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1	Time-Lapse Gravity Monitoring of CO2 Migration Based on Numerical Modeling of a
2	Faulted Storage Complex
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## 18 Abstract

19 In this study, the performance of both surface and borehole time-lapse gravity monitoring to detect  $CO_2$ 20 leakage from a carbon storage site is evaluated. Several hypothetical scenarios of CO<sub>2</sub> migration in a leaky 21 fault, and thief zones at different depths at the Kimberlina site (California, USA) constitute the basis of the 22 approach. The CO<sub>2</sub> displacement is simulated using the TOUGH2 simulator applied to a detailed geological 23 model of the site. The gravity responses to these  $CO_2$  plumes are simulated using forward modeling with 24 sensors at ground surface and in vertical boreholes. Results of inversion on one scenario are also presented. 25 The surface-based gravity responses obtained for the different leakage scenarios demonstrate that leakage 26 can be detected at the surface in all the scenarios but the time to detection is highly variable (10 to 40 years) and dependent on the detection threshold considered. Borehole measurements of the vertical component of 27 28 gravity provide excellent constraints in depth when they are located in proximity of the density anomaly 29 associated with the presence of CO<sub>2</sub>, thus discriminating multiple leaks in different thief zones. Joint 30 inversion of surface and borehole data can bring valuable information of the occurrence of leakages and 31 their importance by providing a reasonable estimate of mass of displaced fluids. This study demonstrates 32 the importance of combining multiphase flow simulations with gravity modeling in order to define if and

33 when gravity monitoring would be applicable at a given storage site.

## 34 **1. Introduction**

35 Leakage of CO<sub>2</sub> from storage reservoirs has been identified in previous studies as one of the potential obstacles to large-scale Carbon Capture and Storage (CCS) deployment (Hepple and Benson, 2005; Herzog, 36 37 2011). Impacts of unexpected CO<sub>2</sub> migration into groundwater resources (Birkholzer et al., 2009; Keating 38 et al., 2013; Kim et al., 2018; Lions et al., 2014), risk management (Anderson, 2017; White and Foxall, 39 2016), economic issues and liability of CO<sub>2</sub> leakage (Bielicki et al., 2016; Bielicki et al., 2014; Pollak et al., 2013) are all topics related to  $CO_2$  leakage discussed in the recent literature. The ability to detect and 40 41 quantify these potential leaks using geophysical or geochemical monitoring methods remains nonetheless 42 challenging. Continuous advancements in instrumentations have demonstrated that time-lapse gravity is a 43 viable method for effective reservoir monitoring but only a limited number of studies focus on the feasibility 44 and effectiveness of this method to detect unforeseen upward CO<sub>2</sub> migration out of the reservoir. This study 45 is motivated by the need to understand the limits and expectations of the method for leak detection, and 46 ultimately to understand requirements, both spatial and temporal, for time-lapse gravity surveys design for

47 efficient monitoring of leakage.

48 The concern of  $CO_2$  leakage out of a reservoir is intrinsically related to  $CO_2$  properties. Due to  $CO_2$ 49 buoyancy, any manmade or natural pathways can lead to upward migration of CO<sub>2</sub> and potentially a loss of 50 CO<sub>2</sub> containment in a storage complex (IPCC, 2005). Preferential leakage pathways may therefore include 51 poorly plugged wellbores (Jordan et al., 2015), or permeable structural features, such as geological faults 52 or fractures (Lewicki et al., 2006). Because hydraulic properties of those leakage pathways may change with time in response to changes in rock stress, fluid pressure or fluid temperature (Nicol et al., 2017), CO<sub>2</sub> 53 migration may occur during or after the injection phase of a project. The risks associated with CO<sub>2</sub> leakage 54 55 include accumulation of  $CO_2$  in overlying geological formations with a potential deterioration of 56 groundwater resources (Keating et al., 2010; Lawter et al., 2016; Yang et al., 2014a; Yang et al., 2014b) or interference with other subsurface activities (Bielicki et al., 2014). If not partially diverted sideways into 57 intermediate aquifers in "secondary trappings" (Bielicki et al., 2016), the upward migrating  $CO_2$  could 58 59 eventually be discharged to the atmosphere, resulting in a failure in reducing greenhouse gas emissions, 60 and potentially present hazards to human health and the environment (Anderson, 2017; Deng et al., 2017).

61 CO<sub>2</sub> injection in a storage complex and CO<sub>2</sub> and brine leakage drive changes in subsurface properties,

62 including changes in pressure,  $CO_2$  saturation, pH, or total dissolved solids. A broad range technologies can

be deployed at storage sites to track these changes (Chadwick et al., 2009; Furre et al., 2017; Hannis et al.,

64 2017; Harbert et al., 2016) with three primary monitoring objectives: containment assurance, conformance assurance and contingency monitoring. The role of containment monitoring is to demonstrate that injected 65 66  $CO_2$  is effectively and safely contained within the storage complex during and long after the injection phase 67 of the project and must provide accurate estimates of the mass of CO<sub>2</sub> stored. Conformance monitoring is intended to compare the forecast from modeling to the observed behavior of  $CO_2$  in the storage complex. 68 This comparison is used for calibration and prediction with the aim of demonstrating that the long-term 69 predictions are valid. A third category of monitoring, contingency monitoring, is required in the event of 70 71 observations from the existing monitoring network that indicate that the storage complex has failed, leading 72 to  $CO_2$  migration through the overburden and potentially into the atmosphere or the ocean for offshore 73 carbon storage reservoirs. Compliance to these CO<sub>2</sub> storage performance criteria is captured in regulatory 74 and policy frameworks (e.g., European Union CCS Directive, 2009; U.S. EPA, 2010) and seeks to minimize 75 the risk of leakage from the storage complex and to quantify and mitigate any unforeseen leaks that arise.

Several studies related to the evaluation of monitoring technologies for  $CO_2$  leakage focused on monitoring technologies at the surface or in the shallow subsurface, such as soil-gas, atmospheric, microbiology monitoring, fluid pressure measurements or geochemical sampling (Romanak et al., 2012). Any unforeseen signals from these monitoring techniques would indicate that  $CO_2$  has reached or is about to reach the surface. Although near-surface monitoring is essential for public acceptance, liability, and accounting purposes (Feitz et al., 2014), early detection of  $CO_2$  migration from the storage reservoir is critical for contingency actions in order to avoid potential adverse impacts.

83 Several studies have focused on the feasibility of leak detection by monitoring for pressure changes in 84 permeable aquifers overlying the storage reservoir (Chabora and Benson, 2009; Jung et al., 2013, 2015; 85 Namhata et al., 2017). These studies have demonstrated the effectiveness of downhole monitoring of 86 pressure changes to detect unexpected migration of  $CO_2$  out of the reservoir; however an important 87 limitation of the method relies on the fact that pressure measurements are point measurements by definition, 88 limiting therefore the volume of investigation. Conversely, deep-subsurface geophysical monitoring 89 technologies, such as 3D seismic or time-lapse gravity, allow the investigation of a large volume in the 90 subsurface. They have been primarily used for tracking CO<sub>2</sub> migration in the storage reservoir to understand 91 reservoir dynamics and therefore help predict future behavior. It is still a challenge for these deep-92 subsurface monitoring technologies to reliably detect changes at a satisfactory resolution in the overburden 93 that can indicate CO<sub>2</sub> movement out of the storage reservoir. Wang et al. (2018) showed that the reduction 94 in noise levels of seismic data is critical to detect supercritical CO<sub>2</sub> leakage in a deep formation. Similarly, 95 numerical studies successfully demonstrated that surface gravity surveys are well adapted for detecting the bulk of the CO<sub>2</sub> plume in the storage reservoir (Gasperikova and Hoversten, 2008; Jacob et al., 2016; 96 97 Krahenbuhl et al., 2011), but are not suitable to reveal small-to-moderate CO<sub>2</sub> accumulations associated 98 with leakage (Jacob et al., 2016).

