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1 CO₂ storage and potential fault instability in the St. Lawrence Lowlands sedimentary basin
2 (Quebec, Canada): insight from coupled reservoir-geomechanical modeling

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8 A coupled reservoir-geomechanical (TOUGH-FLAC) modeling is applied for the first time in the St.
9 Lawrence Lowlands region to evaluate the potential shear failure along pre-existing high-angle
10 normal faults and tensile failure in the caprock units (Utica Shale and Lorraine Group) associated
11 with CO₂ injection into the sandstone reservoir (Covey Hill Formation) of the Early Paleozoic
12 sedimentary basin. Field and subsurface data are used to estimate sealing properties of two
13 reservoir-bounding faults (Yamaska and Champlain Faults). The spatial variations in fluid
14 pressure, effective minimum horizontal stress and shear strain are calculated for different
15 injection rates using a simplified 2D geological model of the Becancour area located ~110 km to
16 the SW of Quebec City. The simulation results show that initial fault permeability affects the
17 timing, localization, rate and length of fault shear slip. Contrary to the conventional view, our
18 results suggest that shear failure may start earlier in time in the case of a permeable fault rather
19 than in the case of a sealing fault depending on the site-specific geologic setting. In the
20 simulations, shear slip is nucleated along a 60-m-long fault segment in a thin and brittle caprock
21 unit (Utica Shale) trapped below a thicker and more ductile caprock unit (Lorraine Group), and
22 subsequently progressing up to the surface. In the case of an assumed sealing fault, shear failure
23 occurs later in time and it is localized along a fault segment (300 m) below the caprock units. The
24 presence of the inclined low-permeable Yamaska fault close to the injection well causes
25 asymmetric fluid pressure build-up and lateral migration of CO₂ plume away from the fault that
26 reduces the overall risk of CO₂ leakage along faults. The fluid pressure-induced tensile fracturing
27 occurs only under extremely high injection rates; and it is localized below the caprock units,
28 which remain intact preventing upward CO₂ migration.

29

30 1. INTRODUCTION

31 The changes in fluid pressure and shear stress accumulation may trigger reactivation of
32 faults, which are optimally oriented relative to in-situ stress fields (Davies et al., 2013; Miller et
33 al., 2004; Sibson, 1992; Streit and Cox, 2001). The high fluid injection rates and low permeability
34 of reservoir formation may contribute to the risk of induced seismicity (Berry and Hasegawa,
35 1979; McClain, 1970). The incidents of fault reactivation and induced earthquakes related to
36 large-volume fluid injection or gas extraction are well known in sites of Snipe Lake and Strachan
37 (Alberta), Wilmington (California), Rangely and Denver (Colorado), midcontinent region of the
38 United States, In Salah (Algeria) (Baranova et al., 1999; Ellsworth, 2013; Healy et al., 1968; Hsieh
39 and Bredehoeft, 1981; Mathieson et al. 2010, 2011; Milne, 1970; Nicol et al., 2011; Raleigh et al.,
40 1976; Shemeta et al., 2012; Suckale, 2010; Wyss and Molnar, 1972).

41 Even if no harmful induced seismicity has been associated with global carbon capture and
42 storage (CCS) demonstration projects as of February 2011 (Committee, 2012; NETL, 2013), the
43 continuous CO₂ injection at high rates under high pressures for very long periods of time may
44 lead to increase of fluid pressures in storage reservoirs and thus to potential fault reactivation.
45 The CO₂ volume stored in deep saline aquifers in industrial projects to date varies from about
46 0.7-1 Mt/yr. (e.g. Snøhvit and Sleipner, Norway; In Salah, Algeria; Illinois, U.S.; Quest, Alberta) up
47 to 3-4 Mt/yr. (Gorgon, Western Australia) (GCCSI, 2012). The maximum period of injection time
48 in operating CCS projects to date varies from 17 years in deep saline aquifers (Sleipner, Norway)
49 to 40 years in enhanced oil recovery (EOR) project (Val Verde, Texas) (GCCSI, 2012). The risks of
50 induced seismicity associated with CO₂ storage may be minimized through careful site
51 characterisation and numerical modeling.

