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Mechanistic Modeling of CO₂ Well Leakage in a Generic Abandoned Well
Through a Bridge Plug Cement-Casing Gap

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1

2 **Abstract**

3 Both known and unmapped plugged and abandoned wells are potential leakage pathways for CO₂
4 from geologic carbon sequestration (GCS) sites. Although many abandoned wells have cement
5 bridge plugs installed to prevent leakage, the seal between the cement and the inner casing wall is
6 subject to failure. In this study, we carried out detailed T2Well simulations of cases of sudden non-
7 Darcy flow of CO₂ and brine leakage up the gap between a cement plug and the inner steel casing
8 wall that becomes a fully connected flow path during the post-injection period. The goal of our
9 study was two-fold: (1) to understand the dynamics, rates, and the characteristic temporal signals
10 associated with the onset of leakage through various gap-aperture sizes, and (2) to suggest potential
11 monitoring strategies based on the findings. Simulation results show that the leakage of CO₂ and
12 brine upward is transient with interesting phase interference behavior. Time-dependent oscillatory
13 flows with varying pressure, temperature, and flow rates of CO₂ and brine show strong dependence
14 on gap aperture. Phase-change and decompression lead to very low temperatures at the top of the
15 well for gap apertures larger than 4 mm suggesting that remote thermal monitoring at the ground
16 surface may be an effective way of monitoring even if well locations are not known a priori.
17 Pressure in the well is also indicative of CO₂ leakage. The temporal patterns of changing
18 temperature and pressure may be useful diagnostic signals for leakage detection. Finally, these
19 transient leakage signals may provide information on the cause of leakage and/or characteristics
20 of the flow path that could inform effective remediation design and execution approaches.

21 **Introduction**

22 Both known and unknown (unmapped) plugged and abandoned wells are widely recognized as
23 potential pathways for CO₂ and brine to leak from geologic carbon sequestration (GCS) sites into
24 potable groundwater aquifers and even back into the atmosphere (Gasda et al., 2004). Wells are
25 often abandoned by a procedure involving emplacement of a cement bridge plug at depth, above
26 which the well is filled with fluids such as brine, drilling mud, or corrosion-inhibiting fluid. The
27 purpose of the cement bridge plug is to seal off the well from the reservoir, hydraulic
28 communication to which is provided by perforations. The purpose of the fluid above the bridge
29 plug is to maintain pressure and prevent rapid corrosion of the steel casing. Experience has shown
30 that cement-casing interfaces are subject to debonding and other processes over time that lead to
31 failure to seal that creates a leakage flow path for formation fluids and CO₂ upward past the plug
32 into the fluid-filled well.

33 Before a plugged and abandoned well that is leaking up its inner casing string to the surface or into
34 shallow soils above a buried well top can be fixed, the leakage must be detected and stopped.
35 Challenges arise because CO₂ leakage rates through degraded cement seals may be small and fluid
36 leakage manifestations on the ground surface from plugged and abandoned wells may be difficult
37 to detect within natural background variations of moisture and CO₂ concentration. In this study,

1 we have carried out detailed non-Darcy flow simulations of the transient period following the onset
2 of CO₂ and brine leakage up the gap in a bridge plug between cement and inner casing wall and
3 into the open fluid-filled column of a prototypical abandoned well. We vary the plug gap aperture
4 and simulate two different bridge-plug lengths (10 m and 30 m) to investigate sensitivity of leakage
5 signals to plug-gap properties. One purpose of this study is to provide information on expected
6 leakage behavior dynamics and the temporal signals associated with non-isothermal CO₂ and brine
7 leakage that can be used to design near-surface monitoring approaches for leakage detection.
8 Through mechanistic modeling of viscous two-phase flow in the well-reservoir system, the reasons
9 for various interesting dynamic behaviors can be explained. The simulation approach is general
10 enough that the plug gap can also be conceived as being a fracture in the cement bridge plug with
11 axial length equal to the plug thickness and horizontal length equal to one-half of the plug
12 perimeter.

13 **Background and Prior Work**

14 Integrity failures in pre-existing wells of all kinds (abandoned, idled, shut-in, operating) completed
15 to reservoir depth within the footprint of the CO₂ free-phase and/or pressure plumes of GCS sites
16 are widely recognized as a potential cause of CO₂ and brine leakage from future large-scale GCS
17 operations. There are several components of wells and critical interface seals that can fail over
18 time and allow leakage to occur as summarized by Gasda et al. (2004). Of the several well integrity
19 failure modes, failures resulting in open gaps and annuli, e.g., between cement and casing or
20 between cement and formation, are considered by researchers studying CO₂ and brine leakage in
21 the GCS context to be most likely to result in large leakage flow (Kutchko et al., 2007; Bachu and
22 Bennion, 2009). Laboratory and field studies in the GCS context have found that chemical
23 reactions between cement and carbonic acid (CO₂ dissolved in water) can degrade cement integrity
24 (net dissolution) and in other cases lead to precipitation and self-sealing of gaps and spaces (Carey
25 et al., 2007; Crow et al., 2007). Nevertheless, the large number of documented cases of sustained
26 casing pressure (SCP) in oil and gas wells (Bourgoyne et al., 1999; Choi et al., 2013; Lackey et
27 al., 2017) suggests that gaps and annuli are generally present in wells (Huerta et al., 2009). At least
28 one example exists in the GCS context of poor bonding of cement to steel casing that can lead to
29 gaps and annular spaces that compromise well integrity (e.g., Oldenburg et al., 2011).

30 Given the general concern for the integrity of existing wells, a large body of work exists focusing
31 on the evaluation of the leakage rates and total leakage that could occur as a result of well integrity
32 failure, along with remediation approaches (e.g., Wojtanowicz et al., 2001). Early studies were
33 aimed at evaluating and mitigating sustained casing pressure (SCP) in oil and gas wells (e.g., Xu
34 and Wojtanowicz, 2001), and these methods were further developed more recently (Huerta et al.,
35 2009; Tao et al., 2010). As interest in GCS grew in the early 2000's, new semi-analytical
36 approaches to modeling well leakage related to CO₂ and brine were developed and applied (e.g.,
37 Nordbotten et al., 2004; 2005). In addition, numerical methods including consideration of two-
38 phase flow were developed and applied (e.g., Pruess, 2003; Celia et al., 2005; Ebigbo et al., 2007).

1 Reduced order models (ROMs) for well leakage and aquifer impact have been developed by the
2 U.S. Department of Energy's National Risk Assessment Partnership (NRAP) for quantification of
3 the uncertainty of estimated leakage impacts (Pawar et al., 2016). Despite the large number of
4 studies and solution approaches, all of the prior well leakage models except for NRAP's open-well
5 leakage ROM (Pan and Oldenburg, 2016) have assumed that well leakage flow was through an
6 effective porous medium, i.e., by the process of Darcy flow. While this assumption may be
7 adequate for many cases involving SCP and/or low-flow-rate or incipient leakage through fine
8 cracks or through tortuous paths in degraded cement, CO₂ and brine leakage through finite-
9 aperture gaps and annuli between cement and casing should formally be modeled as viscous flow
10 rather than Darcy flow.

11 In the study presented here, we simulate the onset and transient period of well leakage by single-,
12 two-, and three-phase viscous (non-Darcy) flow in gaps or annuli of various apertures along a
13 cement plug at the cement-casing interface within an idealized abandoned well. The conceptual
14 model we assume is that the cement plug was sealing the abandoned well effectively up until some
15 time during the post-injection period of the GCS project when the gap became fully connected
16 across the plug and the well started to leak. Leakage along such a gap leads to reservoir fluid (CO₂
17 and/or brine) entering the fluid-filled column above the plug where non-Darcy pipe flow occurs
18 by pressure gradient or buoyancy forces. At certain conditions, two types of CO₂-rich phases can
19 exist, namely, gaseous CO₂ and liquid CO₂, which can lead to a three-phase (aqueous, gaseous CO₂
20 and liquid CO₂) system at different depths in the well. In all cases, we simulate the entire coupled
21 reservoir-well (plug gap and well column) system upward to the top of the well at the ground
22 surface considering coupled reservoir flow (Darcy flow) and open gap and column flow (non-
23 Darcy flow). As it will be shown, these gap-leakage flow processes occur over time scales much
24 smaller than expected chemical reaction time scales which were not included in our model. In
25 order to focus on the flow processes and transient leakage signals, we also neglect for now
26 geomechanical processes. To our knowledge, this is the first study that simulates the mechanistic
27 non-isothermal process of three-phase flow in a narrow gap related to CO₂ and brine well leakage
28 from a hypothetical GCS reservoir.

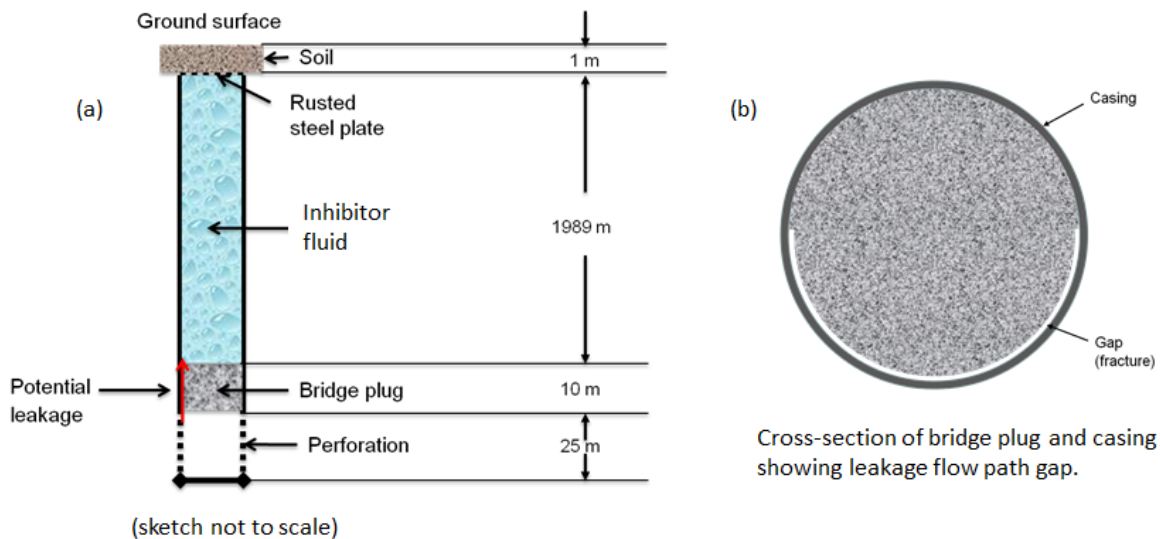
29 **Conceptual Model**

30 The prototypical abandoned well system that we simulate is shown in Fig. 1. In the system, a 1989
31 m-long column of inhibitor fluid (assumed to be pure water in this study) fills an open well above
32 a 10 m-long cement bridge plug with an open gap (e.g., due to debonding) over part of its
33 circumference (50%). Although the current U.S. regulations require longer cement plugs for
34 abandoned wells (e.g., extending 100 ft above oil bearing strata), many older wells abandoned
35 prior to the 1950s either were not plugged at all or were plugged with very little cement in them
36 (NPC, 2011). The requirement on length of cement plug is rather vague prior to the 1970s in the
37 U.S. The longer the cement plug is, the lower the chance to be subject to through-going gaps and
38 the greater the resistance is to leakage flow if a gap were to develop. We use a 10 m-long cement

1 plug to reflect poor plugs in those older wells that are more vulnerable to leakage without losing
 2 the general features of leakage through a failed plug in abandoned wells. Additional results for a
 3 30 m-long plug are presented for comparison.