99 To demonstrate the ability of the gravity monitoring method to detect  $CO_2$  leaks from a storage complex, 100 several hypothetical scenarios of  $CO_2$  injection in a storage reservoir and migration along a leaky fault into thief zones at different depths at the Kimberlina site (California, USA) have been developed for the present 101 study. The CO<sub>2</sub> migration is simulated using the TOUGH2-MP/ECO2N simulator (Pruess, 2004; Zhang et 102 al., 2008), based on a detailed geological model (Wagoner, 2009) and the rock properties presented in the 103 papers by Zhou and Birkholzer (2011) and Wainwright et al. (2013). The responses of gravity to these CO<sub>2</sub> 104 105 plumes are simulated using a forward modeling approach with instrumentation at ground surface and in vertical boreholes. Results of inversion on one scenario are also presented to illustrate the potential of the 106 107 method in estimating the mass of leaked CO<sub>2</sub>.

## 108 2. Gravity method: A well-known and still promising method

## 109 **2.1 Monitoring of CCS site with time-lapse gravity surveys**

110 Injection of  $CO_2$  in a reservoir induces fluid displacement and changes in saturation that lead to a mass redistribution in the subsurface. Because the Earth's gravitational field is directly related to the mass 111 distribution, repeated gravity surveys can be used to monitor mass balance changes over time and, in the 112 113 case of carbon storage, fluid migration in the subsurface associated with CO<sub>2</sub> injection. The technique consists of measuring the downward acceleration of gravity (gz) at a series of specific locations using high-114 115 precision gravimeters and repeating the measurements at defined times, with the aim of assessing the 116 changes in gravity between measurements. Gravity measurements are made either at the ground surface or in boreholes. 117

- 118 Land-based gravity surveys can commonly achieve micro-Gal (µGal) accuracy with measurements repeatability as low as 3 µGal (Krahenbuhl et al., 2011; Van Camp et al., 2017). Borehole gravimeters like 119 Gravilog<sup>TM</sup> (Nind et al., 2013) can operate in small diameter boreholes that deviate from vertical by up to 120 121 ~60°. Emerging three-axis microgravity technology microelectromechanical system (MEMS) gravimeter and subsequent modeling studies indicate that valuable direction/azimuthal information could also be 122 123 recovered for reservoir surveillance although no actual field experiment has been implemented (Lofts et al., 2019). As highlighted in Krahenbuhl and Li (2012), these continuous advancements in both applications 124 125 and in instrumentation demonstrate that the gravity method is transitioning from a traditional exploration tool to a reservoir management and monitoring tool, including for carbon storage. 126
- 127 For instance, a comprehensive acquisition of gravity measurements to monitor gas production and  $CO_2$ 128 injection as part of a time-lapse gravity strategy occurred in 2002, on the offshore site of Sleipner in the 129 Norwegian North Sea (Nooner et al., 2007). This initial survey was followed by repeat surveys in 2005, 2009 and 2013 (Alnes et al., 2011; Furre et al., 2017). Although the implementation of gravity surveys 130 131 offshore was technically challenging (e.g., noise, establishing a benchmark height, etc.), the interpretation 132 of time-lapse gravity data in combination with seismic data provided a unique dataset, leading to the 133 determination of  $CO_2$  density and supporting the notion that the gravity method is well suited for 134 conformance monitoring. The first time-lapse gravity survey using a borehole gravimeter applied to a  $CO_2$ storage site was conducted at the Cranfield site, Mississippi, as part of the Southeast Partnership test 135 136 (Dodds, et al., 2013). The results showed a significant decrease in density contrast following the injection, 137 consistent with the CO<sub>2</sub> locations predicted from reservoir simulations.
- 138 Fabriol et al. (2011), Gasperikova and Hoversten (2008), Jacob et al. (2016), and Krahenbuhl et al. (2011)
- 139 numerically assessed the performance of the gravity method for monitoring carbon storage sites and
- 140 discussed the benefits and limitations of using time-lapse gravity surveys. Benefits include the possibility
- 141 to recover, relatively easily, the mass of stored  $CO_2$  at a cost that is much less than cost-prohibitive seismic 142 methods. Limitations include the inadequately low depth resolution for surface surveys, the limited density
- 142 includes. Elimitations include the inadequately low depth resolution for surface surveys, the innited density 143 contrast that may exist in some formations due to the presence of multiple fluids (e.g., Sleipner), or due to
- the depth of injection. More recently, Wilkinson et al. (2017) also using a numerical modeling approach,
- demonstrated that a gravity anomaly due to leakage from a deep reservoir could be detected from the surface
- 146 provided that there is an accumulation of  $CO_2$  in a shallow aquifer.
- 147 Additionally, gravity being by essence sensitive to the mass distribution in the subsurface, any natural or
- 148 manmade phenomena leading to a redistribution of mass contributes to the overall gravity response
- 149 observed during time-lapse gravity surveys. The discrimination between other sources contributing to the
- 150 gravity response at ground surface, such as seasonal or long-term temporal changes in groundwater mass,
- 151 or the elevation changes at the survey stations, must also be taken into considerations. The contribution
- 152 from the near-surface hydrologic phenomena are highly variable and site-specific but they can be spatially
- 153 correlated and controlled by topography (Hare et al., 1999) and can be filtered or numerical modeling of

154 their effects can be attempted. The variation of stations elevation between two consecutive surveys is 155 another source of important gravity anomaly because the elevation of the instrument affects gravity measurements (0.3086 mGal/m). At large scale these variations can be either positive (uplift) due for 156 157 example to the poroelastic effect of  $CO_2$  plume emplaced at shallow depth or negative (subsidence) like the 158 one induced by groundwater pumping being faster than aquifer recharge. All these effects can be corrected 159 by measuring accurately the elevation at each gravity station using differential Ground Positioning System 160 (DGPS) which provides vertical position accuracy at the centimeter level (equivalent to a 3  $\mu$ Gal accuracy 161 for the gravity measurement).

#### 162 **2.2 Density contrast: Key parameter of time-lapse gravity monitoring**

The performance of the gravity method applied at CCS sites relies on the density contrast observed over 163 164 time and associated with the injection of  $CO_2$  that displaces initial fluids. The density of  $CO_2$  varies significantly with pressure and temperature. At atmospheric conditions,  $CO_2$  is a low-density gas. Under 165 166 typical operational conditions encountered at CS sites, CO<sub>2</sub> is injected as a liquid and reaches a supercritical state at pressures greater than 7.39 MPa and temperatures higher than 31.1 °C. These conditions are 167 generally met at a depth greater than 800 m but the exact depth is variable and directly related to the 168 169 geothermal and pore pressure gradient existing at a given site. Because  $CO_2$  is less dense than the in-situ fluids,  $CO_2$  injection results in a bulk density decrease over time, as  $CO_2$  partially or totally displaces brine 170 171 in the pore space. In the event of the existence of a pathway in the impermeable cap rock (e.g., leaky wells, 172 fractures, etc.), buoyant CO<sub>2</sub> migrates to the shallower formations, and may undergo a phase transition from 173 supercritical phase to gaseous phase (Figure 1). When buoyed to shallow formations, its density will 174 significantly decrease, and its volume become much larger. These property changes are the key for 175 considering time-lapse gravity surveys as a valuable monitoring tool with increased likelihood of detecting 176 large volumes of low-density fluid approaching the surface.

