir-scale
8 flow coupled with an analytical model for fault leakage. A brief overview of the governing
9 equations used in these models is presented in this section.

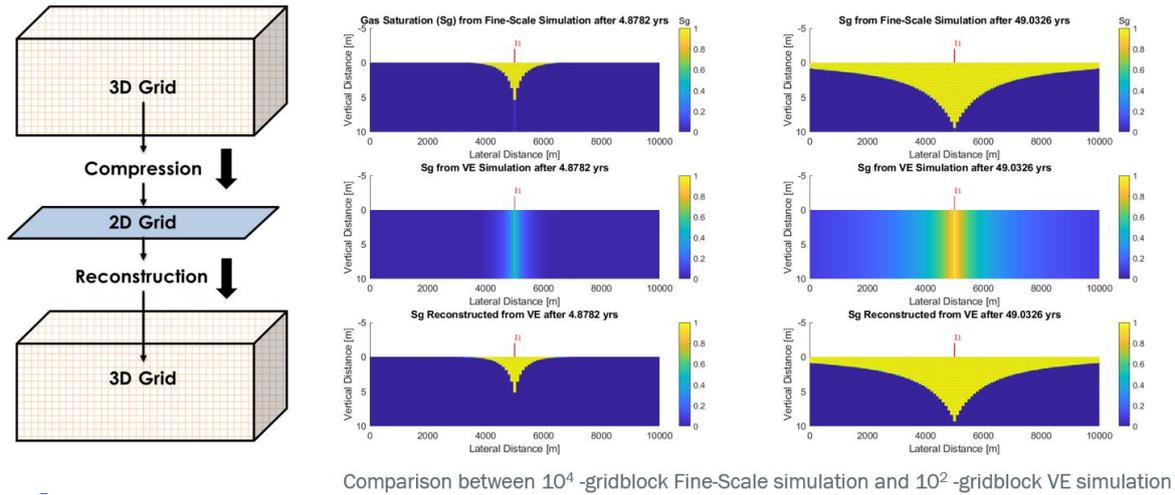
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11 2.1 Vertical Equilibrium Modelling

12 The VE modeling approach for CO₂ storage is a simplification of traditional reservoir
13 simulation methods that is particularly useful for large-scale CO₂ storage projects. This
14 approach hinges on the assumption of VE, which posits that the buoyancy forces acting on the
15 CO₂ cause it to segregate vertically much faster than it can migrate laterally. As a result, the
16 CO₂ forms a thin layer beneath the caprock or under intermediate sealing layers, and the vertical
17 pressure and fluid saturation distributions can be approximated by buoyancy and capillary
18 forces. VE models reduce the dimensionality of the problem by vertically averaging the
19 governing equations, which include conservation of mass and Darcy's law for fluid flow
20 through porous media. This simplification results in a model that requires fewer grid cells and
21 is computationally less intensive compared to full three-dimensional simulations. Post-
22 simulation, the vertical pressure and fluid saturations can be reconstructed from the set of
23 upscaled variables obtained by vertically integrating the conservation equations. Figure 2
24 illustrates the typical compression and reconstruction steps during a VE simulation at early and
25 late times for an example simulation problem. This section provides a concise review of

1 established equations for modeling flow in porous media and the VE simplification approach.
 2 For a more general and in-depth treatment of the derivations and the limits of the VE
 3 assumption, we refer the reader to the relevant literature (Yortsos 1995; Nordbotten & Celia,
 4 2011;).

5



6

7 Figure 2 – Illustrative representation of the concept of VE model compression and
 8 reconstruction in a CO₂ injection simulation. The top panel shows an illustrative representation
 9 of the 3D simulation grid. The middle panel depicts the corresponding 2D grid generated by
 10 VE compression. The bottom panel presents the reconstructed 3D simulation grid obtained by
 11 solving the 2D VE model equations. These panels represent the grid configuration at both early
 12 and late stages of the CO₂ injection simulation. In this example, the VE compression reduces a
 13 10^4 -cell 3D grid to a 10^2 -cell VE grid, achieving significant computational efficiency without
 14 substantial information loss.

15

16 Consider the three-dimensional mass conservation equation for two immiscible and

17 incompressible fluid phases α , CO₂ ($\alpha = g$) and brine ($\alpha = w$) as

$$\frac{\partial(\phi s_\alpha)}{\partial t} + \nabla \cdot u_\alpha = q_\alpha, \quad (1)$$

18 where ϕ is the porosity, s_α is the saturation of phase α , u_α is the Darcy velocity of phase α ,
 19 and q_α is a source/sink term in units of volume of phase α per time. The porous medium is
 20 assumed to be a rigid medium under isothermal conditions. The volume balance is established
 21 by

$$s_g + s_w = 1. \quad (2)$$

1 The Darcy velocity is given by

$$\mathbf{u}_\alpha = -\frac{k_{r\alpha}}{\mu_\alpha} \mathbf{k}(\nabla p_\alpha - \rho_\alpha \mathbf{g}), \quad (3)$$

2 where μ_α is the viscosity of phase α , $k_{r\alpha}$ is the relative permeability of phase α , \mathbf{k} is the
 3 permeability tensor, p_α is the fluid pressure of phase α , ρ_α is the density of phase α , and \mathbf{g} is
 4 the gravity acceleration vector. The phase pressures are related by the capillary pressure
 5 function

$$p_c = p_g - p_w. \quad (4)$$

6 Additional assumptions are that the capillary pressure and relative permeability can be
 7 represented by algebraic functions. These functions solely depend on saturation and its history.
 8 Equations (1) to (4) form a set of 10 equations with 10 unknowns that need to be solved for in
 9 three dimensions. The fluid saturation distributions and pressures are obtained by solving this
 10 system, provided that: 1) specific functions are chosen to represent relative permeability and
 11 capillary pressure, 2) initial conditions for pressure and saturation throughout the reservoir are
 12 provided, and 3) appropriate boundary conditions are specified along the edges of the reservoir
 13 model.

14 In subsurface flow processes, the lateral dimension of interest is typically orders of
 15 magnitude larger (hundreds of meters to kilometers) compared to the vertical dimension (meters
 16 to tens of meters). This disparity leads to a more rapid redistribution of fluids vertically,
 17 allowing for the approximation of VE (Nordbotten & Celia, 2011; Nordbotten & Dahle, 2011).
 18 Consider the reservoir domain to be bounded by impermeable, horizontally oriented layers with
 19 a constant uniform thickness H . The two fluids (brine and CO₂) are separated by a sharp
 20 interface within this reservoir. A cartesian coordinate system is employed, with the z-axis
 21 oriented in opposition to the gravitational vector (positive z upwards). Furthermore, for

1 simplicity in the presentation here, constant permeability and porosity are assumed within the
2 vertical direction, though VE is not limited to those assumptions (Nordbotten & Celia 2012).