4 The perforated bottom section of the well is in hydraulic connection with the permeable CO₂-filled
 5 reservoir. As with many plugged and abandoned wells, there is no wellhead and the top of the
 6 casing is conceptualized as being covered by a permeable rusted steel plate and 1 m of soil (Fig.
 7 1a), both of which we model as porous media coupled to the open well. The thickness of the semi-
 8 circular gap between the cement plug and the casing wall is varied as a parameter in the
 9 simulations. Reservoir fluids (CO₂ and brine) have the potential to leak up the gap between the
 10 cement of the bridge plug and the inner casing wall into the column of inhibitor fluid and onward
 11 to the ground surface through the permeable materials (rusted steel plate and soil) at the top of the
 12 well. Note that although this is a coupled well-reservoir model, we do not intend to simulate the
 13 full development process of the CO₂-filled reservoir. Instead, we investigate possible dynamic
 14 behaviors of leakage when plug failure takes place in an abandoned well connected to a CO₂-filled
 15 reservoir during the post-injection period of the GCS reservoir.

16



17

18 Figure 1. (a) Conceptual model of prototypical abandoned well with bridge plug below long open section, and (b) cross section of bridge plug
 19 showing the gap (over one-half of the circumference) the aperture of which was varied in the simulations shown here. The reservoir and other
 20 formations (cap rock, soil etc.) are included in the model (see Figure 2 and related text for details of the integrated well-reservoir model used in
 21 this study).

22

23 The properties of the modeled system for the 10 m-long plug are presented in Tables 1 and 2. We
 24 note that all of the layers in the model (Table 2) are assumed to have pore compressibility of $3 \times 10^{-9} \text{ Pa}^{-1}$, and that all layers have thermal conductivities of $3.0 \text{ W}/(\text{m } ^\circ\text{C})$ and specific heats of $1000 \text{ J}/(\text{kg } ^\circ\text{C})$.

26

1
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Table 1. Well and plug properties.

Feature	Value
Well length	2024 m (from -1 m to -2025 m)
Casing ID	0.15962 m (7-inch casing, wall thickness = 9.09 mm)
Bridge plug	10 m thickness (from -1990 to -2000 m)
Perforation	25 m (from -2000 m to -2025 m)
Wall roughness of well	45×10^{-6} m
Wall roughness of plug gap	100×10^{-6} m
Gap aperture	Various
Effective porosity	Various, a function of aperture
Effective perimeter of gas	Various, a function of aperture
Rusted steel plate at top of the abandoned well	Assumed same permeability as cover soil (100 Darcy)

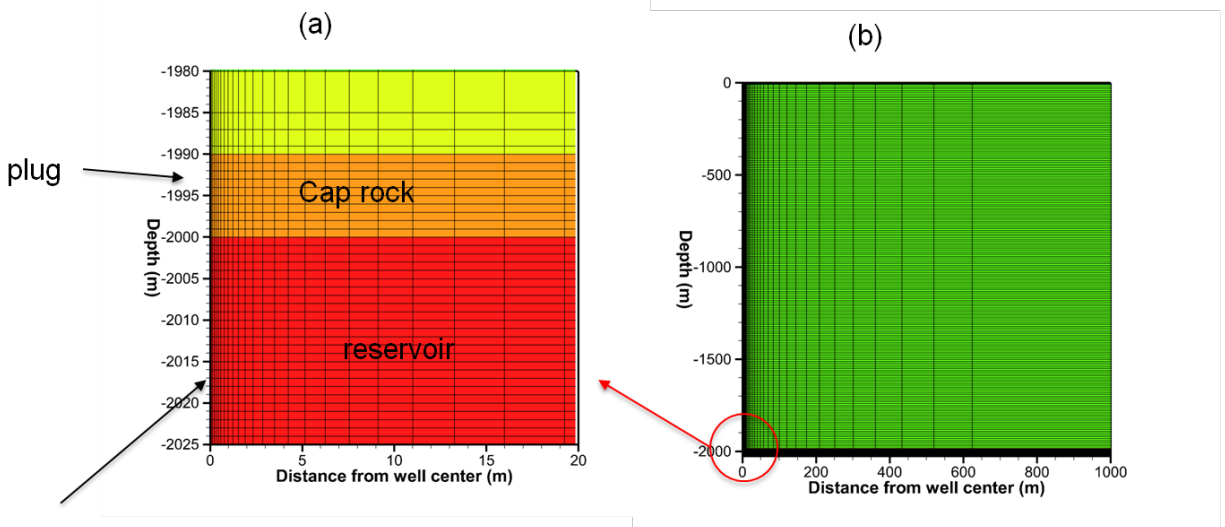
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Table 2. Layer properties.

Layer	Depth (m)	Porosity	Lateral permeability (m ²)	Vertical permeability (m ²)
Reservoir sand	2000-2025	0.25	10^{-12}	10^{-12}
Cap rock	1980-2000	0.05	10^{-18}	10^{-18}
Overburden	10-1980	0.05	10^{-18}	10^{-18}
Soil2	1-10	0.45	10^{-15}	10^{-15}
Soil1	0-1	0.45	10^{-10}	10^{-10}

5

6 All formation layers above the reservoir are saturated with water under hydrostatic pressure. The
7 bottom formation layer is modeled (with 25 grid layers) to represent a GCS reservoir with a given
8 initial gas (CO₂-rich phase) saturation (0.5 in this study) and initial pressure at the bottom grid cell
9 equal to the hydrostatic pressure. Because of the existence of gas phase, the initial pressure at the
10 top of the reservoir is slightly (1 bar) larger than the hydrostatic pressure that would exist at the
11 same depth (1986 m below land surface) if the reservoir were fully saturated with water. The
12 wellbore above the reservoir (including the plug) is initially saturated with water under hydrostatic
13 pressure whereas the wellbore below the plug is under the same conditions as the reservoir. The
14 geothermal gradient is 30 °C/km and the ambient temperature at land surface is assumed to be 25
15 °C. The entire domain is under natural ambient thermal conditions initially. Conditions at the top
16 of the model are held at atmospheric pressure and ambient temperature (25 °C). In all cases we use
17 a radially symmetric (RZ) grid with variable radial and vertical grid spacing (Fig. 2). a no-flow
18 boundary is assigned along the lateral boundary at 1000 m away from the well.



Perforated
well

1
2 Figure 2. Radially symmetric *RZ* grid used in the simulations. Horizontal grid resolution varies
3 from 0.1 m near well to ~200 m in the far field while the vertical resolution varies from 1 m below
4 a depth of -1995 m (the top of the plug) to 10 m above -1985 m and 1- ~2 m near land surface. (a)
5 locally zoomed view of the region including the well perforation zone and the plug and (b)
6 overview of entire simulation domain.

7 **Methods**

8 We simulate three-phase brine-CO₂ flow in the prototypical leaking well with T2Well, a numerical
9 simulator for solving the equations of non-isothermal, multiphase, and multi-component flows in
10 integrated wellbore-reservoir systems (e.g., Pan et al. 2011 a, b; Pan and Oldenburg, 2014). T2Well
11 extends the numerical reservoir simulator TOUGH2 to calculate the non-Darcy flow in open
12 (viscous) flow regions (i.e., not porous media) such as within well tubing, annuli, or cement-casing
13 gaps and in connected porous media simultaneously and efficiently by identifying “wellbore”
14 regions within the numerical grid in which two-phase viscous (non-Darcy) flow is simulated while
15 generalized multiphase Darcy flow is simulated elsewhere. TOUGH2 uses a mass-conserving
16 integral finite difference method with implicit time stepping to solve the multicomponent flow
17 equations, and a residual-based convergence criterion with Newton-Raphson iteration to handle
18 non-linearity (Pruess et al., 2012).

19 Within the wellbore sub-domains, T2Well solves a 1D momentum equation of the fluid mixture
20 (which may be three-phase) as described by the extended drift-flux model (DFM). The velocity of
21 the mixture is obtained by solving the momentum equation numerically while the individual phase
22 velocities are calculated from the mixture velocity and other fluid-flow parameters as defined by
23 the three-phase DFM. The three-phase DFM is formulated as a two-step extension of the two-
24 phase DFM in which the two-phase DFM is first applied to get the aqueous phase velocity and the

1 non-aqueous (CO₂-rich) phase velocity. If the non-aqueous phase is a mixture of gas and liquid
2 CO₂, the two-phase DFM is then applied to obtain the liquid phase velocity and gas phase velocity
3 with proper parameters from the non-aqueous phase velocity. A mixed implicit-explicit scheme is
4 applied to facilitate the solution of the momentum equation within the Newton-Raphson iteration
5 framework of TOUGH2. Specifically, the pressure gradient, the gravity component, and the time-
6 derivative of momentum are treated fully implicitly while the spatial gradient of momentum is
7 treated explicitly. The friction term is calculated with a mixed implicit-explicit scheme (Pan et al.
8 2011a). Although the wellbore flow model is one-dimensional and cannot describe two- or three-
9 dimensional flow phenomena, the drift-velocity-model implemented in T2Well does parameterize
10 the two- or three-phase flow instabilities and turbulence and even two-phase counter-flow to model
11 the important multiphase flow phenomena. This wellbore-domain approach is coupled seamlessly
12 with the standard TOUGH2 porous media approach to simulate coupled wellbore-reservoir flow
13 problems. The approach has been demonstrated over the years for problems related to wellbore
14 leakage and injection relevant to geologic carbon sequestration (Pan et al. 2011b), oil reservoir
15 blowout (Oldenburg et al. 2011), and gas reservoir blowout (Pan et al., 2018a). The rigor of the
16 flow modeling in T2Well is complemented by the accuracy of the equation of state (EOS) modules
17 used for the fluid compositions and phase relations. In this study, we make use of a research version
18 of ECO2M (Pruess and Spycher, 2007; Pan et al., 2017) which models three fluid phases (aqueous,
19 gaseous CO₂, and liquid CO₂), and three chemical components (H₂O, CO₂, and salt) with recent
20 improvements and extensions (Pan et al., 2018b). ECO2M is capable of modeling three-phase
21 aqueous systems containing gaseous, supercritical, or liquid CO₂, including two simultaneously
22 co-existing phases of CO₂. Note that the current ECO2M has a lower limit in temperature and
23 cannot simulate the scenarios with frozen or hydrate-forming conditions. As a result, any possible
24 blocking of leakage due to such conditions (forming of ice or hydrate) is not considered in this
25 study. We refer the reader to Pan and Oldenburg (2014) for a complete description of the methods
26 used in T2Well.