177 The goal of time-lapse gravity monitoring at storage sites is to determine temporal gravity anomalies related 178 to the injection of CO<sub>2</sub> and exclusively associated with the redistribution of fluids (i.e., CO<sub>2</sub> and brine) in 179 the pore space. Gravity measurements are performed exactly at the same spatial positions in each individual 180 survey. Corrections typically depending on the location at the surface of the Earth remain constant over 181 time and *ipso facto* accounted in time-lapse processing (Davis et al., 2008). Assuming that porosity changes 182 are negligible over time, the bulk density change  $\Delta \rho$  between two time steps within a saline formation, such 183 as the Vedder sandstone considered for the simulations at the Kimberlina site (see section 3), is only 184 dependent on the change in fluid density (i.e., CO<sub>2</sub> and brine) and can be expressed as:

185 
$$\Delta \rho = \Delta S_{CO_2} \phi (\rho_{CO_2} - \rho_{brine}) \tag{1}$$

where  $\Delta S_{CO_2}$  is the change in CO<sub>2</sub> saturation,  $\phi$  is the porosity,  $\rho_{CO_2}$  is the CO<sub>2</sub> density and  $\rho_{brine}$  is the 186 brine density (Eiken et al., 2008; Jacob et al., 2016). This density change directly influences gravity 187 188 variations. As stated previously, equation 1 is based on the assumption that porosity changes caused by 189  $CO_2$  injection are negligible. Kabirzadeh et al. (2017) studied the effect of porosity variations in the 190 reservoir and their impact on the gravity response, but unless important deformations of the ground surface 191 are observed (on the order of tens of centimeters), this effect seems to be very limited. As other potential 192 field methods, gravity is inversely proportional to the square of the distance between the source and the 193 observation station. Downhole gravity measurements being closer to the sources present a signal larger than 194 at the surface and can potentially detect much smaller changes in the subsurface mass distribution than 195 surface measurements.



197 Figure 1. Brine Density (blue) and CO<sub>2</sub> density (pink) as a function of depth at the Kimberlina site. Geothermal gradient is 26.8

198 °C/km, average surface temperature is 21.8°C. The salinity gradient is very low at 6.7 ppm/m and geothermal gradient is high,

199 which explains why the density of brine slightly decreases with depth. Colored area represents the increasing density contrast as

200 *depth decreases, enhancing the potential for detection of leakage using the gravity method.* 

#### **3. Modeling CO<sub>2</sub> injection and leakage at Kimberlina**

#### 202 **3.1 Geological setting**

203 The performance of time-lapse gravity monitoring is evaluated for a number of CO<sub>2</sub> leakage scenarios 204 developed on a hypothetical reservoir-scale model initially established for the Kimberlina storage complex 205 (Zhou and Birkholzer, 2011). The Kimberlina site is located in the southern San Joaquin Valley in 206 California between the Sierra Nevada Mountains to the east and the Coast Ranges to the west (Figure 2). 207 The southern part of the San Joaquin Valley is filled by more than 7000 m of Tertiary marine and non-208 marine sediments. The targeted storage formation is the Vedder Formation, a large permeable sandstone 209 formed by marine and coastal marine sediments. Other permeable formations include the Olcese Formation, 210 the Santa Margarita Formation and the Etchegoin Formation, which are three sandstone formations located 211 above the reservoir. Several thick sealing shale units overlie the Vedder Formation, including the Freeman-Fruitvale shale, the Round Mountain shale and the Macoma shale. The stratigraphy was thus considered of 212 213 particular interest to safe storage of large quantities of  $CO_2$ . This is counterbalanced by the existence of 214 numerous faults in this part of the basin, such as the Pond-Poso-Creek fault zone, which adds structural 215 complexities and operational risks as CO<sub>2</sub> migrates through the reservoir. The Pond-Poso Creek fault zone 216 is part of a northwesterly-striking normal faulting system, dipping to the southwest at 50 to 70 degrees 217 (Wagoner, 2009). This area also includes numerous wells, and well leakage is also a risk at this site but this 218 possible leakage pathway is beyond the scope of this paper.

219 Based on the initial large geological model and flow model developed by Zhou and Birkholzer, (2011), a

220 25-layer submodel (38 km  $\times$  38 km), referred to as the Kimberlina 2 model, was developed for this study

with a focus on the Vedder Sandstone near the Pond-Poso-Creek fault. The Vedder top updips northeast at

222 7°. The model was rotated so that the northern part of the fault aligns with X-Y direction. The Kimberlina

223 2 model was then used to simulate CO<sub>2</sub> storage in the Vedder Sandstone and hypothetical scenarios of

subsequent leakage through the fault into the three permeable sandstone formations identified above and referred to now as thief zones (Figure 3). These simulated three dimensions (3D)  $CO_2$  plumes were then used to calculate the vertical component of gravity.



227

Figure 2. Location of the Kimberlina Project in the San Joaquin Valley (a). The Pond-Poso-Creek fault System bounds the storage
 complex on the east. (b) The model was rotated and subsequently used to conduct fluid flow simulations with TOUGH2-MP. The
 CO<sub>2</sub> saturation 40 years after the beginning of the injection is shown.



Figure 3. Conceptual cross-section of the southern part of the San Joaquin Valley showing potential CO<sub>2</sub> leakage pathways
modeled in the hypothetical scenarios. The scenarios used for the simulations consist of CO<sub>2</sub> injection into the injection zone and
CO<sub>2</sub> leaked through the Pond-Poso-Creek fault into up to three thief zones: Olcese Formation (thief zone 1), Santa Margarita
Formation (thief zone2), and Etchegoin Formation (thief zone 3). These formations are dipping and thus depth ranges are given
instead of single values.

#### 237 **3.2 Model parameters**

238 The injection of  $CO_2$  into the deep Vedder Formation was simulated at a rate of 2.5 million metric tons (Mt) of CO<sub>2</sub> per year for 60 years, followed by a 140-year post-injection monitoring period. All the fluid 239 flow simulations were performed with TOUGH2-MP/ECO2N, the massively parallel version of the 240 241 TOUGH2 code (Zhang et al., 2008) to predict the dynamic CO<sub>2</sub> storage in the subsurface. The initial 242 conditions were set with linear geothermal, pore pressure and salinity gradients (26.8 °C/km, 10.5 243 MPa/km and 6.7 ppm/m, respectively). Dissolution of CO<sub>2</sub> into brine is taken into account until 70 years but, due to problems of convergence of the solutions at the front of the plume for the various leakage 244 scenarios, it was not considered for time greater than 70 years. It must be noted though that the 245 246 dissolution rate being very moderated after 70 years, this doesn't impact the results in terms of 247 quantification of the  $CO_2$  free gaseous phase. Table 1 provides additional information about the main 248 parameters used to develop the Kimberlina 2 multi-phase flow model.

Table 1. Parameters used for the Kimberlina 2 model simulations

Model Parameters	
Model dimensions	38 km × 38 km / 25 layers
Number of elements	2 562 357
Study area	$12.5 \text{ km} \times 16 \text{ km} \times 3 \text{ km}$
Initial Conditions	
Surface temperature	21.8 °C
Geothermal gradient	26.8 °C/km
Salinity Gradient	6.7 ppm/m
Hydrostatic Pressure Gradient	10.5 MPa/km
Reservoir Parameters	
Reservoir	Vedder Sandstone
Injection zone depth	~ 2500 m
Reservoir depth	1600 to 3000 m
Reservoir thickness	50 m
Reservoir porosity	26 %
Reservoir permeability	$Kx = Ky = 307 \text{ mD}, Kz = Kx \times 0.2$
Injection Parameters	
Well Location	x = 0, y = 0
$CO_2$ injection rate	2.5 Mt/yr
Injection duration	60 yr
Post-injection duration	140 yr
Total injected CO <sub>2</sub> volume	150 Mt
Thief Zones Parameters	
Olcese permeability	$Kx = Ky = 170 \text{ mD}, Kz = Kx \times 0.1$
Olcese porosity	33.6 %
Santa Margarita permeability	$Kx = Ky = 200 \text{ mD}, Kz = Kx \times 0.1$
Santa Margarita porosity	27.5 %
Etchegoin permeability	$Kx = Ky = 120 \text{ mD}, Kz = Kx \times 0.1$
Etchegoin porosity	32 %

#### 251 **3.3 Leakage scenarios**

252 To perform the assessment of the gravity method for CO<sub>2</sub> leakage detection, the study area focuses on the

253 injection point and the fault, which represents a 12.5 km by 16 km area. A first set of simulations was

designed to track CO<sub>2</sub> plume evolution in the storage formation while the Pond-Poso-Creek fault remains

255 sealing (baseline scenario). Then, changes in the fault permeability through leaky windows were 256 introduced, assuming leakage into up to three thief zones. Only a section of the fault is conductive while

the remainder remains sealing. These conductive sections, or windows, are either termed "Location 1" or

- 258 "Location 2". For each leakage scenario, the changes in the fault permeability occurred at 70 years, 10
- 259 years after the end of the injection. The deepest thief zone considered in these scenarios is the Olcese
- 260 formation, lying between 1100 and 1600 m deep (due to steeply dipping strata). The middle thief zone,
- the Santa Margarita formation, lies between 600 and 1200 m and the shallowest thief zone, the Etchegoin

formation, is located between 150 and 500 m below the ground surface (Figure 3).