3 This vertical integration seeks to establish governing equations for the horizontal plane
4 that utilize variables representing the average behavior throughout the reservoir thickness. Fine-
5 scale quantities capture the variations within the vertical dimension, while coarse-scale
6 quantities represent the horizontally averaged behavior. Under the assumption of vertical
7 hydrostatic equilibrium, Equation (3) indicates that the pressure gradient in each phase balances
8 the gravity ($u_{\alpha z} = 0$). This characteristic allows for the determination of pressure at any vertical
9 position by integrating the pressure from a reference level. To facilitate analysis, we normalize
10 the z -axis with respect to the reservoir height H . Here, $z = 0$ is assigned to the bottom and $z =$
11 1 to the top of the reservoir. Consequently, the top of the reservoir is chosen as the reference
12 position for pressure integration as

$$P_\alpha = p_\alpha(z = 1). \quad (5)$$

13 The reconstructed pressure is then given as

$$p_\alpha(z) = P_\alpha + \rho_\alpha g H (1 - z). \quad (6)$$

14 The other coarse-scale quantities are introduced by integrating the fine-scale quantities.
15 This is done under the assumption of a homogeneous system with isothermal and
16 incompressible fluid. We can obtain the coarse-scale equivalents after normalizing the vertical
17 axis to the reservoir height and writing the equations in dimensionless form. For such systems,
18 the coarse-scale equivalents of porosity Φ , permeability K , and viscosity M_α are simply a
19 product of their respective fine-scale counterparts with reservoir height. This is because the
20 averaging or integration process does not introduce any scaling factors in this case. The spatially
21 dependent quantities are given as

$$S_\alpha = \frac{H}{\Phi} \int_0^1 \phi s_\alpha dz, \quad (7)$$

$$U_\alpha = H \int_0^1 u_{\alpha||} dz, \quad (8)$$

$$K_{r\alpha} = \frac{H}{K} \int_0^1 k_{||} k_{r\alpha}(s_\alpha(z)) dz. \quad (9)$$

1 The subscript $||$ denotes the variables in horizontal components such that U_α is a two-
 2 dimensional vector instead of three dimensions. With these definitions, Equations (1) to (4)
 3 after integrating over the vertical extent are given as

$$\frac{\partial(\Phi S_\alpha)}{\partial t} + \nabla_{||} \cdot (U_\alpha) = Q_\alpha, \quad (10)$$

$$S_g + S_w = 1, \quad (11)$$

$$U_\alpha = -K \frac{K_{r\alpha}}{M_\alpha} \nabla_{||} P_\alpha, \quad (12)$$

$$P_c(\bullet) = P_g - P_w, \quad (13)$$

4 where (\bullet) is used to highlight the upscaled dependence of the capillary pressure function that is
 5 yet to be determined. Equation (9) demonstrates that reconstructing the vertical, fine-scale
 6 saturation distributions, $s_w(z; x, y)$, is necessary to determine the effective parameter functions
 7 employed in a purely coarse-scale model. Fortunately, the assumption of hydrostatic fluid
 8 distribution facilitates this reconstruction process. By examining Equation (6), we observe that
 9 the fine-scale capillary pressure, $p_c(z; x, y)$, must compensate for the buoyancy force arising
 10 from the density difference. This relationship allows for the construction of the fine-scale
 11 capillary pressure and its subsequent connection to the coarse-scale capillary pressure as

$$p_c(z; x, y) = P_c(x, y) - (\rho_w - \rho_g)gH(1 - z). \quad (14)$$

12 A well-defined relationship between capillary pressure and water saturation enables the
 13 establishment of invertible $p_c - s_w$ mappings. These mappings allow for the reconstruction of
 14 the vertical saturation distribution, $s_w(z; x, y)$, given a specific coarse-scale capillary pressure
 15 P_c . Furthermore, Equation (7) can be employed to obtain a $P_c - S_w$ relationship. By leveraging

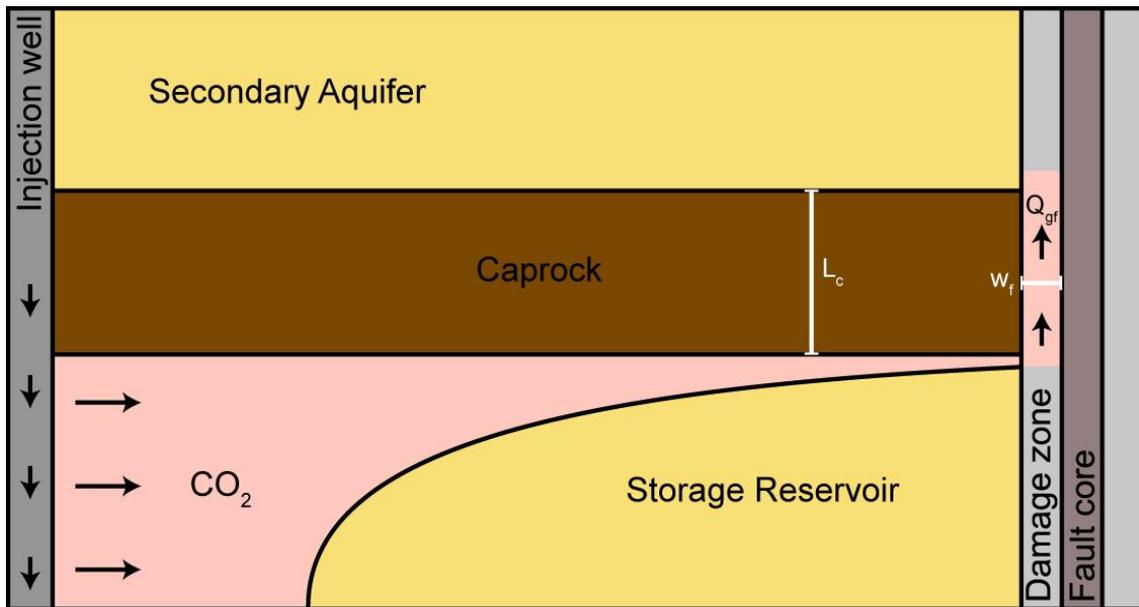
1 this relationship, the fine-scale saturation distribution $s_w(z; x, y)$ is determined for a given
2 coarse-scale saturation S_w . Consequently, coarse-scale relative permeabilities $K_{r\alpha}$ are
3 dependent on coarse-scale saturations only.

4

5 2.2 Fault Leakage Function

6 This section details the steady-state analytical solution used to estimate leakage rates
7 along the fault. The fault is conceptualized to connect the storage reservoir with a secondary
8 aquifer at a shallower depth, which acts as sink for the leaking CO₂. Only faults of shorter
9 lengths such that the CO₂ fluid properties remain nearly constant are considered here, while the
10 long-range fault leakage (faults that connect the reservoir to the surface or seafloor) with
11 variable CO₂ fluid properties and decompressive cooling has been investigated previously
12 (Pruess, 2011; Ramachandran et al., 2017). The leaky fault is conceptualized as consisting of a
13 low-conductivity (i.e., low permeability) core that prevents flow across the fault. This core is
14 surrounded by two high-conductivity (i.e., high-permeability) damage zones that permit flow
15 vertically along the fault as shown in Figure 3 (Faulkner et al., 2010). This damage zone is
16 referred to here as "the fault zone" or simply "the fault", and the low-conductivity core is
17 represented as a no-flow boundary in the model. Hence the fault leakage will predominantly
18 occur along the damage zone which is hypothesized as an equivalent porous medium with
19 appropriate rock properties describing it. Estimating the hydraulic properties of the fault,
20 particularly within the fault core and damage zone, is crucial for accurately modeling fault
21 leakage. While insights can be gained from studying outcrop analogues, inherent uncertainties
22 remain at the finer scale. Several researchers have developed stochastic modeling approaches
23 to predict the fault properties, such as permeability, among other parameters (Berge et al., 2022;
24 Gasda et al., 2022; Salo-Salgado et al., 2023; Rizzo et al., 2024). However, for this specific
25 model, we are assuming constant fault properties throughout the simulation. The flow along the

1 fault is described using Darcy's law by considering the pressure differential across the storage
 2 reservoir and the secondary aquifer, and the flow is assumed to occur only in the vertical
 3 direction. Once the CO₂ plume reaches the base of the fault within the aquifer, it is hypothesized
 4 to form a thick layer, acting as a barrier for aqueous phase entry into the fault (Kang et al.,
 5 2014). As a result, the aqueous phase flux along the fault is considered negligible and excluded
 6 from the model.



8
 9 Figure 3 – A schematic representation of a vertical cross section of a storage reservoir
 10 containing a fault (gray). The black line represents the interface between CO₂ and the brine
 11 phase. CO₂ leaks along the damage zone of the fault once it reaches the base of the fault within
 12 the reservoir.