27 **Results**

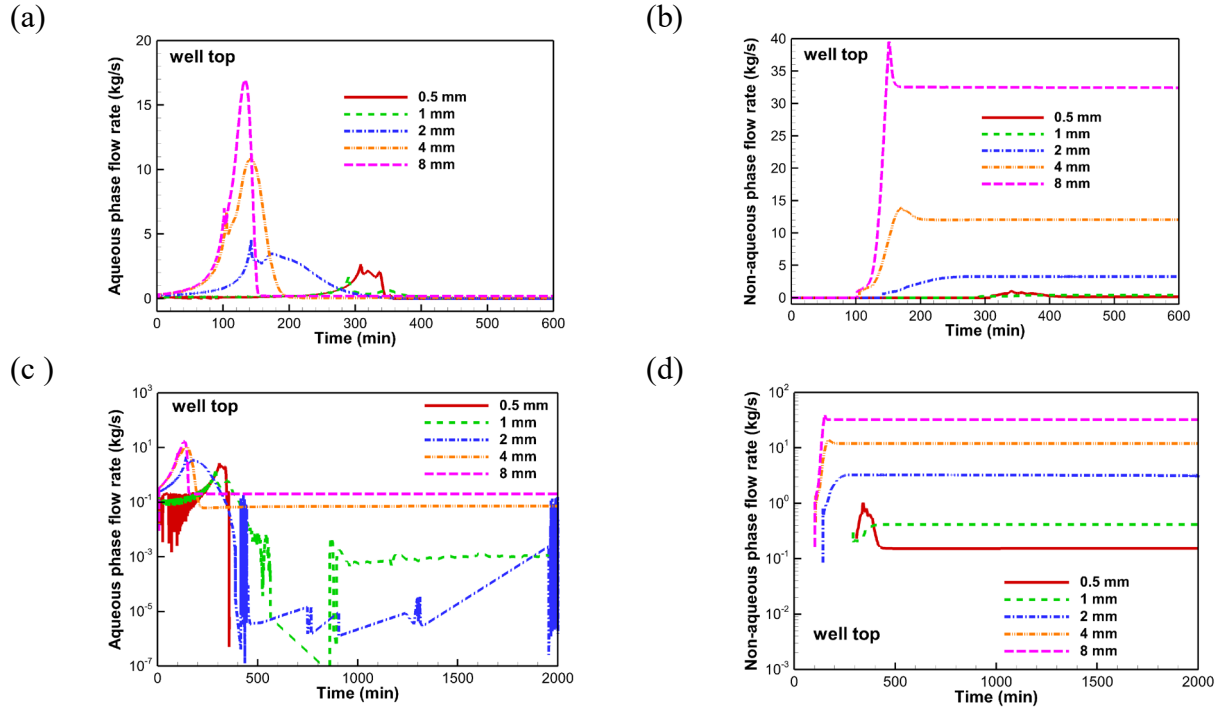
28 **Introduction**

29 Before leakage control methods can be applied, leakage must be detected and the well must be
30 located. In order to develop and improve CO₂ and brine leakage detection and abandoned well-
31 locating methods, it is useful to know generally what such leakage signals look like so they can be
32 distinguished from background variations (Oldenburg et al., 2003; Cortis et al., 2008). The
33 mechanistic simulations presented here provide information on the pressure, temperature, and fluid
34 compositional transient signals for the case of an abandoned well leaking CO₂ and brine along a
35 gap in a bridge plug. These results are not meant to be used for quantifying leakage rates from any
36 particular single well nor extrapolated to estimate leakage from multiple wells because the
37 properties of the well modeled are idealized and not site-specific. Instead, the results are meant to
38 be used to gain insight into the signals of leakage originating by this failure mode and to explain

1 the mechanistic origins of the signals including their transient behaviors as a function of well
2 system properties, with a focus on gap aperture. Insights gained from the results can be used to
3 design monitoring and leakage quantification approaches that are especially challenging for
4 unknown and abandoned wells.

5 The coupled three-phase flow system is complex resulting in the need for many figures to describe
6 the results. We have organized the presentation into three tiers of results. The first tier summarizes
7 the dynamic behaviors in terms of aqueous phase and CO₂-rich phase leakage rates as affected by
8 the fracture aperture in the plug. The second tier analyzes the temporal evolution of well status in
9 each individual well with particular aperture that causes particular characteristics in leakage
10 behaviors. The third tier further analyzes different patterns of the friction and gravity pressure
11 drops along the plug with different apertures which create unique characteristic leakage dynamics
12 in the system that are very promising for leak detection.

13 We present in Fig. 3 the aqueous (H₂O-rich) phase and non-aqueous (CO₂-rich) phase flow rates
14 at the top of the well for five different gap apertures. In general, the leakage starts with one or two
15 peaks of water eruption prior to breakthrough of CO₂-rich phase. This erupted water originates as
16 water contained in the well above the plug prior to leakage onset. As shown in Figure 3, the larger
17 the gap aperture is, the larger the eruption strength and the earlier the eruption occurs. For example,
18 the aqueous mass flow rate reaches 16.97 kg/s at about 130 min for the 8 mm aperture whereas the
19 aqueous mass flow rate only reaches 1.73 kg/s at 290 min in the case of the 1 mm aperture (Figure
20 3a). For a 0.5 mm aperture, the aqueous phase flow starts as a strong oscillatory flow with a very
21 small flow rate (Figure 3c). However, the magnitude of the flow rate during its single peak is larger
22 than that in the 1 mm case although its after-peak aqueous phase flow rate is practically zero. After
23 the short-lived transient water eruption, the aqueous phase flow rate greatly reduces to a small
24 value associated with almost constant non-aqueous phase (CO₂-rich) flow. The non-aqueous phase
25 (i.e., CO₂-rich phase) mass flow rate peaks immediately after breakthrough and then gradually
26 reaches a stable value in most cases except for the cases of 1 or 2 mm gap aperture for which the
27 early peak does not occur. The peak values of non-aqueous phase flow rate are 39.56, 13.88, 3.31
28 0.42, and 1.03 kg/s for gap apertures of 8, 4, 2, 1, and 0.5 mm, respectively. The corresponding
29 stable flow rates are 32.5, 12.1, 3.3, 0.42 and 0.15 kg/s, respectively. The response in flow rate to
30 gap-size variation is not linear.



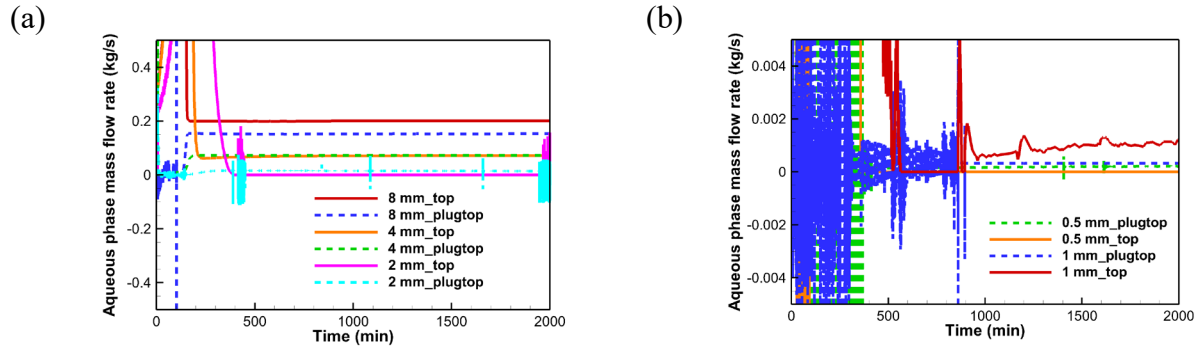
1 Figure 3. Simulated mass flow rates of aqueous and non-aqueous phase at the wellhead as a function of time for the five gap apertures. (a)
 2 aqueous phase flow rate, (b) non-aqueous (CO₂-rich) phase flow rate, (c) aqueous phase flow rate (log-scale) and (d) non-aqueous phase flow
 3 rate (log-scale).

4

5 The gap size does not only affect the timing and magnitude of aqueous phase eruption but it also
 6 regulates the dynamics of the aqueous phase flow rate and the final aqueous phase flow rate (Figure
 7 3c). As shown in Figure 3c, the final aqueous phase flow rate decreases quickly with decrease of
 8 gap size for all cases in general although it does so in a manner of irregular oscillations in cases
 9 with intermediate gap size (e.g., 1 mm and 2 mm). As the aperture is reduced to 0.5 mm, the
 10 aqueous phase leakage rate is practically zero after a relatively big eruption at early time associated
 11 with the breakthrough of CO₂-rich phase.

12 Comparing the aqueous phase flow rate at the well top and plug top (Figure 4) reveals complicated
 13 dynamics in phase changes in the well above the plug as a function of gap aperture. For the 8 mm
 14 aperture, the aqueous phase flow rate at the wellhead (i.e., well top) is slightly higher than that at
 15 the plug top which implies that water vapor has condensed in the well above the plug (Figure 4a).
 16 This difference does not occur for the 4 mm gap in which the aqueous phase flow rates are identical
 17 at the wellhead and plug top. When the aperture is reduced to 2 mm, the aqueous phase flow rate
 18 out of the plug top is larger than that at the wellhead most of the time although the rate itself is
 19 very small. The aqueous phase leak at the wellhead for the 2 mm gap behaves more like a geyser
 20 (Figure 4a) and water may flow downward in the well during those oscillation periods. As the
 21 aperture is reduced to 1 mm, the aqueous phase flow rate at the plug top is quite stable but small
 22 after early time eruption whereas the aqueous phase flow rate at the wellhead is slightly larger with

1 obvious oscillations (Figure 4b). However, as the aperture is further reduced to 0.5 mm, the
 2 aqueous phase flow rate at the plug top still shows strong oscillations although they tend to
 3 decrease with time significantly (Figure 4b) while the aqueous phase flow rate at the wellhead is
 4 practically zero (Figure 3c & 4b). In smaller gap-aperture cases (1 and 0.5 mm), the aqueous phase
 5 flow rate at the plug top at early time shows strong oscillatory behavior (Figure 4b).