263 A total of 7 leakage scenarios are evaluated. The first set of leakage scenarios is for location 1, located 2.9 264 km east from the injection well (Figure 4). The scenarios studied include CO<sub>2</sub> migration into either Olcene or Etchegoin formations or both (Table 2). The sealing formations above the secondary leak are intact, 265 hence no CO<sub>2</sub> comes to the surface. The second set of leakage scenarios is for location 2 located 6 km 266 267 southeast of the injection well (Figure 4). This set includes secondary CO<sub>2</sub> accumulations in one of the three 268 thief zones (Olcese, Santa Margarita or Etchegoin), and in three thief zones simultaneously (Table 2). The 269 masses of leakage considered in these scenarios could seem large (e.g., over 12 Mt of leaked CO<sub>2</sub> after 130 270 years of leakage in the Olcese Formation); however, these scenarios are hypothetical and are being 271 evaluated to assess the effectiveness of gravity monitoring to detection  $CO_2$  into overlying thief zones.

272

273 For each leakage scenario evaluated in this study, the time-dependent  $CO_2$  mass leaked into these zones is 274 plotted in Figure 5, along with the minimum depth reached by the CO<sub>2</sub>. The total CO<sub>2</sub> mass leaked in each thief zone differs. At both leakage locations, a total of over 12 Mt of CO<sub>2</sub> leaks into the Olcese Formation, 275 276 the deepest thief zone. At the locations 1 and 2, about 4 Mt of CO<sub>2</sub> leaked into the Etchegoin Formation, 277 the shallowest thief zone. At the location 2, one scenario considers a leakage of more than 10 Mt of  $CO_2$ 278 into the Santa Margarita Formation, the intermediate thief zone. Two scenarios consider simultaneous 279 leakage. At the location 1, Etchegoin and Olcese formations are the two thief zones active for leaked  $CO_2$ 280 to migrate into, with respective total  $CO_2$  mass leaked of 3.5 and 9.1 Mt. At the location 2, a scenario 281 considered the three thief zones as being simultaneously active with a CO<sub>2</sub> mass leaked of 4.1 Mt in the 282 Olcese formation, 5.4 Mt in the Santa Margarita formation and 4.2 Mt in the Etchegoin formation (Table 283 2). Although  $CO_2$  upward migration is initiated at 70 years for all leakage scenarios, the actual time of arrival of the  $CO_2$  into the respective thief zone(s) is highly dependent on the depth of these leakage 284 intervals. For instance, Figure 5 shows that CO<sub>2</sub> reaches the Olcese and the Santa Maragarita thief zones 285 286 only 2 to 5 years after the beginning of the leak while  $CO_2$  is reaching the shallowest thief zone (i.e., 287 Etchegoin formation), at 100 years, 30 years after the leak was initiated. The mechanism leading to the different time of arrival of the  $CO_2$  into the thief zones is not critical for this study; however, knowing if 288 the gravity method could detect it when  $CO_2$  enters the thief zones is key. 289



Figure 4. a) CO<sub>2</sub> saturation at 160 years resulting from a leak occurring at location 1 in the Etchegoin formation. b) CO<sub>2</sub> saturation
 at 160 years resulting from a leakage occurring at location 2 in the three thief zones

<sup>293</sup> Table 2. Leakage scenarios with thief zones active for leaked CO<sub>2</sub> to migrate into with respective total leaked CO<sub>2</sub> mass in Mt.

Total leaked CO <sub>2</sub> mass (Mt) entering the thief zones						
Scenario	#	Olcese (OL)	Santa Margarita (SM)	Etchegoin (ET)		
Baseline	0	-	-	-		
Location 1						
OL	1.1	12.6				
ET	1.2	-	-	3.7		
OL + ET	1.3	9.1		3.5		
Location 2						
OL	2.1	12.2	-	-		
SM	2.2	-	10.2	-		
ET	2.3	-	-	4.5		
OL + SM + ET	2.4	4.1	5.4	4.2		



296

Figure 5. Evolution of leaked CO<sub>2</sub> mass entering thief zones (bottom) and minimum depth reached by the CO<sub>2</sub> (top) as a function of time for each leakage scenario considered in location 1 (left) and location 2 (right). The dash-dot lines are used for the scenarios involving multiple thief zones, red color is for CO<sub>2</sub> reaching the Olcese Fm, Orange the Santa Margarita Fm and green the Etchegoin Fm.

#### **301 3.4 Simulation results: CO<sub>2</sub> behavior in the subsurface**

#### 302 **3.4.1 Baseline – Non-leakage scenario**

303 The non-leakage scenario simulates the development of the CO<sub>2</sub> plume in the reservoir for the expected 304 conditions of operations and post-injection of the hypothetical Kimberlina CCS site. This scenario 305 constitutes the reference case, or baseline, that will be used to evaluate the difference in gravity response corresponding to CO<sub>2</sub> leakage. In this baseline scenario, the sealing Pond-Poso-Creek fault acts as a 306 307 boundary in the reservoir and leads to a gradual accumulation of CO<sub>2</sub> along this fault. CO<sub>2</sub> reaches the fault 308 about 40 years after the beginning of injection (Figure 6). Because of the updipping stratigraphy of the 309 Vedder Formation and CO<sub>2</sub> buoyancy, CO<sub>2</sub> gradually reaches the shallower parts of the reservoir 310 (approximately 1,500 m deep) laterally along the fault to the southern part of the model domain, with  $CO_2$ 311 saturation ranging from 0.5 to 0.6 (Figure 6). Net density changes within the reservoir are shown in Figure 7 at the end of the injection and at the end of the monitoring period (200 years). The maximum density 312 changes are located at the injection point with values approaching -75 kg/m<sup>3</sup>. The net density changes are 313 314 small in most parts of the reservoir, with values ranging from -20 to -60 kg/m<sup>3</sup> (Figure 7).



Figure 6. Plan view from above of time-dependent CO2 saturation within the storage formation (baseline scenario) at 10, 40, 60

- and 200 years. CO2 accumulates along the sealing fault and migrates to the shallower portion of the dipping reservoir. Locations
- of CO<sub>2</sub> leakage (not active) are indicated for reference.