13
 14 Several researchers have indicated that the CO₂ needs to overcome the capillary entry
 15 pressure of the fault, commonly referred to as the fault displacement pressure, for it to leak
 16 (Espinoza et al., 2017; Zheng & Espinoza, 2022). This capillary entry pressure is controlled by
 17 an effective aperture of the fracture network and as such strongly depends on the geomechanical
 18 properties of the fault as well as the pressurization of the target reservoir. For simplicity, we
 19 keep this parameter constant here. We base the flux calculation on the model presented by
 20 Neufeld et al. (2009), with slight modifications to account for the reservoir overpressure caused

1 by injection. This model describes leakage through fissures between two aquifers, with one
 2 being the targeted CO₂ storage site. We model the driving potentials ψ as

$$\psi = \Delta\rho g h_g + (P_w - P_{w0}) - p_e, \quad (15)$$

3 where $\Delta\rho = \rho_w - \rho_g$ is the density difference between brine and CO₂, h_g is the height of CO₂
 4 which is obtained from the coarse-scale gas saturation S_g (after accounting for the reservoir
 5 rock-fluid characteristics), of the reservoir block connected to the fault block, P_w is the brine
 6 pressure in the reservoir, P_{w0} is the initial brine pressure in the reservoir, and p_e is the capillary
 7 entry pressure of the fault/fractures. The vertical gas leakage flux Q_{gf} along the fault is given
 8 as

$$Q_{gf} = \begin{cases} 0, & \psi \leq 0 \\ \frac{A_f k_f (\psi + \Delta\rho g L_c)}{\mu_g L_c}, & \psi > 0 \end{cases}, \quad (16)$$

9 where A_f is the area of the fault perpendicular to flow, k_f is the vertical fault permeability and
 10 L_c is length of the caprock or the length of the fault connecting the reservoir to the secondary
 11 aquifer. This formulation accounts for the capillary entry pressure required for CO₂ to enter the
 12 fault. This approach relaxes the assumption of VE at the grid block where the fault is connected,
 13 allowing for non-zero vertical flow. However, for steady state single phase flow, fault leakage
 14 does not have a significant effect on reservoir predictions (Kang et al., 2014). By incorporating
 15 these key factors, the model aims to provide a more realistic representation of the fault leakage
 16 process.

17

18 2.3 Model Implementation

19 The leakage along the fault is numerically simulated as a fault leakage function, which
 20 is represented as a source/sink term in the material balance equations (Equation 10). This
 21 methodology circumvents the explicit discretization of faults, thereby capturing their impact on
 22 fluid flow and replicating their influence without requiring a computationally intensive, fully

1 discretized fault representation. The fault leakage function is related implicitly to the primary
2 unknowns of the reservoir model using the gas saturation and the overpressure terms of the grid
3 blocks adjacent to the fault. The flow rate at the fault-reservoir interface is represented as shown
4 in Equation 16. From a simulation perspective, fault leakage occurs when the leakage
5 constraint, expressed as $\Delta\rho gh_g + (P_w - P_{w0})$, exceeds the fault capillary entry pressure p_e and
6 the upscaled gas saturation is greater than zero. However, numerical experiments have
7 demonstrated that this criterion can result in unstable behaviour, characterized by frequent
8 fluctuations (appearance and disappearance of the fault leakage term) during the iteration
9 process and between time steps, which causes convergence issues and increases simulation
10 time. To address this problem, the implementation of a smoothing function for the leakage rate
11 term enables the adoption of a more robust fault leakage function. We use a smoothing function,
12 such that $\hat{Q}_{gf} = Q_{gf}f(\psi)$ with the smoothing function $f(\psi) = (1 - e^{(-\xi\psi)})$ and the smoothing
13 parameter ξ . In our simulations we use $\xi = 10^{-3} Pa^{-1}$ to regulate the fault leakage rate upon
14 the initial occurrence of a non-zero fault leakage term. Under rigorous consideration, permitting
15 the leakage constraint to marginally exceed p_e without initiating fault leakage introduces a
16 minor inaccuracy in leakage rates. However, this approach has a negligible impact on long-term
17 simulation results while significantly improving the efficiency of the simulations with respect
18 to timesteps and convergence. The fault permeability assigned to the fault leakage term
19 represents the combined effect of the fault core permeability and the surrounding damage zone
20 permeability. This combined parameterization simplifies the model while preserving the
21 essential flow characteristics associated with the fault system. The resulting reservoir is
22 discretized based on a finite volume discretization using the two-point flux approximation
23 method, as implemented in the MRST (Lie, 2019) framework.

1 3 Results and Discussion

2 In this section, we present the results obtained from applying the fault leakage function
3 coupled with the VE reservoir model to several CO₂ injection scenarios.

4

5 3.1 Test case – comparison with 2D simulations

6 The test case presented in this section are designed to validate the fault leakage modeling
7 methods presented in section 2. A 2D two-phase numerical model is used to simulate the fault
8 leakage rates within the simplified CO₂ storage setting (Figure 4a). The objective of this test
9 case is to compare the fault leakage rates between the 2D numerical simulation with an explicit
10 representation of the fault and the VE model with the fault leakage function proposed in this
11 work. The test case simulates fluid flow through a conceptual model comprising two horizontal
12 aquifers separated by a caprock and connected by a vertical, conductive fault. The bottom
13 aquifer serves as the storage reservoir, while the top aquifer is the top reservoir. The fault is
14 treated as an equivalent porous medium with the reservoir, fault, fluid, and rock-fluid properties
15 as specified in Table 1. Although the permeability of the aquifers and faults is simplified for
16 comparative purposes, it is crucial to emphasize that the primary focus is on the interaction of
17 these components, rather than precise geological representation. We expect that varying these
18 parameters within reasonable bounds would not significantly alter the leakage rate comparison.

19 A numerical grid of 12,000 cells discretizes the system with a resolution of 1 m x 1 m x
20 0.25 m (x, y, and z directions, respectively), resulting in a physical model with dimensions of
21 100 m x 30 m, consisting of three layers, each 10 m thick. The fault zone, located on the right
22 side of the model, is 5 m wide and 10 m long. The system is assumed to be in hydrostatic
23 equilibrium with 100% water saturation initially, and the relative permeability is governed by
24 the Brooks-Corey model with parameters described in Table 1. No-flow boundaries are
25 assumed at the top, bottom, and the right side (representing the no flow across the fault core).

1 The left boundary is treated as an open boundary with the pressure maintained as hydrostatic.
 2 The system is initialized with a constant CO₂ column height at the left boundary of the storage
 3 reservoir. This column height and the boundary pressures can be varied to simulate buoyancy-
 4 driven and pressure-driven conditions, allowing for a comprehensive evaluation of the fault
 5 leakage modeling approach.

6

7 Table 1 – Summary of model parameters used for fault leakage function validation simulation
 8 described in section 3.1.