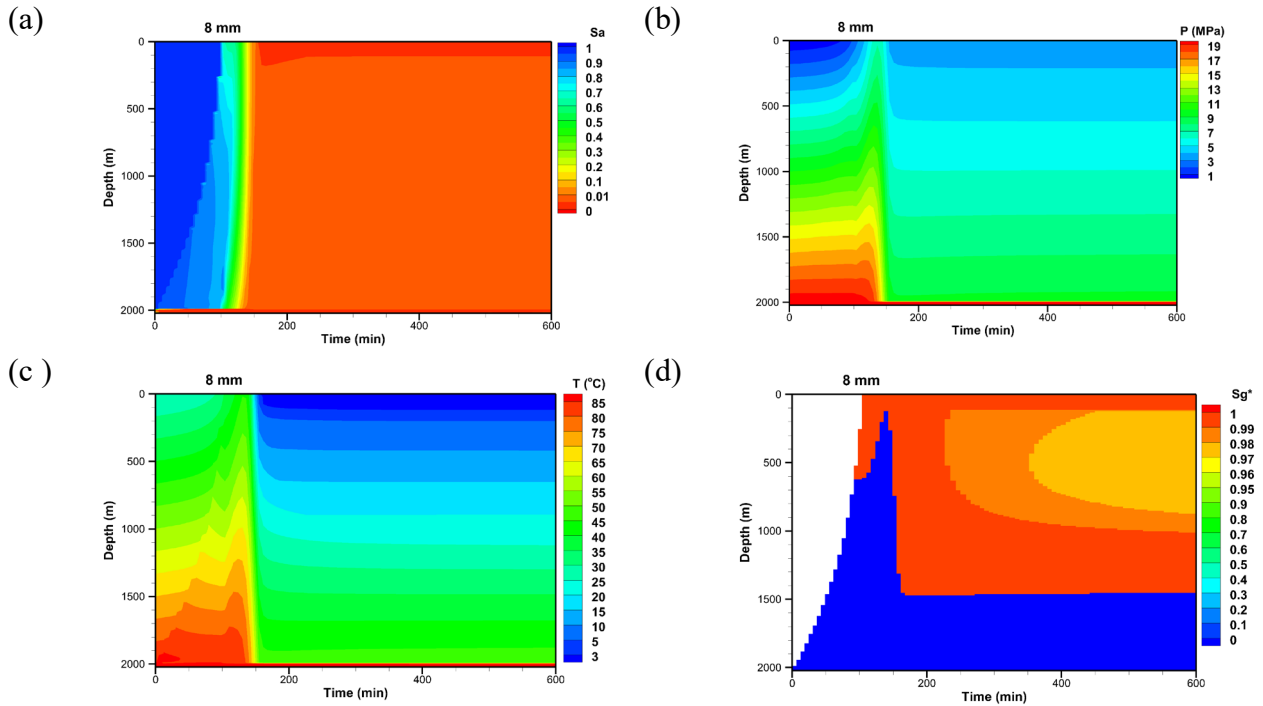
6 Figure 4. Simulated mass flow rates of aqueous at wellhead (top) and top of plug (plugtop) as a function of time for the four gap apertures. (a)
 7 larger aperture (8, 4, and 2 mm) and (b) smaller aperture (1 and 0.5 mm).

8

9 The complicated leakage behaviors observed to vary with gap aperture originate from variations
 10 in the non-isothermal phase change processes occurring in the well as the leakage progresses. In
 11 the following paragraphs, we will analyze the temporal evolution of aqueous phase saturation,
 12 pressure, temperature, and gaseous CO₂-ratio profiles in the well, case by case, to understand the
 13 mechanisms behind the leakage behaviors found in each case.

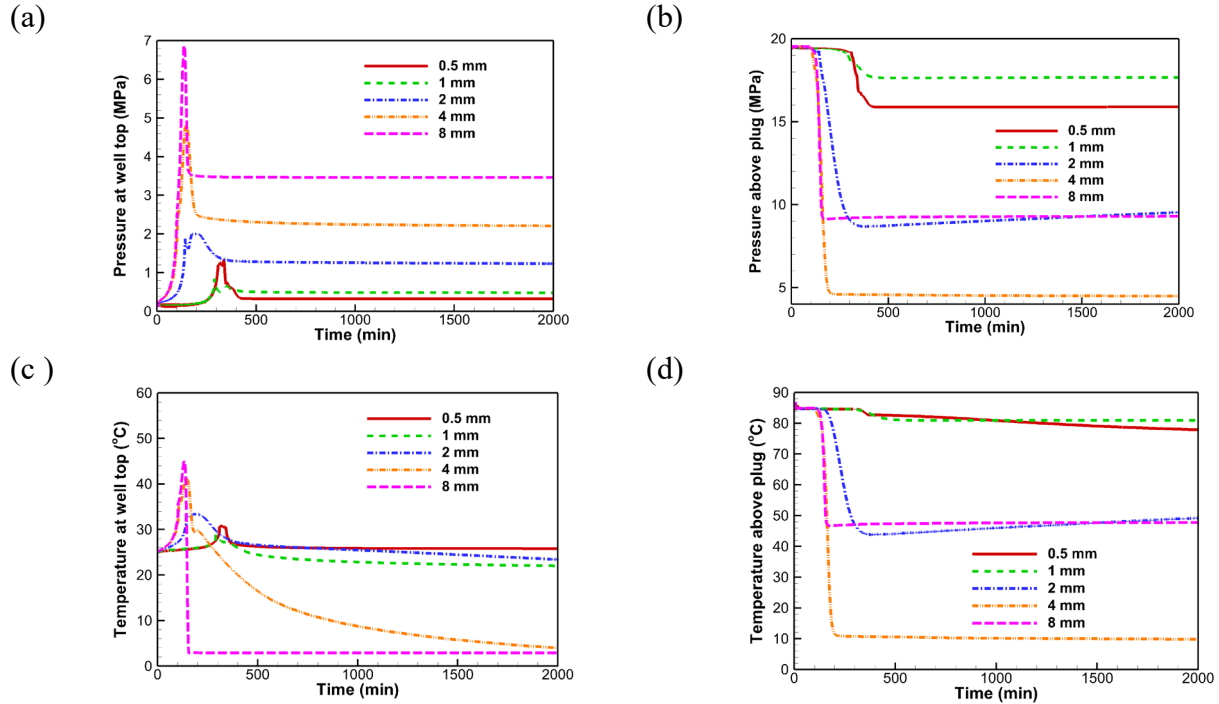
14 In the case of the 8 mm gap aperture (Figure 5a), the initially water-filled well (above 2000 m, i.e.,
 15 the plug and above) becomes very dry (aqueous saturation ~0.001 or less) after 150 min because
 16 the water has been lifted out of the well by the leaking “gas” (CO₂-rich phases) in the big eruption.
 17 As a result, the pressure above the plug drops significantly after the big eruption of water (Figure
 18 5b) although the pressure right above the plug is still around 9 MPa because of small resistance to
 19 the flow due to the large aperture (Figure 6b) and around 3.6 MPa at well top (Figure 6a). Before
 20 the water eruption, the temperature in the well increases in general as warmer fluid flows upward
 21 although the trend is complicated by the presence of CO₂-rich phase which is lighter than water
 22 (Figure 5c). The CO₂-rich phase accelerates the upward flow which brings more enthalpy from
 23 below resulting in an increase of local temperature shown as the first peak (Figure 5c) along the
 24 aqueous phase saturation line (Figure 5a or 5d). However, increases in temperature tend to be
 25 canceled or suppressed by the expansion cooling of the CO₂-rich phase as the CO₂-rich phase
 26 saturation further increases especially in shallow regions of the well until the water flow rate
 27 reaches the peak value at eruption when the CO₂-rich phase finally reaches the well top. After that
 28 the temperature above the plug drops to below 50 °C (Figure 5c and 6d) because of expansion
 29 cooling. The temperature decreases with elevation (Figure 5c) and reaches about 3 °C (the lower
 30 limit of the equation of state in the simulator) at the well top implying that dry ice or CO₂-hydrate

1 could form under this larger aperture leakage scenario. Furthermore, as shown in Figure 5d,
 2 although CO₂ transforms from supercritical to gas around the depth of 1500 m, there is a large
 3 region above the depth of 1000 m where a small amount of liquid CO₂ coexists with gaseous CO₂.
 4 This two-phase CO₂ region disappears near the top of the well (<100 m) and the continuous
 5 evaporation of liquid CO₂ at that depth is responsible for the super-cooled condition of the well
 6 above this point (the actual temperature could be lower than what is shown considering the 3 °C
 7 lower-temperature limitation of the simulator).



8 Figure 5. Evolution of profiles of (a) aqueous phase saturation, (b) pressure, (c) temperature, and (d) the ratio of gaseous CO₂ saturation within
 9 CO₂-rich phase ($S_g^* = S_g/(S_g+S_L)$, S_g is the saturation of gaseous CO₂ while S_L is the saturation of liquid or super-critical CO₂) in the well for
 10 the 8 mm gap-aperture case. The white region indicates no free CO₂ phase exists (i.e., $S_a = 1$).

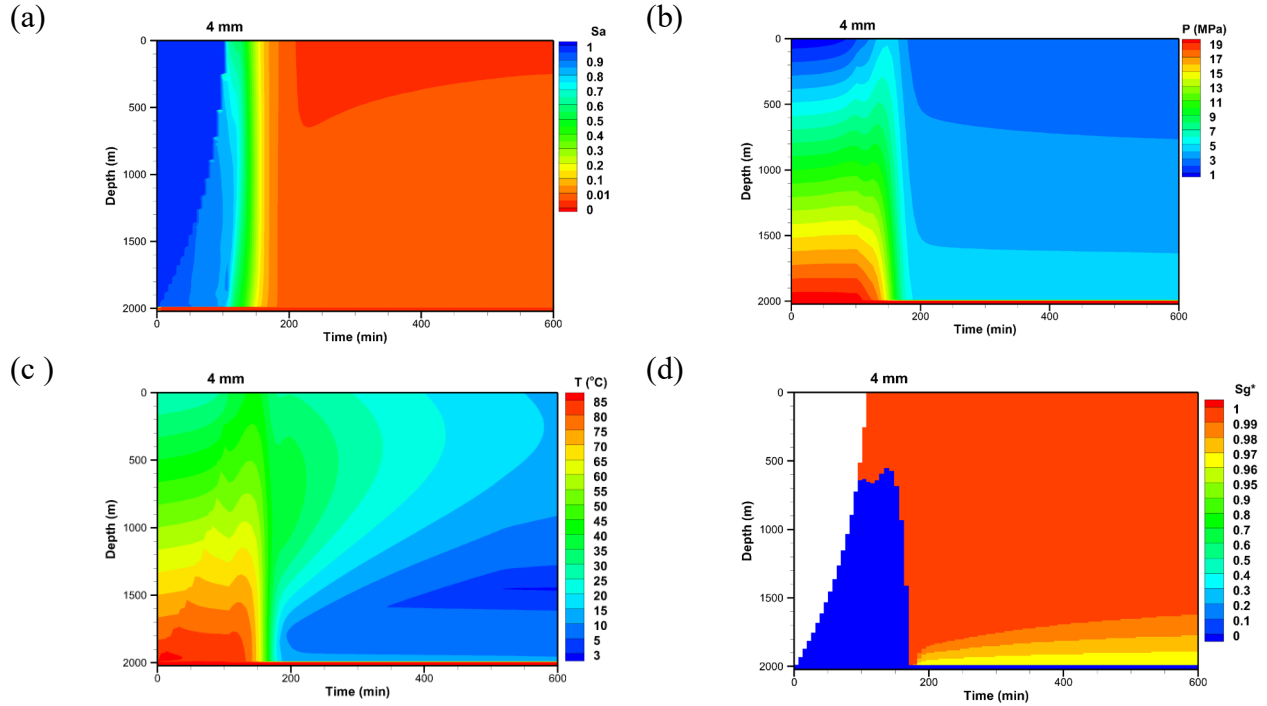
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1 Figure 6. Simulated (a) pressure at well top, (b) pressure right above plug, (c) temperature at well top, and (d) temperature right above plug for
 2 different gap apertures.