319

320 *Figure 7. Plan view from above of the net change in density (kg/m<sup>3</sup>) at 60 years (end of injection) and 200 years (end of monitoring)* 

#### 321 **3.4.2 Leakage scenarios at location 1**

In the first set of leakage scenarios (location 1, Table 2),  $CO_2$  migrates and accumulates along the fault and 322 323 toward the shallower parts of the storage formation in a similar way to the baseline scenario. At 70 years, 324 the leaky fault progressively leads to the development of secondary CO<sub>2</sub> plumes in the thief zone(s), either Olcese, Etchegoin or both.  $CO_2$  saturation ranges from 0.3 to 0.5 in the secondary  $CO_2$  plumes, plotted in 325 Figure 8 (top). Although the total leaked  $CO_2$  mass in the Etchegoin formation is smaller (about 2 Mt at 326 327 200 years) than that in the Olcese formation (12.36 Mt at 200 years), the largest extent of the plume is observed in the Etchegoin formation. While CO<sub>2</sub> saturation values are relatively comparable in the two thief 328 329 zones, the net density changes observed are significantly different, reaching a maximum change of about 330 -64 kg/m<sup>3</sup> in the Olcese Formation (Thief zone 1), and -150 kg/m<sup>3</sup> in the Etchegoin Formation (thief zone 331 3). These differences observed in the two formations are directly associated to the change of  $CO_2$  density 332 properties with depth, illustrated in Figure 1.



Figure 8. Plan views from above of  $CO_2$  saturation (top) and net density changes in  $kg/m^3$  (bottom) at 160 years for the three leakage scenarios evaluated at location 1. Only the  $CO_2$  saturation and net density changes associated with leakage into the thief zone(s) are plotted.

### **337 3.4.3** Leakage scenarios at location 2

For the second set of leakage scenarios (location 2, Table 2), a similar  $CO_2$  behavior is observed in the reservoir, with secondary plumes developing either in the Olcese, Santa Margarita, Etchegoin or in all three thief zones (Figure 9). Similar ranges of  $CO_2$  saturation are observed in all three thief zones, with maximum saturation of 0.6 observed in the vicinity of the injection point. The net density changes are however significantly different, with maximum density changes reaching more than -58 kg/m<sup>3</sup> in the Olcese, -92 kg/m<sup>3</sup> in the Santa Margarita and -158 kg/m<sup>3</sup> in the Etchegoin formations.



Figure 9. Plan views from above of CO<sub>2</sub> saturation (top) and net density changes in kg/m<sup>3</sup> (bottom) at 160 years for the four leakage
 scenarios evaluated at location 2. Only the CO<sub>2</sub> saturation and net density changes associated with leakage into the thief zone(s)

348 are plotted

## 349 4. Gravity Forward Modeling

350 GRAV3D v5.0 (UBC-Geophysical Inversion Facility, 2017) was used for carrying out forward modeling

of the vertical component of the gravity response  $(g_z)$  to a 3D volume of density contrast.  $g_z$  is computed using an analytical solution from Haaz (1953), with a calculation based on a collection of rectangular prisms with varying densities.

354 For each leakage scenario, a density model was built based on the outputs of the TOUGH2-MP Kimberlina

- $2 \mod 1$  is a second se
- The model domain was discretized into a 3D orthogonal mesh, with cells of dimensions  $50 \text{ m} \times 50 \text{ m} \times 25$ m. Each cell was given a density anomaly, or density contrast, corresponding to the density difference
- 557 III. Each cell was given a density anomaly, of density contrast, corresponding to the density difference
- between the time step considered and the pre-injection phase (i.e., time = 0 year). A grid of  $12,500 \times 16,000$ m with station spacing of 200 m was used to compute the surface gravity anomaly.
- 360 Threshold values of 4, 7 and 10 µGal are chosen to assess the performance of the gravity method to detect
- $CO_2$  leaks. These values are in the ranges of repeatability level reported at the  $CO_2$  injection site of Sleipner
- 362 (Landrø and Zumberge, 2017), or at Prudhoe Bay (Alaska) for monitoring of water flooding operations
- 363 (Ferguson et al., 2007).

The vertical component of gravity was also calculated in vertical boreholes deployed in the vicinity of the injection point and of the fault in order to assess the performance of the method to detect  $CO_2$  with measurements taken every 20 m.

## 368 5. Forward modeling Results

# 5.1 Using time-lapse gravity for reservoir monitoring: time to detection, frequency of surveys and contribution of borehole measurements

The gravity anomaly associated with the CO<sub>2</sub> migration in the Vedder Formation while the Pond-Poso-371 372 Creek fault remains sealed is calculated using the forward modeling steps described above. The CO<sub>2</sub> plume 373 growth, migration in the dipping reservoir and accumulation along the structural feature can be detected 374 from surface measurements as plotted in Figure 10. The magnitude of the gravity anomaly grows to a maximum of -33 µGal reached at 90 years, 20 years after the leak is initiated. This maximal value is found 375 up dip of the injection point for all time steps. The CO<sub>2</sub> plume reaches the Pond-Poso-Creek fault after 40 376 vears of injection and the  $CO_2$  accumulation along the sealed fault becomes detectable in the gravity 377 378 response at 90 years, with the development of an asymmetrical anomaly, while injection operations are 379 over. Over time, the buoyancy-driven plume migrates into the shallower parts of the reservoir and the 380 associated gravity anomaly magnitude increases. In the baseline scenario, the maximum gravity response 381 occurs at 80 years, with an anomaly of  $-33 \mu$ Gal, up dip of the injection point, corresponding to a net change of density of -90 kg/m<sup>3</sup> in the reservoir. Then the signal magnitude decreases due to the spreading of the 382 plume to southeastern and upper part of the reservoir. 383

384 The time to detection and frequency of gravity surveys can be obtained from the profile of the evolution of 385 the maximum surface gravity anomaly over time (Figure 11). The time to detection of the  $CO_2$  injected in 386 the reservoir was determined for three threshold values (i.e., 4, 7 and 10  $\mu$ Gal) and is illustrated in Figure 387 11 and reported in Table 3. Using a threshold of 4  $\mu$ Gal, the gravity anomaly associated with the CO<sub>2</sub> 388 injected in the reservoir can be detected as soon as 6 years after injection starts (15 Mt of CO<sub>2</sub> injected), compared to 10 and 15 years for thresholds of 7 and 10 µGal respectively (25 and 37.5 Mt of CO<sub>2</sub> injected). 389 390 Additionally, the change of gravity anomaly over time is shown in Figure 11 where a steep gradient of -0.67 µGal/yr occurs during the first 30 years of injection (yellow points and line) and a shallower slope of 391 392 -0.32 µGal/yr (orange line) occurs during the following 30 years. These gradients show that surface gravity 393 surveys could be conducted every 6, 10 or 15 years for thresholds of 4, 7 and 10 µGal in order to detect the 394 maximum change in the signal during the first 30 years of injection whereas the frequency of surveys could 395 be decreased after 30 years as the evolution of gravity over time is less significant. During the post-injection period, the slope is even smaller (about 0.1 µGal/yr) and the frequency of surveys can be set to a minimum 396 397 value. However, both monitoring strategy and frequency of surveys should also take into account the 398 tracking of the shape of the plume and not only the detection of the maximum of signal magnitude. Should 399 any divergence from the prediction be detected on the plume shape, the monitoring would need to be

400 pursued at the same or even greater frequency.



Figure 10. Change in gravity over time for the baseline (no leak) scenario relative to the pre-injection stage. Note the development of an asymmetrical, south east trending, gravity response due 1) to the presence of the sealing fault along which the CO<sub>2</sub> accumulates, and 2) to the geometry of the reservoir itself. Injection point ("Inj."), locations 1 and 2 ("Loc1" and "Loc2") and maximum CO<sub>2</sub> plume extent (black dashed line) are plotted for reference.



407 Figure 11. Evolution of the maximum surface gravity anomaly over time for the baseline scenario. The 4, 7 and 10 μGal detection
 408 thresholds are also indicated (see text for explanation).