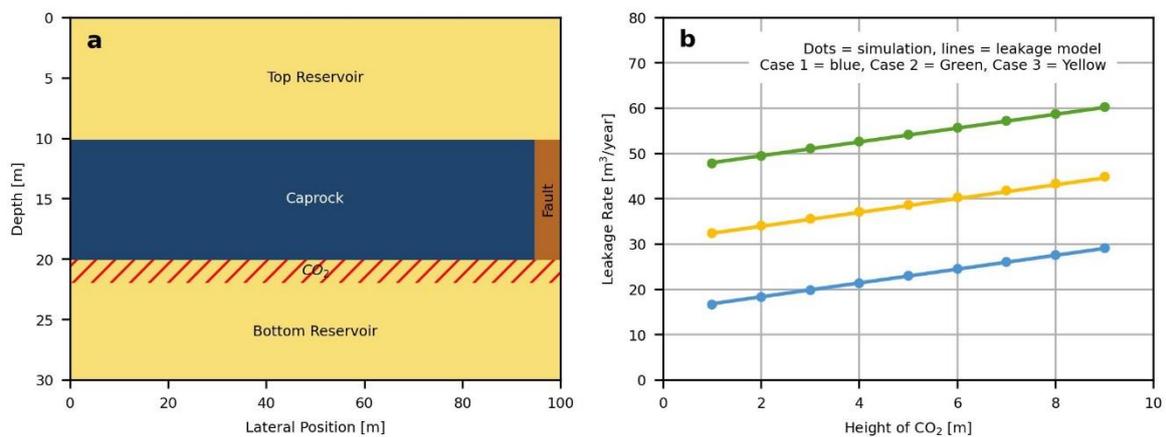
Property	Value
Bottom Reservoir and Top Reservoir Properties	
Top reservoir porosity	0.3
Bottom reservoir porosity	0.3
Top reservoir permeability (D)	10
Bottom reservoir permeability (D)	10
Reservoir overpressure (bars) (case 2 and 3)	1
Caprock properties	
Caprock permeability (mD)	1×10^{-6}
Caprock porosity	0.3
Fault properties	
Fault porosity	0.03
Fault permeability (mD)	1
Fault width (m)	5
Fault length (m)	10
Fault capillary entry pressure (bars) (case 3)	0.5
Bottom Reservoir, Fault and Top Reservoir Relative Permeability Properties	
Residual gas saturation	0
Residual brine saturation	0
Gas end-point relative permeability	1
Brine end-point relative permeability	1
Gas relative permeability exponent	1
Brine relative permeability exponent	1
Fluid properties	
Gas density (kgm ⁻³)	500
Brine density (kgm ⁻³)	1000
Gas viscosity (Pa.s)	0.5×10^{-6}
Brine viscosity (Pa.s)	0.9×10^{-5}

9

10 Three specific parametrizations are considered to compare the performance of the fault
 11 leakage modeling approach, 1) The reservoir and boundary pressures is hydrostatic. The
 12 pressure of the CO₂ column is derived solely from density differences, and the flow is driven

1 by buoyancy. This parametrization mimics the migration phase of CO₂ storage. 2) The reservoir
 2 pressure is hydrostatic, but the boundary pressure is elevated to mimic the typical pressure
 3 increase observed during injection. The pressure of the CO₂ column is derived from both, the
 4 density differences, and the pressure elevation. 3) Similar to Case 2, the third scenario contains
 5 an additional capillary entry pressure for the fault, which acts as a pressure barrier that the CO₂
 6 must exceed to enter the fault zone. The 2D numerical simulation are run to steady-state
 7 conditions for each of the three cases. The leakage rate, specified as the flow leaving from the
 8 top of the fault, is then compared to the leakage rate obtained from the VE model with the fault
 9 leakage function (Figure 4b). The proposed fault leakage function compares well with the
 10 numerical simulations for all the three scenarios considered in this test case and demonstrates
 11 that it is robust and suitable for capturing the key factors influencing fault-related CO₂ leakage,
 12 i.e., buoyancy, pressure gradients, and capillary entry pressure. Moreover, the model's
 13 computational efficiency is improved by bypassing the explicit representation of the fault and
 14 top reservoir. This validation gives confidence that our model can be applied to field-scale CO₂
 15 storage simulations.

16



17

18 Figure 4 –Grid representation of 2-D fine scale simulation (a) and fault leakage rate comparison
 19 between numerical simulation and VE model with fault leakage function (b). The three cases

1 considered are: (1) hydrostatic reservoir and boundary pressure, (2) elevated reservoir boundary
2 pressure, and (3) fault capillary entry pressure.
3

4 It is important to highlight the potential limitations of the steady-state, single-phase fault
5 leakage assumption used in our modeling approach. For instance, in the overpressure
6 parametrization (2) with a 5-meter CO₂ column height, the calculated leakage rate is 53 m³ per
7 year. Accounting for the fault dimensions, this corresponds to a CO₂ Darcy flux of 0.03 m per
8 day. This implies that it takes approximately 344 days (~1 year), for the CO₂ to travel the 10-
9 meter distance separating the bottom reservoir and the top reservoir. Although faults are
10 typically characterized by very low porosity, and the impact of CO₂ accumulation within the
11 fault on the leakage rate may be minimal (Faulkner et al., 2010; Caine et al., 1996), there
12 remains a significant delay in reaching the top reservoir that is not captured because the current
13 approach presupposes instantaneous leakage once the CO₂ reaches the base of the fault. This
14 raises a pertinent question regarding the definition of leakage - whether it occurs once CO₂
15 enters the top reservoir or once it enters the fault from the bottom reservoir. However, the
16 current modeling approach does not explicitly account for these dynamic effects during the fault
17 leakage process. While acknowledging these limitations is crucial, it is equally important to
18 contextualize the scale of typical CO₂ storage simulations, which extend from few decades to
19 few centuries. Within this broader temporal framework, the steady-state, single-phase
20 assumption may offer a reasonable approximation that allows us to screen leakage rates across
21 a broad range of possible reservoir scenarios before commencing more detailed simulation
22 studies that capture the full physics of fault leakage in a specific reservoir scenario. This
23 consideration underscores the necessity of balancing model complexity with computational
24 feasibility, particularly in the context of large-scale, long-term CO₂ storage simulations.

25

1 3.2 Test case – convergence analysis

2 The following test case aims to elucidate the impact of grid resolution and time step size
3 on the fault leakage modeling methods presented in Section 2. A 2D, two-phase numerical
4 model is employed to simulate fault leakage rates within a simplified CO₂ storage setting (x
5 5a). This test case, with minor modifications, is based on the scenario described in Section 3.1.
6 It simulates fluid flow through a geological model consisting of a horizontal aquifer located
7 beneath a faulted seal. The aquifer serves as the storage reservoir, and the faulted seal is treated
8 as an equivalent porous medium. The properties of the reservoir, fault, fluid, and rock-fluid
9 interactions are specified in Table 2. While the physical dimensions of the aquifer are 100 m
10 by 10 m, and the fault zone is also 100 m wide and 10 m long, are simplified for convergence
11 analysis, it is important to note that the primary focus is on the interplay of these components
12 without being constrained by precise geological representation. We expect that varying these
13 dimensions within reasonable bounds would not significantly alter the observed convergence
14 behavior. The system is assumed to be in hydrostatic equilibrium with an initial water saturation
15 of 100%. Relative permeability is governed by the Brooks-Corey model, with parameters
16 detailed in Table 2. No-flow boundaries are assumed at the bottom, while the left and right
17 boundaries are treated as open, with pressure maintained as hydrostatic. The system is
18 initialized with a constant CO₂ column height of 5 m at the left boundary of the storage
19 reservoir. This column height and the boundary pressures can be varied to simulate buoyancy-
20 driven and pressure-driven conditions, similar to those in Section 3.1. The grid blocks enclosing
21 the faulted is modified to incorporate the fault leakage function, with properties mentioned in
22 Table 2, to mimic along-fault leakage.