3 If the 8 mm gap aperture is cut in half to 4 mm, the leaking gas is still able to flush the water out
 4 of the well to make a very dry well although it takes about 30 min longer time to do so (Figure 7a).
 5 The pressure drop after the water eruption is more severe for the 4 mm gap than for the 8 mm gap
 6 (Figure 7b) because of the larger resistance to leakage flow through the smaller (4 mm) aperture.
 7 The pressure right above the plug is reduced to 4.5 MPa while the well top pressure drops to 2.2
 8 MPa (Figure 6b, 6a), and pressures at both of these locations are significantly lower than those in
 9 the 8 mm case. Although the evolution of the temperature profile before the water eruption for the
 10 4 mm gap has a similar pattern to that for the 8 mm gap, differences are quite large overall between
 11 the two cases (Figure 6c and 7c). Whereas the coldest point in the 8 mm case is located at the well
 12 top, the coldest point in the 4 mm case is located at about a depth of 1500 m at 600 min, near the
 13 upper margin of the two-phase CO₂ region (Figure 7d). By close inspection of the S_g^* ($S_g^* =$
 14 $S_g/(S_g+S_l)$) plot (not shown here), we observed that CO₂ evolves from supercritical conditions to
 15 enter a two-phase region before reaching the top of the plug in the 4 mm gap-aperture case. The
 16 CO₂ temperature continues to decrease as it flows upward because of the drop in pressure (along
 17 the phase line). After CO₂ passes the upper margin of the two-phase region, expansion cooling
 18 causes further drop in gas temperature. As gaseous CO₂ migrates farther upward, the heat from the
 19 surrounding formations is able to overcome the expansion cooling resulting in a gradual increase
 20 in temperature as CO₂ flows up to the well top. However, this formation-to-well heating effect is
 21 weakening with time so that the cold region shown in Figure 7c gradually expands upward and
 22 reaches the well top at about 2400 min (not shown here) and the well top temperature is eventually

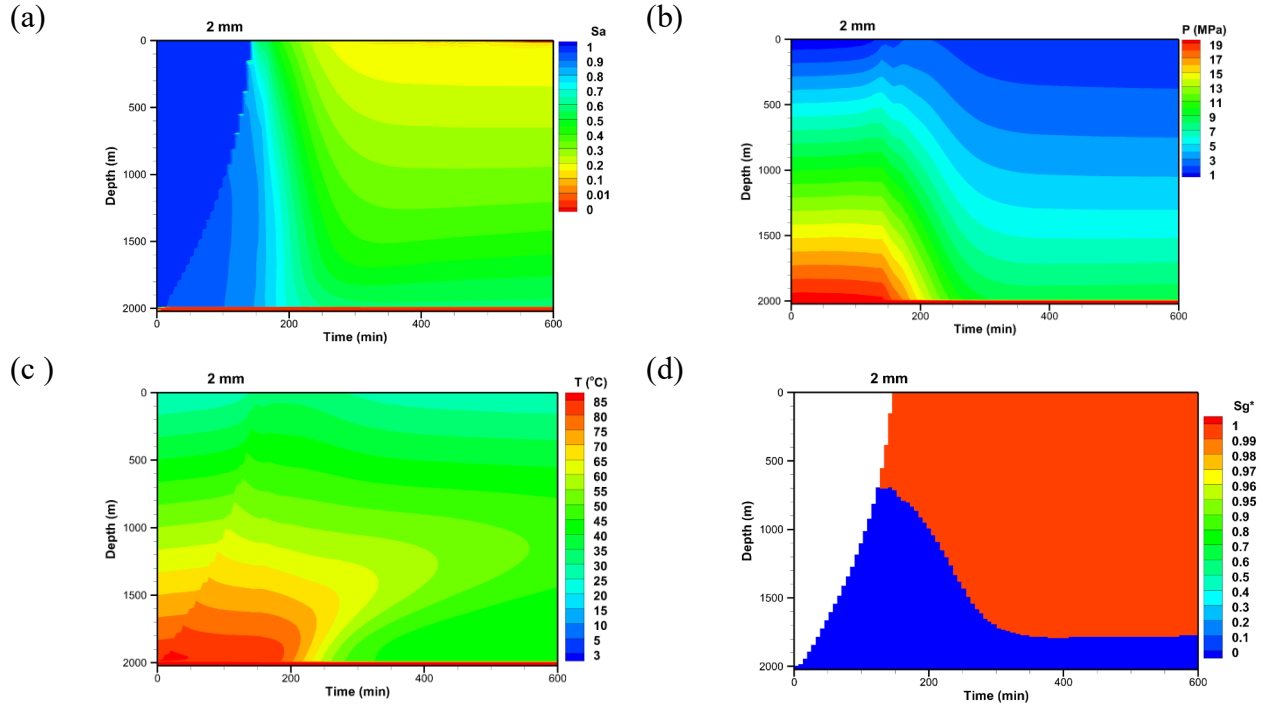
- 1 approaching 3°C (Figure 6c) although the temperature right above the plug is stabilized at 10 °C
- 2 after 200 min (Figure 6d).



1 Figure 7. Evolution of profiles of (a) aqueous phase saturation, (b) pressure, (c) temperature, and (d) the ratio of gaseous CO₂ saturation within
 2 CO₂-rich phase ($Sg^* = Sg/(Sg+S_L)$, Sg is the saturation of gaseous CO₂ while S_L is the saturation of liquid or super-critical CO₂) in the well for
 3 the 4 mm case. The white region indicates no free CO₂ phase exists (i.e., $Sa = 1$).

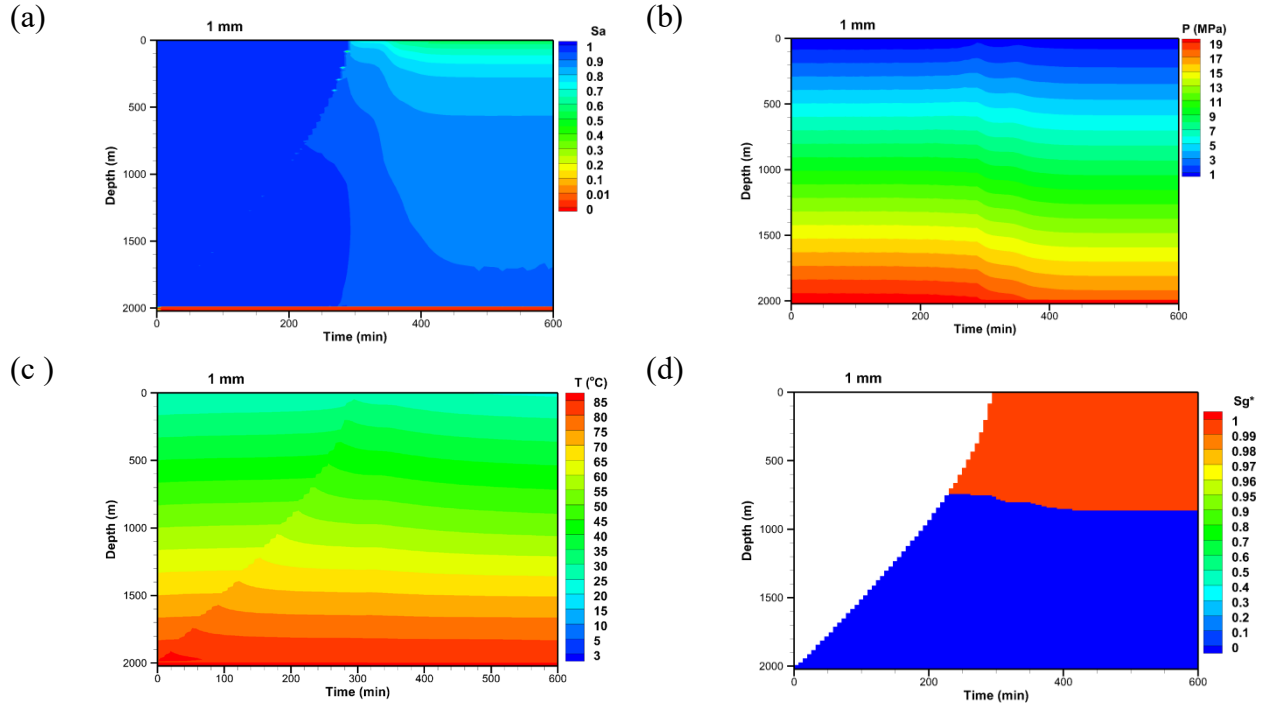
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5 For the 2 mm gap aperture, the leaking gas is not able to lift all of the water above the plug out of
 6 well, unlike in the cases with larger aperture (e.g., 4 and 8 mm). As shown in Figure 8a, significant
 7 aqueous phase still exists in the well after the water eruption around 200 min. Such phase
 8 conditions are reflected in the pressure profiles as shown in Figure 8b. The aqueous phase (denser
 9 than CO₂) increases the gravitational pressure gradient along the well. As a result, although the
 10 well top pressure is about 1.3 MPa in the 2 mm case, much smaller than 2.2 MPa in 4 mm case or
 11 3.6 MPa in 8 mm case (Figure 6a), the pressure right above the plug for the 2 mm gap-aperture
 12 case is around 9 MPa (Figure 6b), a level similar to that in 8 mm case, and is much higher than
 13 that in 4 mm case (~4.5 MPa). While the well-top pressure is mainly controlled by the final leakage
 14 rate, the pressure right above the plug is a result of two interacting factors, the pressure drop
 15 through the plug corresponding to the given flow rate from below and the gravity force asserted
 16 by the water column in the well above the plug. The significant aqueous phase in the well also
 17 alters the temperature profile in the 2 mm case (Figure 8c). Although the temperature right above
 18 the plug drops to below 50 °C due to expansion cooling (Figure 6d), similar to the 8 mm case, the
 19 smaller CO₂-rich aqueous phase saturation (which is under expansion cooling) and smaller leakage
 20 rate in the 2 mm case make it possible for the upward flowing fluid to be heated up by the
 21 surrounding formations especially in the region below 1000 m (Figure 8c). As a result, the well
 22 top temperature in the 2 mm case is close to the ambient temperature although it is slowly
 23 decreasing with time (Figure 6c) as the surrounding formations gradually cool. Different from the
 24 4 mm case, no two-phase CO₂ regions occur in the 2 mm case (Figure 8d). Instead, the CO₂
 25 transitions from supercritical into gaseous phase at 1800 m depth.