Table 3. Time to detection of the CO<sub>2</sub> injected in the reservoir using surface gravity measurements (no leakage), with threshold values of 4, 7 and 10 μGal

Gravity Threshold	Time to detection	Mass of CO <sub>2</sub> injected
(µGal)	(years)	(IVIL)
4	6	15
7	10	25
10	15	37.5

427

413 In addition to surface gravity measurements, time-lapse changes of  $g_z$  in boreholes are calculated in three 414 boreholes. For these borehole measurements, a conservative value of 10 µGal can be considered for the 415 detection threshold. The first borehole is located right at the CO<sub>2</sub> injection point while the others are located at locations 1 and 2 (Figure 12). The results show that very soon after the beginning of the injection, a very 416 417 strong response is observed. For instance, 5 years after the start of injection (12.5 Mt of CO<sub>2</sub> injected), g<sub>z</sub> 418 reaches a magnitude of  $-140 \mu$ Gal at the injection depth. The gravity anomaly keeps increasing over time 419 and reaches a maximum of -180 µGal at 130 years before decreasing again. At location 1, the gravity 420 anomaly starts being detectable at 70 years with a magnitude of about -50 µGal at the depth of 2300 m and reaches a maximum magnitude of about -130 µGal at 180 years. At location 2, the furthest borehole from 421 422 the injection well, the gravity signal indicates an anomaly at a depth of 2000 m which does not exceed -25  $\mu$ Gal. The time to detection of the gravity anomaly is directly related to the migration of the CO<sub>2</sub> plume in 423 424 the reservoir and gives an excellent indication of the depth of the  $CO_2$  in the reservoir. These borehole 425 measurements provide information about the depth and vertical extent of the density anomaly, which could 426 later be used as a constraint in gravity inversions or when modeling surface responses.





## 430 **5.1 Tracking secondary plumes with time-lapse gravity**

The change in the vertical component of gravity for the different leakage scenarios was determined using
both surface-based and borehole data. As the leaky windows become active at 70 years, previous time-steps
are not considered because they are the same as the baseline scenario.

#### 434 **5.1.1 Surface measurements**

435 In the first leakage scenario (location 1), the leak occurs at a depth ranging from 1300 to 1800 m (Figure 5) 436 and about 12 Mt of  $CO_2$  leaks into the Olcese Formation. The baseline model response is subtracted from 437 the response at each time step in order to determine the signal exclusively associated with the leak and

- 438 plotted in Figure 13a for four time-steps: 90, 130, 160 and 200 years. The maximum gravity response over 439 time is reported in Figure 14 and the times to detection of the leak corresponding to the three detection
- thresholds considered (i.e., -4, -7 and -10 µGal) are reported in Table 4. The gravity response associated to 440
- the migration of  $CO_2$  into the Olcese Formation reaches the minimum detection threshold of -4  $\mu$ Gal at 90 441
- 442 years, and -10 µGal at 110 years. Over the following decades, the gravity response remains relatively
- 443
- constant and limited, with a maximum value of -15 µGal observed at 160 years (Figure 13a).

444 Responses associated with the migration of  $CO_2$  into the shallowest thief zone, the Etchegoin formation, 445 and a combined leakage into the Olcese and Etchegoin thief zones are also plotted in Figures 13b,c and 446 Figure 14. While the overall leaked  $CO_2$  mass is considerably lower than for the leak occurring in the Olcese 447 only (4 Mt at 200 years as compared to 12 Mt), the gravity anomaly exclusively associated to the leak 448 becomes detectable as soon as 100 years for a threshold of -4  $\mu$ Gal (Figure 14), which corresponds to the 449 time of arrival of the  $CO_2$  into the Etchegoin formation (Figure 5). The gravity anomaly keeps increasing over time and reaches a magnitude of -170 µGal at 200 years (Figure 13b). In addition to the magnitude of 450 this anomaly, a larger areal extent is observed which is directly related to the larger volume that the  $CO_2$  in 451 a gaseous phase occupies in the porous space at this depth. The asymmetry observed in the gravity anomaly, 452 453 extending along a northwest-southeast profile is directly related to the regional dip and the subsequent

454 buoyancy-driven migration of CO<sub>2</sub> into the shallower parts of the thief zone.

455 Figure 13 and Figure 14 also show the results for the combined-leakage scenario, simultaneously into the Olcese and Echtegoin formations. These results support the fact that the contribution of the leak into the 456 Olcese on the overall vertical component of the gravity response is very limited compared to the 457 458 contribution of the leak occurring in the shallow thief zone. In both cases, the surface vertical component of gravity response demonstrates the presence of a leak. 459



Threshold value (µGal)	Time to detection (years) at location 1			Time to detection (years) at location 2			
	OL	ET	OL+ET	OL	SM	ET	OL+SM+ET
4	90	100	90	90	90	100	90
7	95	110	95	100	100	100	90
10	110	110	100	110	110	100	95

462

OL=Olcese, ET=Etchegoin, SM=Santa Margarita



Figure 13. Difference between the surface gravity response associated with a leak occurring into a) the Olcese thief zone; b) the
Etchegoin thief zones, c) the Etchegoin and Olcese thief zones, and that with the baseline scenario for the same time steps (90, 130, 160 and 200 years).



468 Figure 14. Maximum surface gravity anomaly calculated over time for the different leakage scenarios (left: Location 1 scenarios;
 469 right: Location 2 scenarios). The gravity response from the reservoir has been removed.

471 The same method was used to calculate the surface gravity response for the second set of leakage scenarios

472 (Location 2, Table 2). This leaky window is located ~6 km southeast of the injection well, and the leakage

473 occurs either in the Olcese, Santa Margarita, or Etchegoin formations separately or in all formations at once.

474 The results of maximum surface gravity anomaly and leaked  $CO_2$  mass as a function of time are presented 475 in Figure 14. Maps of the surface gravity anomalies for the four scenarios at four different times are shown

in Figure 15 and times to detection are presented in Table 4. The presence of leakage is established for the

four scenarios with a maximum gravity response located first up dip of the leaky point, and that gradually

478 migrates to where the  $CO_2$  accumulates in the shallower parts of the reservoir.

The four scenarios evaluated at location 2 present similarities to the first set of leakage scenarios described above. The main difference is the magnitude and the shape of the gravity anomalies. Overall, due to the shallower depths at which the well intersects the thief formations, the magnitude of the gravity anomalies is slightly higher for this set of scenarios. For instance, the gravity response reaches a magnitude of -20

483  $\mu$ Gal at 200 years for a leak occurring in the Olcese Formation at location 2, as compared to -15  $\mu$ Gal at

484 location 1 at the same time and for the same mass of CO<sub>2</sub> leaked (12 Mt). Similarly, the magnitude of the

gravity anomaly associated to leak occurring in the Etchegoin formation (Figure 14c), reaches a maximum

486 value of -167  $\mu$ Gal at 200 years at location 1 compared to -204  $\mu$ Gal at location 2. The leak occurring in

487 the Santa Margarita formation only (Figure 14b) leads to a maximum gravity response of -50 μGal observed

488 at 180 years, when 9 Mt of  $CO_2$  leaks out from the reservoir (6% of the total mass injected). An elongation

489 of the anomaly in the southeastern direction is observed. Additionally, in the case of multiple leaks, the

490 presence of  $CO_2$  in the shallowest thief zone is the principal contributor to the surface gravity response.

491 The times to detection for the four scenarios evaluated at location 2 (Table 3) are overall reduced compared

492 to the first set of scenarios, which is directly related to the geometry of the reservoir, and more specifically

493 to the shallower depths of the three thief zones.

494 Although gravity surface measurements cannot discriminate alone the existence and depth of multiple CO<sub>2</sub>

495 accumulations in formations located at different depths, additional value of gravity techniques for leak

496 investigation comes from combining the surface-based measurements presented here with borehole-

497 deployed measures that will be presented in the next section.