23

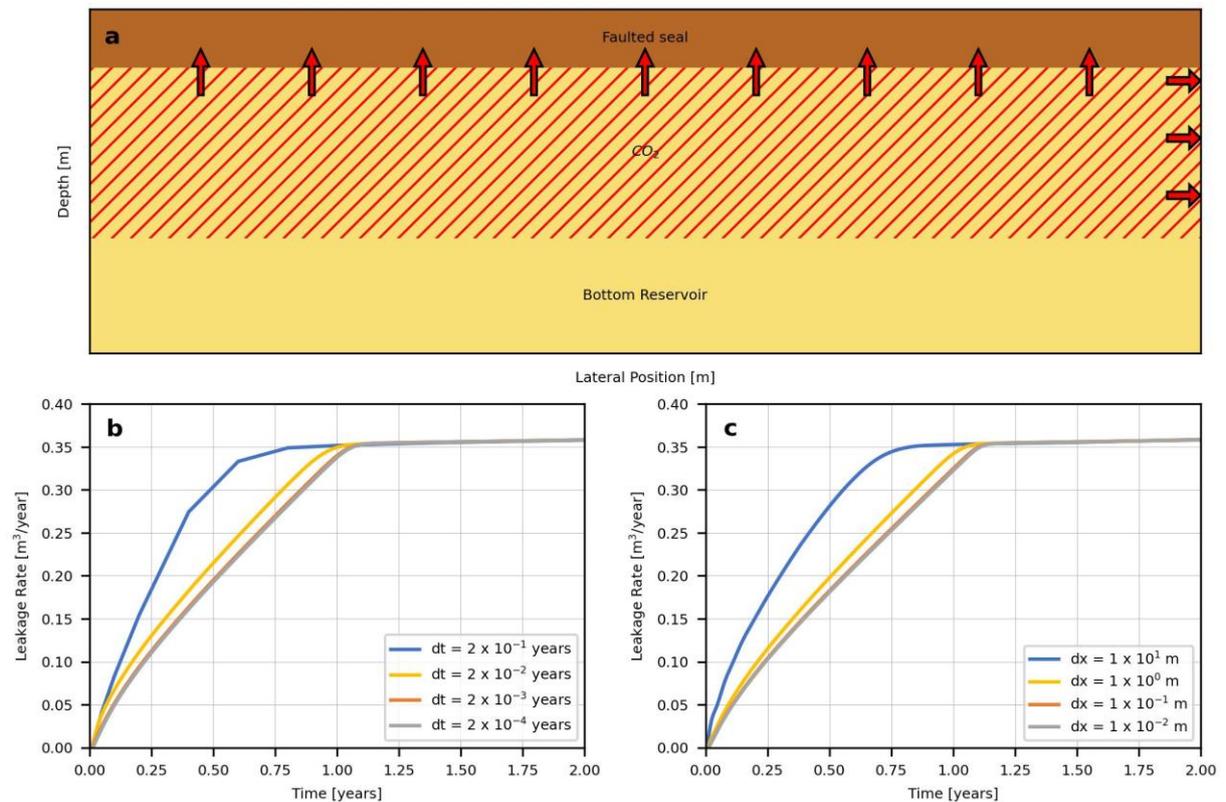
24 Table 2 – Summary of model parameters used for convergence analysis simulation described
25 in section 3.2.

Property	Value
Reservoir Properties	

Reservoir porosity	0.3
Reservoir permeability (mD)	100
Faulted seal properties	
Fault porosity	0.03
Fault permeability (mD)	1×10^{-3}
Fault length (m)	10
Reservoir and Fault Relative Permeability Properties	
Residual gas saturation	0
Residual brine saturation	0
Gas end-point relative permeability	1
Brine end-point relative permeability	1
Gas relative permeability exponent	1
Brine relative permeability exponent	1
Fluid properties	
Gas density (kgm^{-3})	500
Brine density (kgm^{-3})	1000
Gas viscosity (Pa.s)	0.5×10^{-6}
Brine viscosity (Pa.s)	0.9×10^{-5}

1

2



3

4 Figure 5 – Grid representation of VE simulation setup of CO₂ storage with a faulted seal to
 5 assess the impact of grid block dimensions and time step size on fault leakage modeling (a),
 6 fault leakage rate comparison for varying time step sizes for a constant grid block dimension of

1 1 m (b) and fault leakage rate comparison for varying gridblock dimensions at a time step of 4
2 $\times 10^{-3}$ years (c).
3

4 Figure 5b illustrates the leakage rate for two years with time steps varying from 2×10^{-1}
5 years to 2×10^{-4} years and a grid block dimension of 1 m. Figure 5c illustrates the leakage rate
6 for two years with grid block dimensions varying from 1×10^1 m to 1×10^{-2} m and a time step
7 of 4×10^{-3} years. A key observation is that the leakage rate converges towards a consistent
8 solution for both, time and space. Coarser grids and larger time steps lead to overestimated
9 leakage rates in the first year. Subsequently, all time steps and grid block sizes converge toward
10 the same leakage rate predictions. While the total leakage increases with larger time steps and
11 grid sizes, the magnitude of this increase becomes negligible after 100 years of simulation
12 (when the system reaches steady state). For instance, the total leakage after 100 years is only
13 0.0025% higher for the 2×10^{-1} year time step compared to the 2×10^{-3} year time step, and
14 0.0027% higher for the 1×10^1 m grid size compared to the 1×10^{-2} m grid size. Resizing grid
15 blocks proportionally resizes the fault leakage function, ensuring the total fault width remains
16 constant. Consequently, the number of fault leakage terms increases with a higher number of
17 grid blocks. Despite this increase, the impact on total leakage predictions remains relatively
18 low. It is important to acknowledge that this model uses a fault leakage function instead of
19 explicitly representing the faults, to ensure computational efficiency. Despite this
20 simplification, the model is able to approximate the reservoir behavior and leakage rates
21 outcomes with sufficient reliability. This approach facilitates the rapid screening of potential
22 storage sites, enabling the identification of promising candidates. Consequently, resources can
23 be strategically allocated to design comprehensive data acquisition campaigns tailored to the
24 specific geological complexities of selected sites. By expediting the early screening phase, this
25 methodology contributes to the overall acceleration of CO₂ storage project development in
26 geologically complex settings.

1 3.3 Sloping reservoir with a leaky fault

2 The case presented in this section is designed to test the fault leakage function for a
3 gently sloping reservoir with a large fault. The conceptual model comprising of a gently sloping
4 reservoir connected to a secondary aquifer by a fault is shown in Figure 6a. The reservoir is
5 discretized as a VE grid with 2500 cells, each measuring 20 m x 20 m in the x and y directions,
6 respectively, resulting in a physical model with dimensions of 1000 m x 1000 m. The reservoir
7 has a thickness of 10 m and a slope of ~3 degrees. The fault is treated as an equivalent porous
8 medium using the fault function, and the reservoir, fault, fluid, and rock-fluid properties as
9 specified in Table 3. The system is assumed to be in hydrostatic equilibrium with 100% water
10 saturation initially, and the relative permeability is governed by the Brooks-Corey model with
11 parameters mentioned in Table 3. No-flow boundaries are assumed at the top, right and left
12 boundaries. The bottom boundary is treated as an open boundary with the pressure maintained
13 as hydrostatic. Hence this bottom boundary acts as a sink for the heavier brine phase and allows
14 for up-dip movement of CO₂. Unlike previous simulations where the CO₂ injection was
15 controlled by boundary conditions, this simulation uses the rate constrained well for CO₂
16 injection. The injection location is at the coordinate pair (100 m, 500 m) for an injection rate of
17 1229 tons per year over 3 years followed by 97 years of migration. The fault zone is located in
18 the center of the model., i.e., 500 m away from either side boundary in x-direction. The fault is
19 800 m long in the y-direction. The grid blocks enclosing the fault are modified to 1) set the
20 across-fault permeability to zero, mimicking an impermeable fault core, and 2) incorporate the
21 fault leakage function with the properties mentioned in Table 3 to mimic along fault leakage.
22 The goal of this case study is to analyze the evolution of CO₂ leakage rates and assess the impact
23 of fault capillary entry pressure on these rates.

24 VE reservoir simulation is conducted with a time step of one year to evaluate the impact
25 of the fault on the migration of a CO₂ plume within the reservoir. The evolution of the CO₂
26 plume is depicted at the end of the injection period (Figure 6b) and after 97 years of migration

1 (Figure 6c). The simulation results demonstrate the preferential up-dip movement of the CO₂
2 plume within the reservoir. Notably, significant quantities of CO₂ are observed to accumulate
3 at the base of the fault since the impermeable fault core inhibited further across-fault migration
4 within the reservoir. This leads to an increase in gas saturation down dip of the fault until the
5 CO₂ plume migrated laterally to the fault tips, after which it continued its unhindered up-dip
6 movement. Leakage along the fault occurs once the CO₂ reached the fault. The leakage rate
7 reached its maximum and then reduced after the CO₂ migrated around the fault tips. After this
8 point, continued upward migration reduced the amount of CO₂ trapped below the fault,
9 consequently decreasing the leakage rates (Figure 6d). A total of 3680 tons of CO₂ is injected
10 into the reservoir, of which 880 tons has leaked along the fault, accounting for approximately
11 24% of the injected CO₂.