1 Figure 8. Evolution of profiles of (a) aqueous phase saturation, (b) pressure, (c) temperature, and (d) the ratio of gaseous CO₂ saturation within
 2 CO₂-rich phase ($Sg^* = Sg/(Sg+S_L)$, Sg is the saturation of gaseous CO₂ while S_L is the saturation of liquid or super-critical CO₂) in the well for
 3 the 2 mm case. The white region indicates no free CO₂ phase exists (i.e., $Sa = 1$).

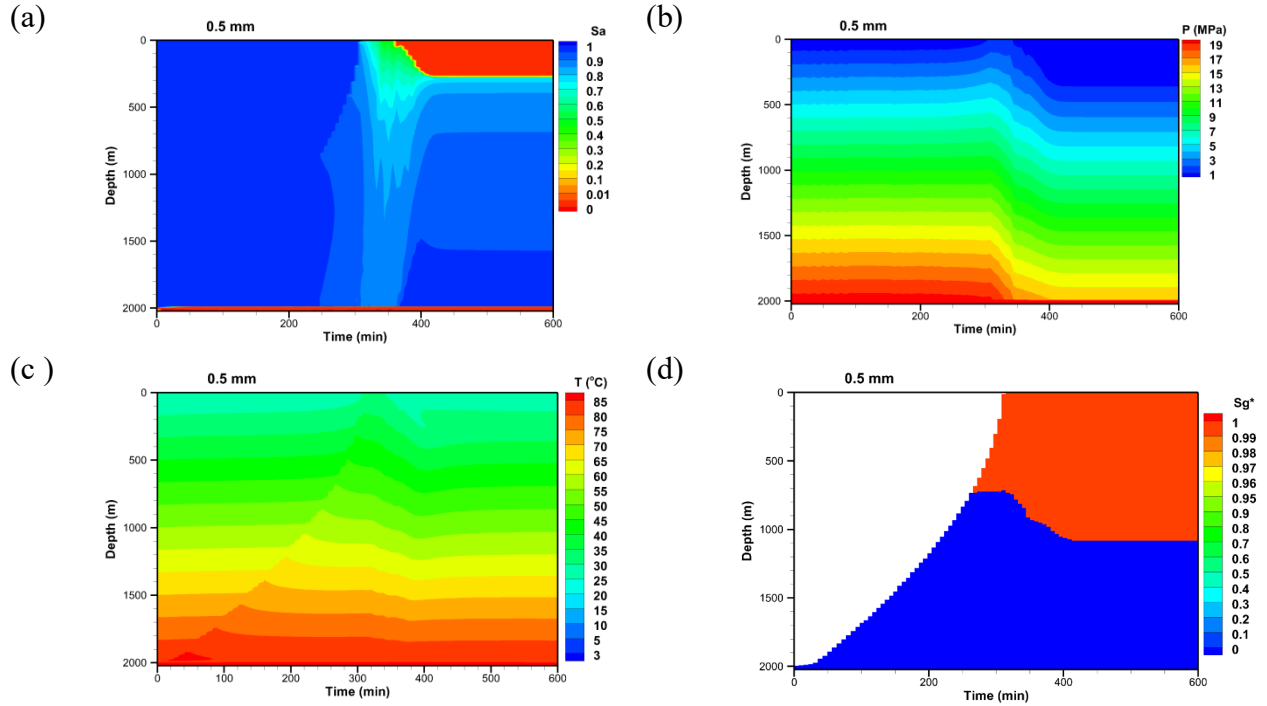
4 As the fracture aperture reduces to 1 mm, the resistance to leakage through the gap increases. As
 5 a result, the leakage rate of CO₂-rich phase only reaches about 0.42 kg/s (Figure 3b and 3d).
 6 Although there are two small peaks of aqueous phase flow at the well top associated with the
 7 breakthrough of CO₂-rich phase (Figure 3a and 3c), the leaking CO₂ is just not able to lift much
 8 water out of the well resulting in a very wet well (high aqueous phase saturation) in the 1 mm case
 9 (Figure 9a). Consequently, the pressure gradient in the well (the section above the plug) is only
 10 slightly increased from the ambient hydrostatic pressure gradient due to leaking CO₂ (Figure 9b).
 11 The pressure right above the plug only drops by 1.8 MPa to 17.6 MPa (Figure 6b) while the well-
 12 top pressure is slightly below 0.5 MPa (Figure 6a). The temperature profile changes little except
 13 for the small peak that occurs associated with the initial rise of CO₂-rich phase (Figure 9c). The
 14 CO₂ converts from supercritical into gaseous at a depth of 850 m (Figure 9d) which is about 950
 15 m shallower than that in the 2 mm case.



1 Figure 9. Evolution of profiles of (a) aqueous phase saturation, (b) pressure, (c) temperature, and (d) the ratio of gaseous CO₂ saturation within
 2 CO₂-rich phase ($S_g^* = S_g / (S_g + S_L)$, S_g is the saturation of gaseous CO₂ while S_L is the saturation of liquid or super-critical CO₂) in the well of 1
 3 mm case. The white region indicates no free CO₂ phase exists (i.e., $S_a = 1$).

4

5 As gap aperture further reduces to 0.5 mm (five times the 100 micron roughness of the gap walls),
 6 the steady-state leakage rate of the CO₂-rich phase is only 0.15 kg/s (Figure 3b and 3d), which can
 7 barely lift any water out of the well top after the early oscillatory period ends as shown in Figure
 8 3c or 4b. However, the CO₂ bubbles seem to accumulate to a significant level (Figure 10a) to cause
 9 an eruption of aqueous phase larger than that in the 1 mm case (Figure 3a). After that, a stable
 10 water table at a depth of 260 m forms implying that the flow becomes a scenario of rising CO₂
 11 bubbles through an almost static water column. This can be seen in Figure 4b where the aqueous
 12 phase flow rate at the well top is zero and at the top of the plug is very small with occasional
 13 downward flow peaks in the 0.5 mm case, which is different from the 1 mm case where a continue
 14 upward aqueous flow exists although at very small magnitude or in a somewhat oscillatory way.
 15 The pressure after early eruption is lower in the 0.5 mm case than that in the 1 mm case (Figure
 16 10b and 9b) although the temperature profiles are very similar (Figure 10c and 9c). The turning
 17 point between gaseous and supercritical CO₂ is located at a depth of 1100 m which is deeper than
 18 that in the 1 mm case but shallower than that in the 2 mm case (Figure 10d, 9d, and 8d).



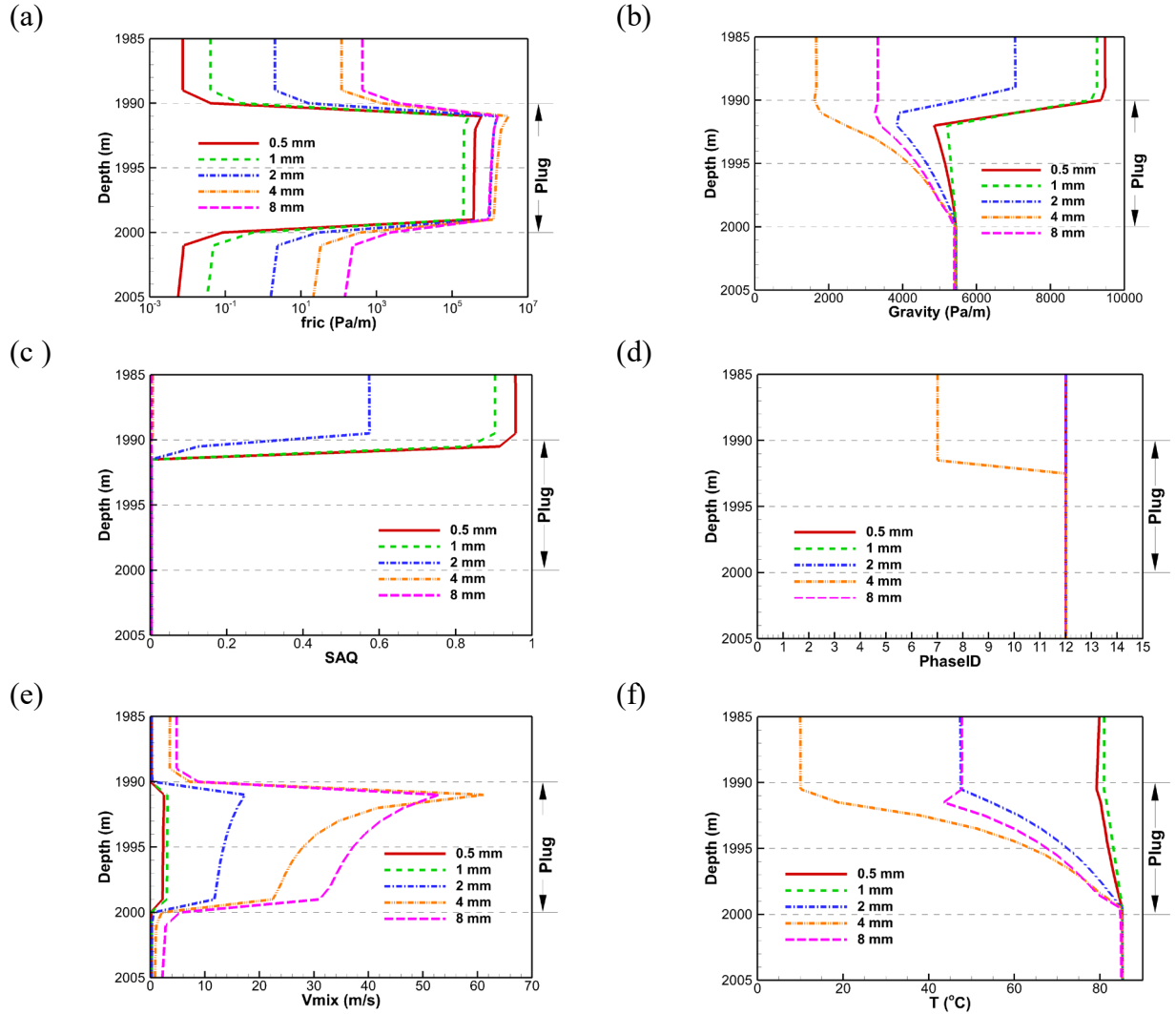
1 Figure 10. Evolution of profiles of (a) aqueous phase saturation, (b) pressure, (c) temperature, and (d) the ratio of gaseous CO₂ saturation within
 2 CO₂-rich phase ($Sg^* = Sg/(Sg+S_L)$, Sg is the saturation of gaseous CO₂ while S_L is the saturation of liquid or super-critical CO₂) in the well of 0.5
 3 mm case. The white region indicates no free CO₂ phase exists (i.e., $S_a = 1$).