52 The hydromechanical behaviour of faults has been studied to assess the risks of induced
53 seismicity and fluid leakage related to CO₂ storage (Chiaramonte et al., 2008; Hawkes et al.,
54 2005; Lucier et al., 2006; Murphy et al., 2013; Rutqvist, 2012; Streit and Hillis, 2004; Vidal-Gilbert
55 et al., 2010; Zhang et al., 2013; Zoback and Gorelick, 2012). Coupled reservoir-geomechanical
56 numerical modeling has been shown to be an effective tool to test fault instability and potential
57 shear failure (Cappa and Rutqvist, 2011b; Rutqvist et al., 2008). The potential for mechanical
58 failure and the type and orientation of failure is to a large extent controlled by the three-
59 dimensional initial stress regime. An extensional stress regime is shown to be favourable for
60 shear failure along high-angle faults (60°) that may cut through overburden rock above the

61 pressurized storage zone (Rutqvist et al., 2008). Fault shear rupture and dilation may induce or
62 enhance fault permeability that in turn facilitates the rupture propagation across the overlying
63 caprock (Cappa and Rutqvist, 2011b; Rinaldi and Rutqvist, 2013). The effect of initial permeability
64 on co-seismic (sudden) fault slip has been investigated by Cappa and Rutqvist (2011a; 2012) and
65 Mazzoldi et al. (2012), indicating relatively minor impact of initial permeability. Additionally, it
66 was found that that high-permeable fault is likely reactivated later in time than low-permeable
67 fault due to easier fluid pressure dissipation along the fault (Cappa and Rutqvist, 2011a).
68 However, the effect of initial fault permeability on timing, localization and rate of fault shear slip,
69 as well as total aseismic fault slip has not yet been fully investigated.

70 The high-angle faults located close to CO₂ injection area are usually considered as a
71 probable pathway for CO₂ or brine migration and leakage due to fault permeability, either initial
72 or induced, triggered by shear reactivation (Chang and Bryant, 2008; Barton, 2011; Hannis et al.,
73 2013; Jordan et al., 2013). Here, we investigate if there are any other possible effects of the
74 presence of inclined fault near the injection zone on fluid pressure build-up and buoyancy-driven
75 CO₂ plume migration path using the real geological setting of the St. Lawrence Lowlands region.
76 The deep saline aquifers of the Early Paleozoic sedimentary basin of the St. Lawrence Lowlands
77 (about 200 km x 40 km) are recognized as the best target for the geological storage of CO₂ in the
78 Province of Quebec based on both geologic and practical criteria (Malo and Bédard, 2012). The
79 Cambrian-Lower Ordovician sandstones of the Potsdam Group (Fig. 1) form 200 to 600 m thick
80 reservoir units in the potential storage area (depths < 4 km). The mean total effective capacity
81 for CO₂ storage in the sandstones of the Potsdam Group is 3.18 Gt at the basin scale (Malo and
82 Bédard, 2012). The Utica Shale and siliciclastic rocks of the Lorraine form a comprehensive
83 caprock system (Fig. 1), whose thickness is ranging from 0.8 km to 3.5 km.

84 The high-angle SW-NE normal faults dipping to the SE affect both the sedimentary
85 succession and the Grenvillian metamorphic basement (Fig. 1). The faults are oriented sub-
86 parallel to oblique (10° to 36°) to the S_{Hmax} stress orientations and are likely near critically
87 stressed for shear slip with slip tendency (shear over normal stress ratio) ranging from 0.34 to
88 0.58 (Konstantinovskaya et al., 2012). Thus, the initial shear over normal stress ratio is less than
89 the range of 0.6 to 1.0 that would substantially increase the likelihood for shear reactivation. The
90 optimally oriented high-angle normal faults in the area might become unstable under the
91 present-day stress field if fluid pressure during CO₂ injection exceeded the critical threshold 18-

92 20 MPa for a depth of 1 km, thus increasing the risks of induced seismicity and CO₂ leakages
93 (Konstantinovskaya et al., 2012).