#### 502 **5.1.2 Borehole measurements**

503 In order to determine if accumulation of  $CO_2$  in multiple formations could be discriminated borehole 504 measurements are considered. The time-lapse changes of  $g_z$  are calculated in the three boreholes presented 505 in section 5.1 assuming simultaneous accumulation of  $CO_2$  into the three thief zones at location 2 (scenario 506 2.4, in Table 2). The results (Figure 16) indicate that the depths of the three thief zones can clearly be 507 distinguished using this method in the wells that intersect the density anomalies. The leak occurring in the shallowest formation (Etchegoin formation, about 500 m deep) yields a significant gravity response with 508 values ranging from -100 to -300 µGal, depending on the time considered. The sensitivity of the borehole 509 510 gravity method with the distance from the edge of the  $CO_2$  plume is not modeled for this scenario, but as 511 demonstrated by Gasperikova and Hoversten (2008), the responses decrease away from the edge of the 512 density anomaly. Several tests (not represented here) have been performed with wells located at increased distances of Location 2 and no borehole-gravity response is observed beyond a distance of 250 m. Overall, 513 it is clear that depths and extent of the density anomalies associated with multiple thief zones can be 514 515 captured using borehole gravity measurements provided they are not too far away for the leakage paths.



516

517 Figure 16. Changes in vertical component of g (gz) in a borehole at Location 1 where leakage is occurring 518 (scenario 2.4, Table 2).

### 519 **6. Inversion: estimating the mass of leakage**

520 The usefulness and sensitivity of the time-lapse gravity method based on forward modeling of density anomalies deduced from a multi-phase flow model of the growth and migration of a CO<sub>2</sub> plume has been 521 522 demonstrated. It is now opportune to test some inverse modeling approaches in order to evaluate the 523 potential of these methods to detect and estimate the change in fluids density in the porous space as given 524 by equation 1 and thus estimate the mass of leaked CO<sub>2</sub>. The gravity anomaly calculated by forward modeling for one scenario and at a specific time step is used and called "observations data" for the simplicity 525 526 of the discussion. The scenario 1.3 (Table 2) has been selected at 160 years, 100 years after the end of the injection. This set of pseudo "observations data" at 160 years, with a standard deviation of 2% added to 527 528 each data, will be inverted with two objectives: 1) getting a reasonable idea of the initial density distribution 529 used to generate the gravity anomaly and 2) testing the best set of parameters to be used in this inversion. 530 In other words, can gravity inversion of time-lapse survey data be able to detect a leakage, determine its 531 location and shape and estimate its corresponding mass?

532 For this approach, the UBC-GIF GRAV3D inversion software is used. The inverse problem is formulated 533 as an optimization problem where a global objective function is minimized. This global objective function

has two components: a data misfit function which is responsible for ensuring the model predicts data that

535 fits the field observations and a model objective function which ensures that the model contains plausible

536 geological structures (UBC-GIF, 2017). In the present case, the model objective function is changed by 537 prescribing the range of minimum and maximum values for the density anomalies and by prescribing or 538 not a density distribution as initial and reference models. This reference density distribution is coming from 539 the modeled baseline scenario at a specific time-step in order to mimic the reality where the operator would 540 only have as a reference the baseline simulation updated by observations. The baseline density distribution

- at 70 years (i.e., 10 years after the end of injection), corresponding to the beginning of leakage, was chosen
- 542 as the reference.

543 The set of observations incorporate both surface and borehole observations. Several cases have been 544 studied: inversion of surface observations alone with or without a reference model and then joint inversion 545 of surface and herebole characterized. There are a surface observations alone with or without a reference model and then joint inversion

of surface and borehole observations. These cases are summarized in Table 5, column 1. It should be noted

- 546 that no inversion of surface observations alone is presented because it results to unrealistic concentration
  - 547 of all the  $CO_2$  close to the surface.
  - 548 Table 5. Equivalent mass of displaced fluids (brine and CO<sub>2</sub>) in Mt for different inversion cases above two depths and for the

550 minimum depth reached by the main plume in the reservoir. Any mass detected above this depth must be considered as

<sup>552</sup> *leakage scenario are provided on line 1 for comparison.* 

	Mass of displaced fluids (Mt) for			
Inversion Cases	depth < 500 m	depth < 1600 m	whole domain	
Reference forward model at 160 years ( <i>Figure 17</i> , leakage at location 1 into Olcese and Etchegoin formations), the inversion results are compared to these values. The corresponding CO <sub>2</sub> masses used for the leakage scenario simulation are in red.	<b>9.5</b> (2.6)	<b>32.4</b> (12.2)	<b>119.5</b> (122.2)	
1) Only surface data – with 70 years baseline scenario as reference ( <i>Figure 18</i> )	1.9	14.7	123.4	
2) Surface data + a dense network of boreholes without reference ( <i>not represented</i> )	11.7	35.8	115.0	
3) Surface data + four boreholes over the leakage zone				
3a) with no reference file ( <i>not represented</i> )	9.4	51.5	110.8	
3b) with 70 years baseline scenario as reference ( <i>Figure 19</i> )	8.7	39.2	115.9	

553

554 The fluid density distribution at 160 years to which the results of the inversion should be compared is

shown in Figure 17.

<sup>549</sup> whole domain. The 500 m depth corresponds to the base of the Etchegoin formation and the 1600 m depth relates to the

<sup>551</sup> anomalous and resulting from a leakage. The masses of  $CO_2$  used in the multiphase flow simulation of the corresponding



558

559

560

Figure 17. Half-plume (cut at y=-50m) for the reference scenario at location 1 at 160 years. The corresponding surface gravity anomaly will be used used for the inversion. The color scale gives the density anomaly compared to baseline scenario at 0 years. The four vertical black lines correspond to the virtual boreholes used in the inversion.

561 Inversion results for two cases are illustrated and discussed. For the first case (case 1, Table 5), one can

562 observe (Figure 18) that the overall shapes of the plume in the reservoir as well as the region interested by

the leakage are in good accordance with the initial model but that the estimated masses for the depths above

564 1600 m don't match the ones used in the reference case.



565 566

567

Figure 18. Density anomaly distribution resulting from the inversion of surface observations only and using 70 years baseline reference model (case 1, Table 5). Left: full plume; right: cross section at y = -50 m.

For the second case (case 3b, Table 5), surface observations are jointly inverted with observations from four boreholes located along a profile crossing the leaked plume using the baseline at 70 years as a reference model. Figure 19 shows a good correspondence of the overall shape of the plume in the main reservoir and a very good definition of the  $CO_2$  plume in both thief zones. The values of the estimated masses (case 3b, Table 5) are in good agreement with the ones obtained in the reference case. The other cases are not represented but one should note that cases 2 and 3a (Table 5) also give satisfactory results.



576 577

Figure 19. Cross section at y=-50 m of the density anomaly distribution resulting from the inversion of surface and four borehole observation without a reference file (case 3b, Table 5). The boreholes are represented as vertical black lines.

578 Inversion of gravity observations gives the best results when borehole data and surface data are jointly used 579 with the baseline density distribution at 70 years as a reference to constrain the model objective function.

### 580 7. Discussion

### **7.1 Approaching the detection threshold of a CCS site with an analytical solution**

The results of the multiphase flow simulations show that once a leak occurs,  $CO_2$  migrates upward and accumulates in overlying permeable thief zones. The buoyancy-driven  $CO_2$  accumulates at the top of the thief zones and the  $CO_2$  plume grows laterally forming elongated or circular shapes with associated thicknesses ranging from 20 to 30 m. Figure 20 shows the minimum leaked  $CO_2$  mass leading to a gravity anomaly greater than 10, 7 and 4 µGal at the surface as a function of the depth of the leak which is defined as the minimum depth reached by  $CO_2$  during its migration toward the surface. Only the scenarios with a leak to a single thief zone were considered here.