4 The gap in the plug is a narrow flow path which is quite different from the open well above and
 5 below the plug from the perspective of flow resistance. We will now inspect the various
 6 components of the pressure loss in the plug gap as compared to those in the open well to capture
 7 the insights of flow dynamics within the plug. As shown in Figure 11, the friction loss is orders of
 8 magnitude higher than the gravity pressure loss through the plug gap whereas the former is often
 9 a fraction of the latter in the well above or below the plug (Figure 11 a and b). In the open-well
 10 section (above or below the plug), the friction loss (Figure 11a) is directly proportional to the
 11 mixture velocity squared (Figure 11e) because the wall roughness is so small (45 microns)
 12 compared to the well diameter (16 cm). However, in the plug gap, because the flow path is very
 13 narrow (0.5-8 mm) compared to the wall roughness (0.1 mm), the larger relative roughness (the
 14 ratio of wall roughness to the size of the flow path) starts to alter the relationship between the
 15 friction loss and the mixture velocity. For example, although the mixture velocity for the 4 mm
 16 gap aperture is smaller than that in the 8 mm case in most of the plug gap (Figure 11e), the friction
 17 loss within the plug in the 4 mm case is significantly larger than that in 8 mm case (Figure 11a,
 18 notice the log scale). Furthermore, even though the mixture velocity within the plug for the 2 mm
 19 gap aperture is about a quarter of that in the 8 mm case, the friction loss within the plug is about
 20 the same in these two cases. As the aperture is reduced more toward the value of the roughness,
 21 although the mixture velocity within the plug in the 1 mm case is slightly larger than that in the
 22 0.5 mm case, the friction loss in the 0.5 mm case is significantly larger than that in the 1 mm case.
 23 In reality, the wall roughness, not to mention the aperture, of a gap between cement and casing or

1 of a fracture in the cement plug may be spatially variable resulting in leakage flow behaviors more
2 complicated than those revealed in these idealized simulations.

3 The gravity pressure loss (Figure 11b) reflects the fluid density changing with depth. Except for
4 the 4 mm case, the CO₂ within the plug remains in supercritical state as it was in the reservoir
5 (Figure 11d). As a result, the gravity pressure loss within the plug increases with the gap aperture
6 in these cases because the total pressure loss is proportional to the fracture aperture in the plug in
7 general. The existence of significant aqueous phase in the upper portion of the plug in the smaller
8 aperture cases (2, 1, and 0.5 mm) greatly increases the density of fluid (water-CO₂ mixture) thereby
9 increasing the gravity pressure loss there. In the 4 mm case, larger friction loss causes the pressure
10 in the upper portion of the plug to drop to subcritical levels so that CO₂ there becomes two-phase
11 (Figure 11d). The transition to gaseous CO₂ greatly reduces the density of the fluid mixture which
12 leads to the smallest gravity pressure loss (Figure 11b) and the largest mixture velocity (Figure
13 11e) in the upper region of the plug gap. The occurrence of two-phase CO₂ also greatly decreases
14 the temperature there in the 4 mm case (Figure 11f). As a result, the temperature at the top of the
15 plug in the 4 mm case decreases to below 10 °C which is about 40 °C below the cases of the 2 mm
16 and 8 mm gap apertures and 70 °C below the 1 mm and 0.5 mm cases.

17



1 Figure 11. Profiles of (a) friction pressure gradient, (b) gravity pressure gradient, (c) aqueous phase saturation, (d) Phase ID (12—supercritical
 2 CO₂-Aqueous, 7—three phases), (e) mixture velocity, and (f) temperature along the plug (1990-2000 m) at 1440 min (1 day).

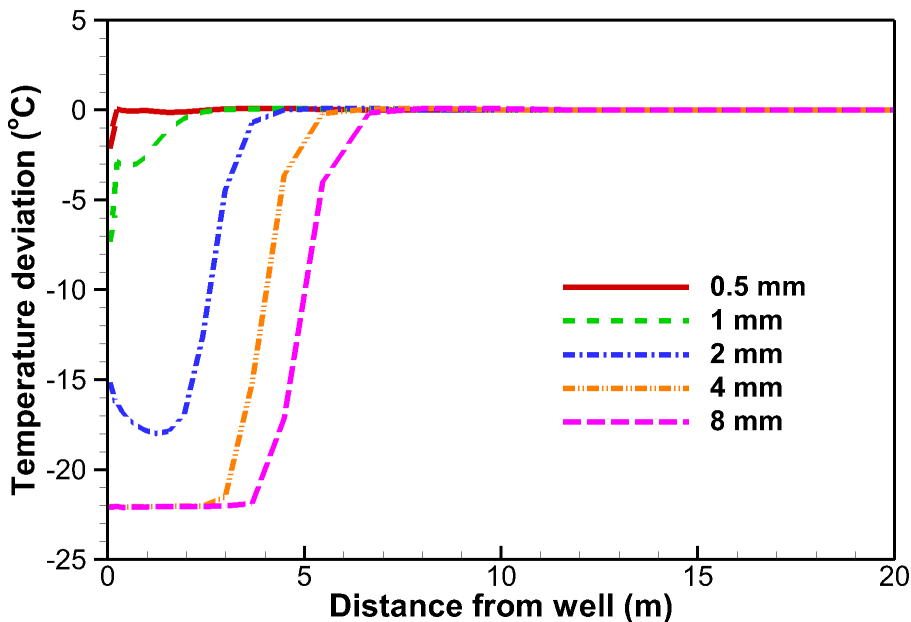
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4 Discussion

5 Discussion of results relative to detection of well leakage

6 The gap between the cement plug and casing, or an equivalent fracture in the plug, is the limiting
 7 feature (bottleneck) for flow of CO₂ leaking up within casing of an abandoned well. In the case of
 8 a relatively large aperture (e.g., 4 or 8 mm), the plug offers little resistance to the leaking CO₂. In
 9 these cases of minimal flow resistance for sudden opening of the gap, the leaking CO₂ is able to
 10 lift the water originally residing in the well above the plug out of the well in a manner of an eruption
 11 (Figure 5a and 7a). After this initial phase of leakage, water plays little role in regulating the
 12 leakage of CO₂ and expansion cooling of CO₂ along the well makes the temperature near the land

1 surface very low, possibly below 3 °C (As shown in Figure 6c, temperature at the top reached the
2 lower limit of the equation of state in our simulator). Such abnormally low temperatures could be
3 a convenient signal of leakage because of the relative ease of measuring temperature over areas of
4 the ground surface. For example, Figure 12 shows the temperature deviation from the ambient
5 temperature in the top (1 m) portion of the soil as a function of horizontal distance from the well
6 at the end of 1 day. As shown in Figure 12, the larger aperture cases (4 and 8 mm) not only have
7 larger temperature drop ($> 20\text{ °C}$) but also a larger anomalously cold region (3-4 m in radius) which
8 provides a promising basis for detecting leaking abandoned wells with soil cover by thermal
9 mapping tools. However, as the aperture decreases, both the cold area and the magnitude of the
10 temperature drop decrease. Especially in the case of 0.5 mm, the maximum temperature drop is
11 about 2 °C and the radius of the cold area is only a fraction of a meter. This is because the CO₂
12 leakage rate is so low in the 0.5 mm case (Figure 3b) that the flow is unable to lift significant water
13 out of the well (Figure 10a). Although the CO₂ bubbles are still undergoing expansion cooling as
14 they slowly migrate upward through the water column, the cooling effects of the limited quantity
15 of CO₂ are not enough to cause a large temperature drop in the soil above the well (Figure 12).
16 The water in the well above the plug becomes an effective barrier for the CO₂ leakage in these
17 small-aperture cases (e.g., 1 and 0.5 mm) by exerting a large pressure on the top side of the plug
18 which greatly reduces the pressure gradient through the plug that drives the upward CO₂ flow.



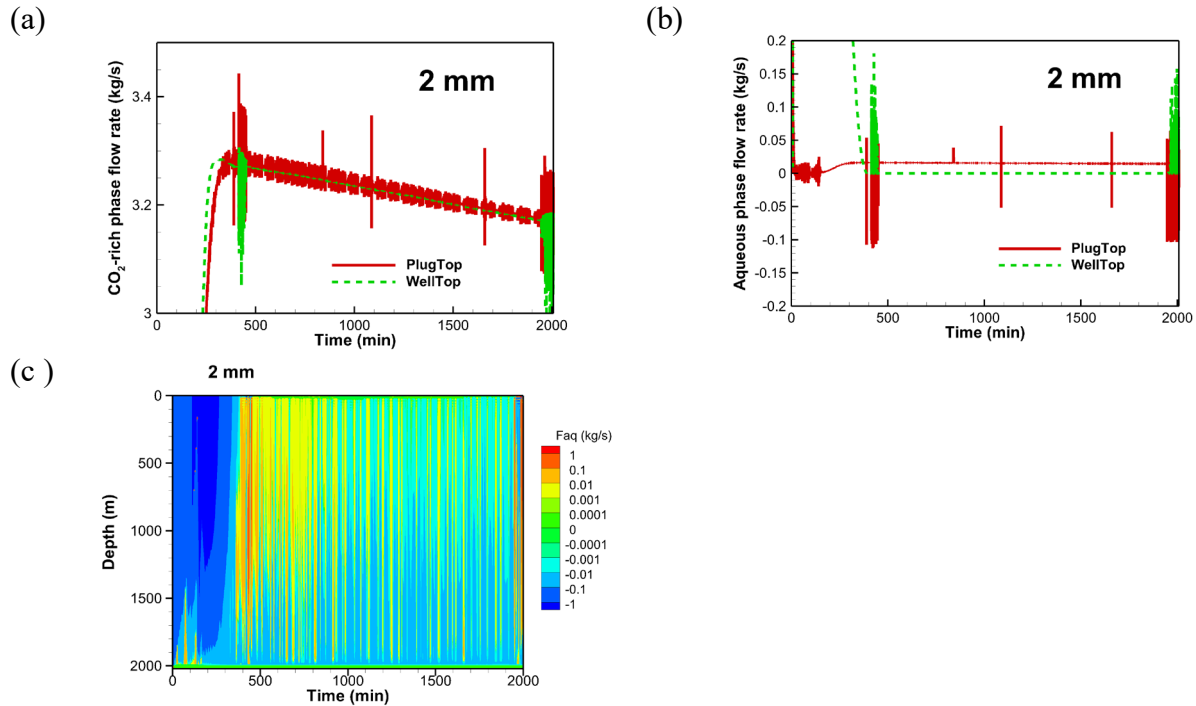
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20 Figure 12. Temperature deviations from the ambient temperature in top soil above the well as a function of horizontal distance from the well
21 center at 1440 min (1 day).