94 In the present study, coupled reservoir-geomechanical numerical modeling is applied to
95 estimate stress changes related to migration of injected CO₂ and associated increase of fluid
96 pressure P_f in order to evaluate the risk of reactivation of high-angle normal faults in the St.
97 Lawrence sedimentary basin. The coupled reservoir-geomechanical simulator TOUGH-FLAC
98 applied in this case is described in detail by Rutqvist (2011).

99 The coupled TOUGH-FLAC modeling is performed for the site of the Becancour area (Fig. 2)
100 using a simplified 2D geological model (Fig. 3). The Becancour area is located at about 110 km to
101 the SW from the Quebec City and it is occupied by the industrial park with relatively high CO₂
102 emissions (between 0.5 and 1 Mt/yr. in 2009) (Malo and Bédard, 2012). The site is easily
103 accessible and has well-developed infrastructures representing one of the best potential sites for
104 CO₂ storage in the St. Lawrence Lowlands (Malo and Bédard, 2012). High density of hydrocarbon
105 exploration wells and seismic lines in the Becancour area made it possible to characterize deep
106 saline aquifers (Tran Ngoc et al., 2012) and to create 3D geological model of the site (Claprood et
107 al., 2012).

108 The model parameters (main boundary conditions, CO₂ injection rate, initial fault
109 permeability, and permeability of reservoir units) are varied to study their influence on fluid
110 pressure build-up, shear failure of faults and tensile fracturing and to estimate the risk of CO₂
111 leakage. Permeability of the SW-NE high-angle normal faults that affect the St. Lawrence
112 Lowlands sedimentary succession (Fig. 1) is not well constrained. To evaluate the possible range
113 of fault permeability that may be applied in the numerical simulations, the field observations on
114 fault zone rocks, sample descriptions from fault-crossing wells are analyzed in this study. The
115 fault seal capacity estimation is carried out for the first time in the region for the Champlain and
116 the Yamaska Faults (Fig. 3).

117 2. MODEL SETUP AND BOUNDARY CONDITIONS

118 The simplified 2D geological model of the Becancour area (Fig. 3) is oriented NW-SE,
119 across the regional structure (Fig. 2), and it extends vertically from the ground surface to a depth
120 of 4000 m and horizontally 20,000 m. The model is built using interpretation of 2D seismic lines
121 (100 km) and well logs (16 wells), analysis of the seismic map of the top of the Grenvillian

122 basement (Fig. 2) and using a 3D geological model of the Becancour area (Claprood et al., 2012).
123 The 2D simplified model geometry is deemed adequate in this case because the geology in the
124 third dimension (along Y-axis) does not change significantly for several km and because the
125 horizontal principal stresses are orthogonal and parallel to the model section (Fig. 2, Line A-B).
126 This implies that the 2D simplification is adequate from mechanical perspective, in particular to
127 investigate the potential for shear fault reactivation. Moreover, the potential for fault
128 reactivation is driven by changes in reservoir pressure, which is simulated explicitly in the 2D
129 model, but with comparison to pressure evolution calculated with an independent axisymmetric
130 model for the same site (Tran Ngoc et al., 2012). As will be discussed later, it is likely that the
131 current 2D model simplification will result in a lower-bound estimate of the maximum
132 sustainable injection pressure and an upper bound estimate of the potential magnitude of shear
133 slip and rupture length. This is because in a full 3D system, some segments of the fault away
134 from the 2D section would not be pressurized, i.e. where the fault would not be reactivated, and
135 this would tend to restrict shear movements along the faults. On the other hand, there are
136 uncertainties related to the exact orientation of the stress field meaning that the principal
137 stresses might not be exactly parallel and perpendicular to the fault strike, which is not always a
138 planar surface, thus leading to strike-slip fault reactivation, an analysis that would require a 3D
139 model analysis.