12

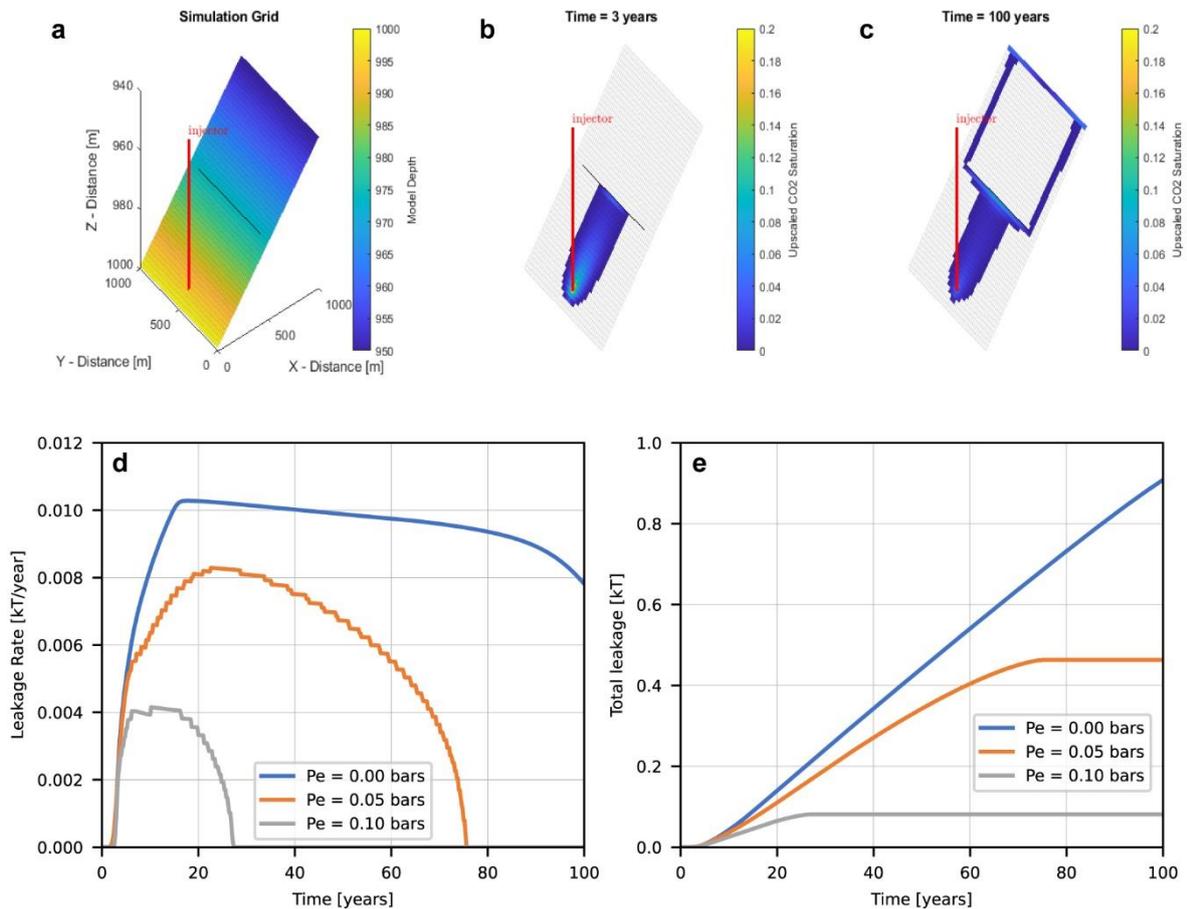
13 Table 3 – Summary of model parameters used for the sloping reservoir simulation case
14 described in section 3.3.

Property	Value
Reservoir description	
Number of cells (NX*NY)	50 x 50
Cell dimensions (DX*DY) (m)	20 x 20
Reservoir height (H) (m)	10
Reservoir slope (degrees)	2.86
Average reservoir depth (m)	975
Porosity	0.3
Permeability (mD)	100
Rock compressibility (Pa ⁻¹)	4.35 x 10 ⁻¹⁰
Fluid properties (at 2000m depth)	
Brine viscosity (Pa.s)	3.13 x 10 ⁻⁴
Gas viscosity (Pa.s)	3.21 x 10 ⁻⁵
Brine density (kgm ⁻³)	1001
Gas density (kgm ⁻³)	389.7
Fault properties	
Fault permeability (mD)	1 x 10 ⁻³
Fault width (m)	5
Fault length (m)	100
Rock-Fluid properties (Brooks-Corey Model)	
Residual gas saturation	0.2
Irreducible brine saturation	0.27
Gas end-point relative permeability	1

Brine end-point relative permeability	1
Gas relative permeability exponent	1
Brine relative permeability exponent	1

1

2



3

4 Figure 6 – Simulation of CO₂ plume migration in a sloping reservoir (note the slope is
5 exaggerated) and leakage along a fault showing the inclined 3D-view of the reservoir and the
6 location of the fault (a), the CO₂ plume saturation distribution at the end of the injection period
7 (b) the CO₂ plume saturation distribution after 100 years of migration (c), the CO₂ leakage rates
8 along the fault for different fault capillary entry pressures (d) and the cumulative CO₂ leakage
9 after 100 years for different fault capillary entry pressures (e).

10

11 The introduction of a capillary entry pressure constraint for fault leakage reveals
12 interesting leakage dynamics. Figure 6d depicts the leakage rates, while Figure 6e shows the
13 cumulative leakage after 100 years for varying fault capillary entry pressures ranging from 0 to
14 0.1 bar. Both the maximum fault leakage rate and cumulative leakage decreases with the

1 increase in fault capillary entry pressure. The scenario with zero fault capillary entry pressure
2 represents unconstrained leakage along the fault, allowing for continuous CO₂ leakage. In
3 contrast, higher capillary entry pressures act as a barrier, limiting the extent of CO₂ migration
4 and leakage through the fault zone. An important observation pertains to the leakage rate
5 reaching zero. This occurs when the trapped CO₂ plume is unable to overcome the capillary
6 entry pressure barrier, effectively stopping further leakage along the fault. The time at which
7 leakage ceases decreases with the increase in fault capillary entry pressure, highlighting its
8 potential for mitigating leakage.

9

10 3.4 Field-scale fault leakage quantification

11 The J area, a conceptual CO₂ storage site within the Malay Basin offshore Peninsular
12 Malaysia, is used to illustrate the fault leakage function coupled with VE models for field-scale
13 fault leakage quantification. The Malay Basin is approximately 500 km long, 200 km wide, and
14 12 km deep, situated in coastal waters less than 100 km from the east coast of Peninsular
15 Malaysia (de Jonge-Anderson et al., 2024b). It is a mature hydrocarbon basin with over 181
16 discoveries since and over 14.8 billion barrels of oil equivalent in recoverable resources since
17 1981 (Madon, 2021). Recently, it has been considered an important area for CCS (Abd Rahman
18 et al., 2022; Hasbollah et al., 2020) due to its numerous mature fields that could be repurposed,
19 providing an abundance of data and production history. Saline aquifers offer great potential,
20 however, limited data and understanding necessitate uncertainty assessment and screening
21 analysis to determine storage traps.