22 The effects of water on the CO₂ leakage become more complicated in the case of the medium-
23 aperture gap (2 mm) because the CO₂ leakage rate is large enough to lift some water out of the
24 well resulting in lower water saturation in the well than the smaller-aperture cases but not a dry

1 well as in larger-aperture cases (Figure 8). As a result, the two-phase interactions between the
2 aqueous phase and the CO₂-rich phase create complicated oscillations in the flow of both the
3 aqueous phase and CO₂-rich phase (Figure 13). These oscillations in flow and temperature at the
4 top of the well may be a useful target for monitoring for well leakage because they may stand out
5 from natural cycles driven by atmospheric pressure, diurnal effects, or precipitation and runoff. As
6 shown in Figure 13, for most of the time the oscillations at the plug top are stronger than those at
7 the well top, except for occasional eruption events (e.g., at around 400 min and 2000 min),
8 implying that the well section above the plug acts as a buffer capable of smoothing out the
9 oscillations. During that period, the water flows upward and downward alternately (Figure 13c)
10 within the well, indicating alternately dominant gas lift (causing upward water flow) and gravity
11 (causing downward water flow) effects. Such alternate upward-downward water flow in the 2 mm
12 case shown in Figure 13c does not occur or becomes less significant after a certain time as we
13 observed in other cases (not shown here). In larger-aperture cases (4 or 8 mm), almost all of the
14 water is lifted out of the well by the leaking gas within a few hundred minutes resulting in a gas-
15 phase dominant flowing well in which the two-phase interaction is minimum (i.e., small amount
16 of condensed water becomes mist dispersed in gas stream). On the other hand, in smaller aperture
17 cases (1 or 0.5 mm), the gas flow becomes bubble flow through an almost static water column
18 after early time in which the magnitude of water flow caused by the bubble flow is very small. In
19 the 1 mm gap-aperture case, there are some oscillations in magnitude of the upward water flow
20 rate at the well top as shown in Figure 4b.

21



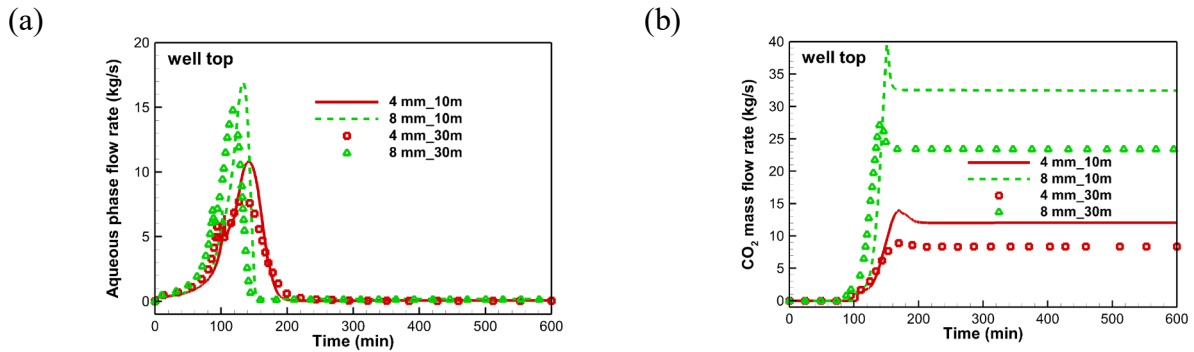
1 Figure 13. Evolution of flow rate in 2 mm case: (a) CO₂-rich phase flow rates through well top and plug top, (b) aqueous phase flow rates through
 2 well top and plug top, (3) contours of aqueous phase flow rate over depth-time space (positive indicating upward flow and negative indicating
 3 downward flow).

4 Assuming an abandoned well can be located, monitoring the pressures in the well may be an
 5 effective way to detect leakage. As shown in Figure 6a and 6b, the well top pressure will increase
 6 and the plug top pressure will decrease significantly in response to leakage past a bridge plug.
 7 The pressure monitoring can detect plug failure even if no CO₂ is released to the atmosphere in
 8 the case that the cap of the abandoned well is an effective seal. Of course, the cost to install such
 9 monitoring system may be high if large number abandoned wells are involved.

10 Discussion of results relative to effects of plug length on leakage

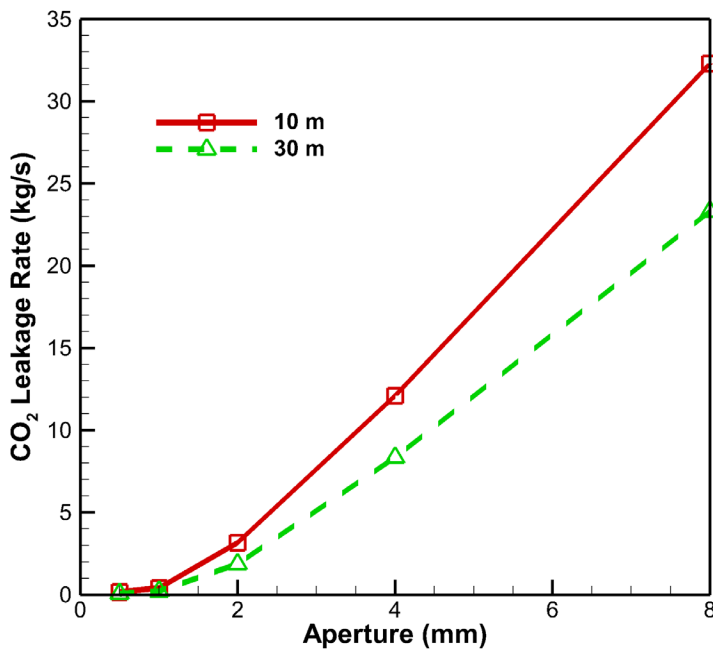
11 In this study, we conceptualize a prototypical abandoned well system with a 10 m-long plug, which
 12 is only about 1/3 of the length required by current U.S. regulation. To understand the effects of the
 13 plug length on the leakage dynamics in a failed abandoned well, we performed another set of
 14 simulations in which the plug length is changed to 30 m but everything else stays the same. As
 15 shown in Figure 14, a longer plug results in smaller leakage rates in both the 8 mm and 4 mm cases
 16 relative to the 10 m-long plug. However, the patterns are similar regardless of plug length. Similar
 17 trends can be seen in smaller aperture cases (not shown here). Furthermore, the leakage rate is
 18 more sensitive to the aperture than to plug length (Figure 15). For example, the final (stable) CO₂
 19 leakage rate in the 8 mm case with 10 m-long plug is about 32.3 kg/s. If the plug length increases
 20 to 30 m (3 times), the CO₂ leakage rate reduces to about 23.3 kg/s, about 72% of the original value.
 21 However, if the aperture reduces to 4 mm (a half) with the same plug length, the CO₂ leakage rate
 22 would reduce to 12.1 kg/s, about 37%. This is because increase of plug length only increases the

1 resistance to the flow linearly whereas decrease of aperture not only increases the friction through
 2 the friction coefficient but also through increase in velocity for the same mass flow rate which
 3 would increase the friction proportional to velocity squared.



4 Figure 14. Comparison of the simulated mass flow rates of aqueous (a) and non-aqueous phase (b) at the wellhead as a function of time for two
 5 big gap apertures with different plug length.

6



7

8 Figure 15. Comparison of the final CO₂ leakage rates as a function of aperture for two plug lengths.

9 **Conclusions**

10 We have used T2Well to simulate the non-Darcy non-isothermal three-phase (aqueous, liquid-
 11 CO₂, and gas-CO₂) flow of CO₂ and brine in a prototypical abandoned well suffering a sudden
 12 failure of a cement plug during the post-injection period at a GCS site. Results show transient

1 leakage rate and signals of pressure, temperature, and saturation at the top of the well as a result
2 of complicated CO₂-water interactions in the open well sections and in the gap or fracture of a
3 bridge plug. The leakage signals and flow rate show strong dependence on gap aperture. The
4 leakage rate increases with the aperture of the fracture in the plug greatly. In larger aperture cases,
5 the water in the well above the plug will be lifted out of the well by the leaking CO₂, resulting in
6 a dry well in which CO₂ flows freely without interference of the aqueous phase. In these cases the
7 CO₂ expansion cooling effect is extremely strong resulting in a significant cold area around the
8 well forms at land surface which implies that thermal mapping could be an effective monitoring
9 technique to detect possible leakage from abandoned wells. While short-lived two-phase CO₂
10 regions occur in the 8 mm gap-aperture case, the two-phase CO₂ region exists consistently at the
11 top of the plug (as well as the nearby section above the plug) in the 4 mm case. The strong cooling
12 due to evaporation of the liquid CO₂ in addition to expansion cooling of gaseous CO₂ in the 4 mm
13 case makes the cold region start at the plug and gradually expand to the land surface. For smaller
14 apertures, both the magnitude of the temperature drop and the size of the cold area at the land
15 surface decrease with aperture because the amount of the leaking CO₂ decreases and water
16 saturation increases. As in the 0.5 mm case, such cooling signals become very weak.

17 During the period with strong interaction between aqueous phase and CO₂-rich phase (usually at
18 early time), the water flow direction can be oscillatory (up and down) at different depths within
19 the well section above the plug, especially in the case of intermediate aperture (e.g., 2 mm) in
20 which case the oscillations never end. In this case, the transient pressure, temperature, and flow
21 rate signals from such a system may stand out from variations arising from natural forcings
22 (barometric pressure, day-night, weather) at the ground surface and provide target strategies for
23 leakage detection monitoring. Furthermore, analysis of the leakage signals may allow diagnosis of
24 the cause and/or source of leakage, characteristics of the flow channel (e.g., its aperture, etc.) that
25 can potentially inform remediation efforts.

26 The results also show that the well top pressure will increase and the plug top pressure will
27 decrease significantly in response to the leakage. Therefore, pressure monitoring in abandoned
28 wells is an effective way to detect potential leakage although deployment of such monitoring
29 system may be costly if large number of wells are involved.

30 ECO2M has a lower limit on temperature and cannot simulate scenarios of water ice conditions or
31 hydrate-forming conditions which may interfere or even block further CO₂ leakage in some cases.
32 Therefore, the leakage behaviors may be very different from those reported here if such conditions
33 occur.

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