140 The model represents a multilayered CO₂ storage system (Fig. 3) built as a 2D plane-strain
141 model with an arbitrary thickness of 100 m along the Y-axis. It includes (from base to top): low-
142 permeable Grenvillian metamorphic basement, sandstone units of aquifer 1 (Covey Hill
143 Formation) and aquifer 2 (Cairnside Formation), intermediate units (sandstones of the Theresa
144 Formation, dolomites of the Beauharnois Formation and argillaceous limestones of the Chazy,
145 Black River and Trenton Groups) and low-permeable units of caprock 1 (Utica shales) and
146 caprock 2 (fine-grained siliciclastic rocks of the Lorraine Group). The intermediate units are
147 characterized by variable and generally low matrix permeability that is locally enhanced by
148 fracturing or secondary porosity. The sandy limestones of the Lower Chazy Group contain thin
149 (first meters) relatively high-permeable levels but they are not distinguished at the scale of the
150 model.

151 The sandstones of aquifer 1 of the Covey Hill Formation (Fig. 3) are targeted for CO₂
152 injection because these rocks are characterized (Table 1) by the highest cumulative thickness

153 (188 m) of permeable (netpay) levels and matrix permeability ($2.6 \times 10^{-16} \text{ m}^2$ or 0.26 mD) if
154 compared to other units, as well as by good porosity (6%). The sandstones of the Covey Hill
155 Formation are located at depths where injected CO_2 would be in supercritical state under the
156 observed fluid pressure and temperature (Table 2) (Tran Ngoc et al., 2012).

157 The average porosity and matrix permeability of rocks in the reservoir and the caprock
158 sedimentary units (Table 1) of the St. Lawrence Lowlands sedimentary succession were
159 determined from available core analyses (Tran Ngoc et al., 2012). The rock mass permeability
160 that takes into account the presence of natural fractures is not well constrained in the Becancour
161 area because drill stem test (DST) data are rather scarce and non-uniform across the
162 sedimentary succession. To overcome the uncertainty, the rock mass permeability of the
163 reservoir units (Covey Hill and Cairnside Formations) is varied as 10-x (k_1) and 100-x (k_2) values of
164 matrix permeability k_m (Table 1), remaining within the known range of DST data from $4 \times 10^{-15} \text{ m}^2$
165 to 10^{-13} m^2 (4 to 100 mD) in the Becancour area (Tran Ngoc et al., 2012). For the overlying units,
166 the matrix permeability is applied. The permeability of the caprock units of the Utica Shale and
167 the Lorraine Group is taken 10^{-18} m^2 (Table 1) as determined from the laboratory analyses.

168 Capillary pressure, CO_2 -brine relative permeability, partial miscibility of CO_2 and brine and
169 reactivity of CO_2 with rock matrix affect fluid pressure build-up under constant injection rates
170 (Burton et al., 2009, Bennion and Bachu, 2008; Mathias et al., 2011a; 2011b; 2013). Capillary
171 properties of sandstones of the Potsdam Group are based on laboratory measurements carried
172 out for core samples using both mercury injection and capillary centrifuge tests (Tran Ngoc et al.,
173 2012). The van Genuchten (1980) model for capillary pressure and the van Genuchten-Mualem /
174 Corey model for relative permeability of gas and liquid phases (Corey, 1954) are fitted to
175 laboratory measurements. Capillary properties for the CO_2 -brine fluid system are obtained based
176 on conversions from air-mercury and air-brine systems, using the experimental correlation of
177 interfacial tension between CO_2 and brine proposed by Bachu and Bennion (2009).

178 Entry pressure (Table 1) is estimated 44.1 kPa in sandstones of the Covey Hill Formation
179 and 40 kPa - of Cairnside Formation (Tran Ngoc et al., 2012), with similar value being applied to
180 other units. Entry pressure for CO_2 in shales is generally higher, ranging from less than 0.1 to 10
181 MPa (Al-Bazali et al., 2005; Busch and Amann-Hildebrand, 2013; Carles et al., 2010; Chadwick et
182 al., 2008; Hildenbrand et al., 2004; Song and Zhang, 2013) and it could be expected value
183 applicable for the modeled fault zones, which are assumed to have the hydrological properties of

184 the Utica shales in the Becancour area (see section 3.1 below). However, the above quoted
 185 values are laboratory scale properties, whereas in the field caprock units and faults include
 186 discontinuities, such as fractures and minor secondary faults that may be slightly more
 187 permeable, resulting in a lower capillary entry pressure. In these simulations we assumed the
 188 same entry pressure of 40 kPa, which is not unrealistic considering a shale permeability of 1×10^{-18}
 189 m^2 (Busch and Amann-Hildenbrand, 2013), but it might be considered as a lower limit value for
 190 the shaly caprock units and the fault zones to simulate the worst scenario when the presence of
 191 natural fractures might facilitate fluid circulation. In any case, a CO_2 injection over-pressure of a
 192 few MPa will be sufficient to break the capillary barrier and the caprock units and faults will be
 193 considered permeability seals, rather than capillary seals (Rutqvist, 2012).