22 The J area lies on the northern margin of the basin, 50 km from the nearest hydrocarbon
23 field with the target reservoir situated at 1984 m depth below the seafloor. The main storage
24 interval consists of a thick and heterogeneous sequence of lower to middle Miocene sandstones,
25 mudstones, and coals, with the sandstones representing the target reservoir. The 3D reservoir

1 grid, depths, petrophysical and reservoir properties are obtained from de Jonge-Anderson et al.
2 (2024a, 2024b). The relevant reservoir properties are summarized in Table 4. Previous storage
3 capacity assessment for this site have identified the best injection location at the coordinate pair
4 (413100 m, 718500 m) (UTM 48 N – reference coordinate system) for an injection rate of 1
5 MT per year over 30 years followed by 970 years of migration (de Jonge-Anderson et al.,
6 2024b), assuming no leakage through the caprock. The top of the reservoir lies at depths
7 between 1500 m and 2500 m below a seafloor depth of 70 m. The reservoir pressure is assumed
8 hydrostatic with a temperature profile following a geothermal gradient of 50°C/km and a
9 seafloor temperature of 24°C (Madon & Jong, 2021). A 26 km-long fault is introduced into this
10 grid as shown in Figure 6a and the fault properties are provided in Table 4. The injection well
11 is located 12 km away from the fault. The grid blocks enclosing the fault are modified to 1) set
12 the across-fault permeability to zero, mimicking an impermeable fault core and 2) incorporate
13 the fault leakage function with the properties mentioned in Table 4 to simulate along fault
14 leakage. The model boundaries are treated as open, with the pressure maintained at hydrostatic
15 conditions. The goal of this case study is to understand the impact of fault leakage on the
16 injection rate and storage capacity within the J area.

17

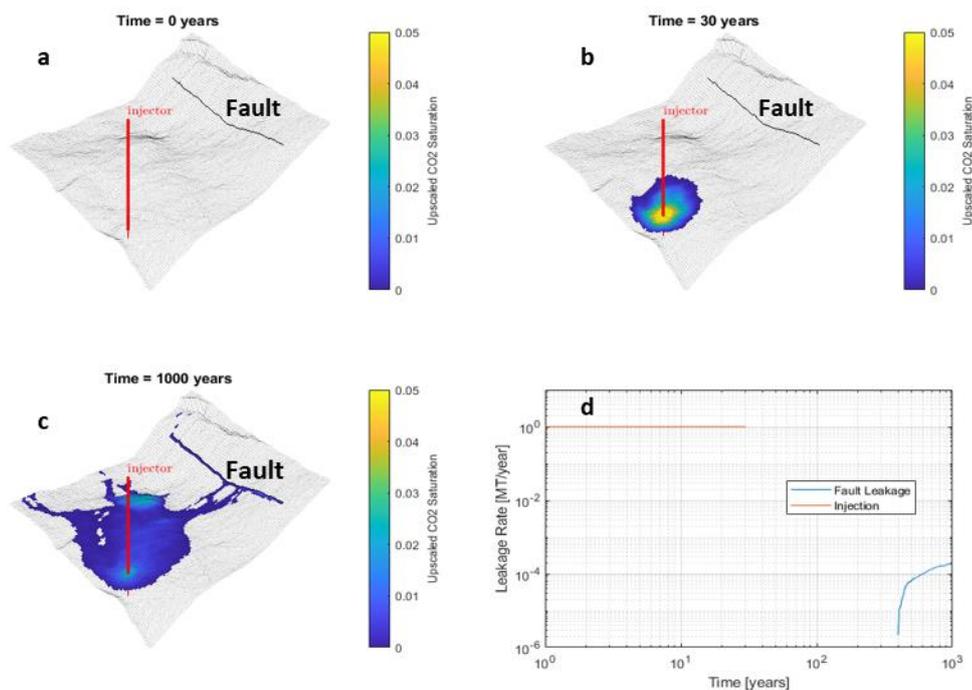
18 Table 4 – Summary of model parameters used for field-scale fault leakage quantification
19 simulation case described in section 3.4 (Adapted from (de Jonge-Anderson et al., 2024b))

Property	Value
Reservoir description	
Number of cells (NX*NY*NZ)	100 x 110 x 5
Cell dimensions (DX*DY) (m)	200 x 200
Area (km ²)	440 (22 x 20)
Average top reservoir depth (m)	1984
Porosity	0.05 – 0.25 (arithmetic mean = 0.145)
Permeability (mD)	1.2 –241 (arithmetic mean = 39.4)
Rock compressibility (Pa ⁻¹)	4.35 x 10 ⁻¹⁰
Seafloor temperature (°C)	24
Temperature gradient (°Ckm ⁻¹)	50
Seafloor Depth (m)	70
Fluid properties (at 2000m depth)	
Brine viscosity (Pa.s)	3.13 x 10 ⁻⁴

Gas viscosity (Pa.s)	3.21×10^{-5}
Brine density (kgm^{-3})	1001
Gas density (kgm^{-3})	389.7
Fault properties	
Fault permeability (mD)	1×10^{-3}
Fault width (m)	5
Fault length (m)	500
Rock-Fluid properties (Brooks-Corey Model)	
Residual gas saturation	0.2
Irreducible brine saturation	0.27
Gas end-point relative permeability	1
Brine end-point relative permeability	1
Gas relative permeability exponent	1
Brine relative permeability exponent	1

1

2



3

4 Figure 7 – Simulation of CO₂ plume migration and leakage along a leaky fault. Inclined 3D
5 view of the reservoir showing the location of the fault (a), CO₂ plume saturation distribution at
6 the end of the injection period (b), CO₂ plume saturation distribution after 1000 years of
7 migration (c) and temporal evolution of the CO₂ leakage rate along the fault (d).
8

8

9

A numerical simulation is performed to assess the impact of a fault on the migration and

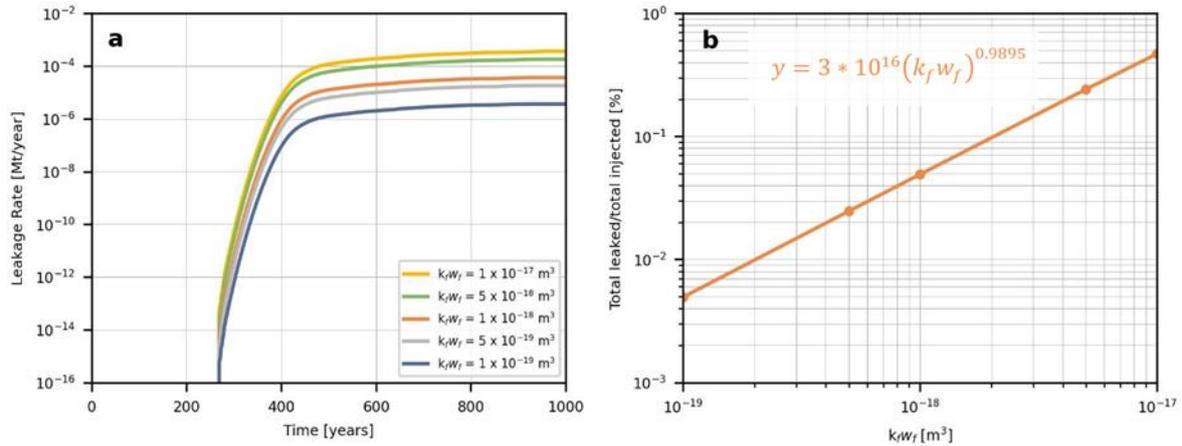
10

leakage of a CO₂ injected into the reservoir (Figure 7a). The evolution of the CO₂ plume is

1 depicted at the end of the injection period (Figure 7b) and after 1000 years of the migration
2 phase (Figure 7c). The simulation results show the CO₂ plume moving up-dip and accumulating
3 within an anticline structure. Considerable amounts of CO₂ accumulate at the base of the fault,
4 with the impermeable fault core preventing further migration across the fault. The CO₂ plume
5 reaches the fault after approximately 400 years and immediately begins leaking through the
6 fault (Figure 7d). The leakage rate increases as more of the migrating CO₂ became trapped at
7 the faulted block representing the hanging wall. By the end of the 1,000-year simulation period,
8 a total of 30 MT of CO₂ has been injected, of which 0.085 MT (0.28%) has leaked along the
9 fault. These results highlight the impact that the presence of a fault can have on the migration
10 and containment of a CO₂ plume in a storage setting and the ability to address this impact
11 quickly as each simulation takes under 30 seconds on Apple MacBook Pro with the Apple M1
12 chip.