589 These results were then compared to those provided by a simplified approach which assumes that  $CO_2$  leaks 590 are comparable to vertical cylinders of length ranging from 20 to 30 m (corresponding roughly to the 591 thicknesses of the CO<sub>2</sub> layer accumulation in thief zones), with homogenously distributed density contrast 592 determined based on the conditions found at Kimberlina for a given depth (e.g., brine and  $CO_2$  densities), 593 for a porosity of 25% and a saturation of 30%. Different values of the cylinder masses are then obtained by 594 varying the radius and thus the volume. To calculate the gravity effect of these vertical cylinders, the 595 analytical solution proposed by Telford (1976) is used and the minimum mass capable of producing an 596 anomaly of 10, 7 and 4 µGal is determined (orange, yellow and green lines in Figure 20). The results of 597 this simplified approach agree very well with the surface gravity responses computed from the Kimberlina. 598 This simplified approach can thus be used to give a rough estimate of the detection thresholds that could be 599 expected for any given storage site with specific conditions of temperature, pressure and salinity gradient.



601 Figure 20. Estimation of the minimum detectable  $CO_2$  mass (in  $10^{-3}Mt$ ) capable to create a gravity anomaly of 10 (orange), 7 602 (vellow) and 4uGal (green) at the surface as a function of depth. Circles, triangles and sauare symbols correspond to the

602 (yellow) and 4μGal (green) at the surface as a function of depth. Circles, triangles and square symbols correspond to the 603 Kimberlina 2 numerical simulations and color lines correspond to the simplified cylinder analytical solution (Telford, 1976), their

604 thickness correspond to the difference between solutions for the two lengths of the reservoir (20 and 30m).

#### **7.2 Strategy to implement a monitoring network**

The spatial extension of the gravity anomaly at the surface depends on the depth, the volume and the 606 607 magnitude of the density anomaly. When planning the station spacing, consideration should be given to the 608 expected anomaly pattern. Designing an appropriate monitoring network would first consist of considering 609 the maximum extent of the main plume obtained by the multiphase flow modeling and also the minimum size of the anomaly of interest that will determine the minimum spatial sampling rate. For Kimberlina, the 610 611 maximum extent of the anomaly corresponds to the large  $12 \times 16$  km area shown in Figure 10. In order to 612 cover this area with an appropriate resolution, a baseline survey consisting of a grid with station spacing of 613 500 m would constitute a reasonable baseline survey before any injection (~800 stations), as illustrated in 614 Figure 21. Such a grid would indeed capture the main pattern.

Regarding the time between two consecutive surveys, results presented in Figure 11 demonstrated that a survey every 6 to 15 years, depending on the detection threshold considered at the site would capture the gravity changes associated to the  $CO_2$  injection. Any deviation from the  $CO_2$  plume baseline scenario for a given time should trigger a redefinition of both the spatial and temporal sampling rates. It is therefore

619 critical to get a high-resolution gravity baseline.

620 These surveys are relatively inexpensive and easy to deploy and could help deciding when and where more

621 expensive seismic surveys should be performed in the case of observed gravity anomalies going above a

622 pre-defined threshold.



Figure 21. Illustration of the importance of the surface station spacing when defining the monitoring network (from left to right, station spacing is respectively 200 m, 500 m and 800m).

626 It was demonstrated that borehole measurements of  $g_z$  provide excellent constrains in depth only when they

are located close (250 m in this study) to the density anomaly associated with the presence of CO<sub>2</sub>. Because

628 the gravity response decreases away from the CO<sub>2</sub> plume, the lateral resolution of the measurements is very

629 limited, and borehole gravity measurements should only be considered for leakage detection when the

630 presence of CO<sub>2</sub> is demonstrated or strongly suspected, and the mass of CO<sub>2</sub> needs to be quantified and the

depth of the leak be determined with accuracy. Recent progress in three-axis microgravity technology could
 permit the deployment of such instrumentation into boreholes to measure the two horizontal components

633 of g sensitive to density anomalies far beyond the borehole (Lofts et al., 2019).

634 Multi-physics models are critical for integrating the geological complexity of a storage site and 635 implementing a risk-based monitoring strategy. When planning the gravity station spacing, consideration 636 should be given to the extent of the predicted anomaly associated to the migration of the  $CO_2$  plume in the 637 reservoir.

- 638 At a large and complex site such as Kimberlina, the presence of the fault is known and should be fully 639 integrated in the risk profile of the site. The models considered in this study were not built to represent the 640 real behavior of a fault but provided means of having CO<sub>2</sub> plumes at certain locations and of demonstrating 641 the sensitivity of the method to various  $CO_2$  plume configurations. In these models, it was observed that although the fault starts being conductive 10 years after the end of the injection, it may require few more 642 643 decades, depending on the detection threshold considered, before any leak can be detected with surface 644 measurements if the  $CO_2$  is migrating toward shallow formations. Conversely, when  $CO_2$  reaches the 645 shallowest formation, even a small to moderate mass of  $CO_2$  triggers an immediate gravity signal that can 646 be measured. While leaks can be detected with surface measurements, their spatial extent may be limited 647 compared to the gravity response associated with the  $CO_2$  plume migration in the reservoir. Additionally,
- should a large leak occur in a deep formation, it is very unlikely that the gravity method could be used as
- 649 an early detection method.
- 650 These observations are all fundamental when designing a monitoring strategy, but also when discussing the
- duration of post-injection site care (PISC) periods on CCS sites. Although the leakage scenarios presented
- in the present study are all theoretical and extreme and meant to assess the sensitivity of geophysical
- 653 methods, they highlight the importance of making risk-informed decisions when designing and optimizing
- the monitoring network. They also illustrate clearly the need for careful simulations to identify the most
- 655 pertinent monitoring tools to be used in early detection of CO<sub>2</sub> leakage.

## 656 8. Conclusions

The performance of both surface and borehole time-lapse gravity monitoring to detect CO<sub>2</sub> leakage from the hypothetical Kimberlina storage site, San Joaquin Valley, California, has been evaluated. Two unique sets of leakage scenarios were developed and tested for one storage formation and up to three thief zones using multi-physics-based simulations that were based on the complex geologic model of the Kimberlina site including a steeply dipping fault. The following main conclusions can be drawn:

- Surface-based gravity monitoring of a CCS site during and after injection provide valuable
   information on the location, shape and volume/mass of the CO<sub>2</sub> plume in the reservoir and can be
   considered as a valid reservoir management tool. In particular this can help with updating the
   predictive scenarios by real time comparison of predicted values with observations.
- 666 \_ The surface-based gravity responses obtained for the different leakage scenarios demonstrate that leakage can be detected at the surface in all the scenarios with the masses of leaked CO<sub>2</sub> considered 667 668 here but the time to detection is highly variable and dependent on the detection threshold considered, location of the leak, and amount of fluid leaked. The magnitude of the gravity signal 669 670 strongly depends on the depth of the leak(s). The areal extent of the anomaly is extremely well correlated to the  $CO_2$  saturation/density changes occurring in the subsurface allowing a precise 671 mapping of the plume front. However, gravity surface measurements cannot alone discriminate the 672 673 existence and depth of multiple distinct leaks. These observations are keys to define the monitoring strategy deployed at CCS sites and demonstrate how monitoring needs to be adapted throughout 674 675 the lifetime of a CCS project.
- 676 The predicted surface gravity changes are small when the source anomaly is located at a depth greater than 1,500 m and a leak occurring at these depths would only be detected if the mass is significant, ranging from about 3 Mt for a detection threshold of 4 μGal to about 8 Mt for a detection threshold of 10 μGal at the hypothetical Kimberlina site, which represent 2 to 5% of the total mass of CO<sub>2</sub> injected.
- The gravity response expected at the surface for a leak occurring in a single thief zone can be assumed to be equivalent to the vertical gravitational effect of a vertical cylinder
- Inversion of surface data alone can bring valuable information on the occurrence of leakages and their spatial extent providing a reference model based on the density distribution at the end of the injection is used. The best estimate of the mass of leaked CO<sub>2</sub> can only be obtained if boreholes data are jointly inverted.

693 Multiphase flow simulations followed by gravity modeling are fundamental in order to define if and when 694 gravity monitoring would be applicable at storage sites. This initial step will help design the spatial and 695 temporal sampling strategy for the gravity surveys.

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