194 The poroelastic constitutive model of the rock mass is applied in simulations, whereas
 195 faults follow an elasto-plastic behavior represented by the anisotropic ubiquitous-joint model
 196 implemented in FLAC3D (Itasca, 2009). The elastic properties (Table 1) of sedimentary rocks have
 197 been determined from triaxial strength tests carried out on core samples in the Weatherford
 198 Laboratory. The values of measured (E , ν) and calculated (K , G , λ) elastic moduli (Table 1)
 199 indicate dolomitic sandstones of intermediate units (Theresa Formation) are more rigid and
 200 more brittle than other aquifer and intermediate units, and calcareous shales of caprock 1 (Utica
 201 Shale) are more brittle than siliciclastic rocks of caprock 2 (Lorraine Group). The rocks of the
 202 Theresa Formation and the Utica Shale are thus expected to be the first units that would be
 203 affected by tensile fracturing in the sedimentary succession of the St. Lawrence Lowlands.

204 The Biot's coefficient α in simulations is assumed equal 1 for all units (Table 1). Its value
 205 may be estimated from the equation (Zoback, 2010):

$$206 \quad \alpha = 1 - K_{\text{dry}}/K_0,$$

207 where K_{dry} is the bulk modulus of dry (drained) rock and K_0 is the bulk modulus of the
 208 rock's individual solid grains. The bulk modulus K_{dry} for the studied sedimentary units is
 209 calculated from values of Young modulus and Poisson's ratio (Zoback, 2010) that were measured
 210 during laboratory tests on drained core samples (K in Table 1). The average bulk modulus of
 211 mineral grains might be approximate as 37 GPa for quartz, 37.5 GPa for average feldspar, 95 GPa
 212 for dolomite, and 77 GPa for calcite ([http://subsurfwiki.org/wiki/Elastic_properties_of](http://subsurfwiki.org/wiki/Elastic_properties_of_common_sedimentary_rock_forming_minerals)
 213 [common_sedimentary_rock_forming_minerals](http://subsurfwiki.org/wiki/Elastic_properties_of_common_sedimentary_rock_forming_minerals)). Applying these values in the above equation,

214 the Biot's coefficient is about 0.56 for sandstones and 0.67 for dolomites, except the Cairnside
215 Formation where it is ~ 0.2 . From laboratory experiments reported in the literature, it is clear the
216 Biot's coefficient could be considerably lower than 1, and it is also stress-dependent along with
217 the stress decency of the bulk modulus (Coussy, 2004). In our simulations, the Biot's coefficient
218 will have an impact on the reservoir strain induced by the fluid pressure (mostly in the vertical
219 direction) and on the poro-elastic stress (mostly induced in the horizontal direction). Regardless
220 of the choice of Biot's coefficient, the Terzaghi effective stress measures the stress level
221 sustained by the solid matrix and it is conventionally used to detect failure in a plastic material
222 (Coussy, 2004; Itasca 2009). Thus, the potential for failure depends mostly on the fluid pressure
223 within the fault in relation to the external stress field with some impact of poro-elastic stress
224 (Rutqvist et al., 2008). Our use of a relatively high Biot's coefficient will result in a relatively
225 larger vertical expansion of the reservoir and a higher induced shear stress on the bounding
226 faults, which in turn might result in an earlier fault reactivation (at a lower injection pressure)
227 and a larger shear displacement once the fault is reactivated.