13 The fault permeability and the thickness of the damage zone play a crucial role in determining
14 the magnitude of CO₂ leakage, as shown in Figure 8. While these parameters do not affect the
15 onset of leakage (Figure 8a). The total amount of leakage decreases, following a power-law
16 trend with an exponent of 0.9895 as the product of fault permeability and damage zone
17 thickness $k_f w_f$ decreases (Figure 8b). While Equation 16 predicted an exponent of 1, the
18 observed deviation suggests that variations in pressure buildup induced by fault permeability
19 also influence leakage rates. These effects are captured within the presented function. The fault
20 permeability is strongly dependent on the thickness of the damage zone, as well as the inter-
21 connectedness and density of the fracture networks within the damage zone, and studies have
22 demonstrated that these fault zone parameters are influenced by the pressure within the
23 reservoir-caprock-fault system (Rutqvist 2012; Vilarrasa et al., 2017).

24



1

2 Figure 8 – Impact of fault properties on CO₂ leakage showing the relationship between fault
 3 permeability, damage zone thickness, and the magnitude of CO₂ leakage (a) and the decrease
 4 in total CO₂ leakage over time with decreasing value for the product of fault permeability and
 5 damage zone thickness $k_f w_f$ (b).

6

7 The capillary entry pressure of the fault is also an important factor to consider for

8 leakage scenarios. High capillary entry pressure can prevent leakage, even where a fault is

9 permeable (Monzocchi et al., 2010; Zheng & Espinoza, 2022). In the preceding simulation for

10 the J area, the fault did not contain entry pressure that needed to be exceeded for CO₂ to leak.

11 The impact of fault capillary entry pressure on leakage was tested by running a series of

12 simulations with increasing fault capillary entry pressure, while keeping all other parameters

13 the same as in Table 4. The resulting leakage rate profile is shown in Figure 9a. As the fault

14 capillary entry pressure increases, the leakage rate decreases, and the onset of leakage is

15 delayed. A fault capillary entry pressure of 1 bar is found to result in a fully sealing fault, with

16 no CO₂ leakage observed for the given injection conditions. These results clearly demonstrate

17 the importance of the fault capillary entry pressure and its significant impact on the leakage

18 behavior. This parameter can be used to help determine the maximum safe storage capacity for

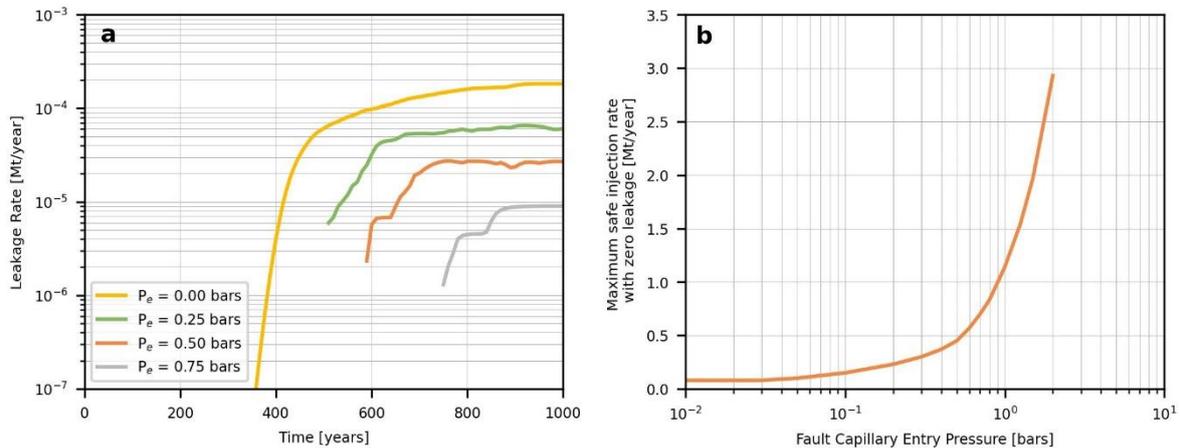
19 a given fault condition. Figure 9b shows the maximum injection rate with zero leakage rate for

20 a range of fault capillary entry pressures. For a fault with a capillary entry pressure of 0.5 bar,

21 leakage is not observed for an injection rate of up to 0.5 MT per year, while for a capillary entry

1 pressure of 1.0 bar, leakage is not observed for an injection rate of up to 1.3 MT per year. This
2 approach provides a valuable tool for screening the maximum safe injection rate and the
3 maximum storage capacity at which the risk of CO₂ leakage along faults is small.

4



5

6 Figure 9 – Impact of fault capillary entry pressure on CO₂ leakage showing the leakage profile
7 for different fault capillary entry pressures where higher entry pressures act as a barrier,
8 delaying and reducing the CO₂ leakage and no leakage occurs for a scenario of 1 bar (a).
9 Maximum injection rate with zero leakage for a range of fault capillary entry pressures where
10 increasing the entry pressure allows for higher injection rates without CO₂ leakage (b).

11

12 4 Conclusions

13 This work presents a fast and computationally efficient tool for simulating fault leakage
14 under uncertainty for realistic, field-scale CO₂ storage applications. Faults are inherently
15 complex, typically characterized by a fault core and a surrounding fractured damage zone, both
16 of which significantly influence fault leakage behavior at the field scale. Explicitly representing
17 these fault complexities along with the multi-layered systems is a computationally intensive
18 method for resolving fault leakage-related uncertainty, especially during the early stages of
19 storage site screening when data availability is limited. The primary contribution of this work
20 addresses this challenge by proposing an approach that integrates an upscaled fault leakage
21 function, specifically tailored to the unique characteristics of the fault core, damage zone, and
22 flow properties, into a VE reservoir modeling framework. This integration provides a valuable

1 tool for incorporating the geological understanding of faults into leakage assessment
2 workflows. The computational efficiency of our proposed approach enables the fast screening
3 of a large number of geological scenarios inherent to multiple potential storage sites, identify
4 those sites that are most promising to develop a secure storage project, and develop more
5 targeted data acquisition and reservoir characterization studies for these sites. Such fast
6 screening of potential storage sites is key to enable the scale-up of CO₂ and reach the gigaton
7 storage needed to reduce global CO₂ emissions.

8 By applying this modeling framework to various CO₂ injection scenarios, we were able
9 to gain insights into the key factors influencing fault-related leakage, such as fault permeability,
10 capillary entry pressure, and the interaction between the fault and the surrounding reservoir.
11 The results from these simulations offer valuable information for the design and risk assessment
12 of CO₂ storage projects in geologically complex settings. While the assumption of constant
13 fault properties simplifies the modeling approach, it may not capture the full heterogeneity and
14 uncertainty associated with real-world fault systems. Future work could explore the impact of
15 incorporating more detailed, stochastic representations of the fault hydraulic properties and
16 geomechanical factors and constraints on the leakage estimates, further enhancing the reliability
17 and applicability of the modeling framework.

18

19 **Acknowledgements**

20 The funding and data underpinning this work was provided by PETRONAS via the
21 PETRONAS Centre of Excellence in Subsurface Engineering and Energy Transition
22 (PACESET), based at Heriot-Watt University. Sebastian Geiger thanks Energi Simulation for
23 supporting his Chair in Sustainable Geoenergy. Florian Doster acknowledge valuable
24 discussions with Michael A. Celia, Jan M. Nordbotten and Mary Kang while formulating the
25 research topic.

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