228 The multilayered storage system is generally flat-lying (Fig. 3) and it is affected by two
229 high-angle (60°) normal faults (Champlain Fault and Yamaska Fault) that extend SW-NE (Fig. 2)
230 and dip to the SE, displacing the sedimentary units downward to the SE. The Yamaska Fault is
231 located at a shorter distance (1.5 km) from the injection zone, while the Champlain Fault is more
232 distant (4.4 km). The normal faults are designed in the model as 30 m wide. According to applied
233 ubiquitous-joint model, a series of parallel weak planes (joints) with a dip angle of 60° and a
234 spacing of 10 m is assigned within the fault. Weak planes are assumed to have a normal and
235 shear stiffness of 5 GPa/m, and designed with cohesion 0.5 MPa, with a friction angle of 25° , a
236 dilation angle of 0° and no tensile strength. For simplicity, the faults are extended up to the
237 surface in the model (Fig. 3), although no upward continuation of fault planes was interpreted on
238 seismic lines (Fig. 1, cross-sections) above the top of the Utica Shale, probably due to syn-
239 sedimentary nature of faults.

240 The block modeled for CO_2 injection in the Becancour area is located between the
241 Champlain and the Yamaska Faults (Fig. 3). The vertical well A198 SOQUIP Petrofina Becancour
242 No 2 is used for simulation of CO_2 injection because it is one of few wells that penetrate the
243 bottom of reservoir unit of the Covey Hill Formation and it is not located too close to the
244 Yamaska Fault (Figs 2, 3). The injection zone or bottom of the injection well is located at $X =$

245 10275 m, Z = - 1180 m, at 1540 m from the Yamaska Fault and at 4430 m from the Champlain
 246 Fault (Fig. 3).

247 The NW-SE West and East Transverse Faults bound the modeled block in the SW and the
 248 NE, respectively (Fig. 2). The East Transverse Fault is suggested from the analysis of the time
 249 structure of the Grenvillian basement (Thériault et al., 2005). The West Transverse Fault is
 250 interpreted as a lineament detected from the remote sensing data (Matton et al., 2011), which is
 251 correlative with a strong linear gradient of the magnetic survey data, and across which high
 252 variation of fluid pressure gradient (Fig. 2) is observed.

253 The average maximum in-situ horizontal stress (S_{Hmax}) in the St. Lawrence Lowlands (Fig. 1)
 254 is oriented $N59^{\circ}E \pm 20^{\circ}$ (Konstantinovskaya et al., 2012). The stress gradients (Table 2) in the
 255 region have been previously estimated for depths < 4 km (Konstantinovskaya et al., 2012) as
 256 $\Delta S_{hmin} 20.5 \pm 3$ kPa/m, $\Delta S_v 25.6$ kPa/m, $\Delta S_{Hmax} 40 \pm 7.5$ kPa/m, that indicates a strike-slip stress
 257 regime with $S_{hmin} < S_v < S_{Hmax}$ (Konstantinovskaya et al., 2012). The 2D model of the Becancour area
 258 is oriented sub-parallel to S_{hmin} (X-axis) and S_v (Z-axis) and sub-orthogonal to S_{Hmax} (Y-axis)
 259 stresses (Fig. 2). As the model is two-dimensional and orthogonal to S_{Hmax} orientation (Fig. 3), the
 260 relation between two principal stresses acting in the model plane ($S_{zz} = S_v$ and $S_{xx} = S_{hmin}$)
 261 corresponds to the extensional stress regime ($\Delta S_{hmin} = 0.7 \Delta S_v$), where ΔS_{hmin} is equal to 18 kPa/m
 262 (Table 2).

263 The average fluid pressure P_{f0} gradient is estimated from the analysis of drill stem test
 264 (DST) data in vertical wells (Konstantinovskaya et al., 2012) and it is about 9.8 kPa/m for the St.
 265 Lawrence Lowlands. The fluid pressure gradient is elevated to an average of 12.17 kPa/m (Table
 266 2) within the modeled block of the Becancour area (Fig. 2) that is compatible with the elevated
 267 brine density 1.13–1.29 g/cm³ and salinity (Table 1) in this area (Massé, 2009). The higher value
 268 of P_{f0} gradient of 15.6 kPa/m is observed to the SW of the West Transverse Fault in the
 269 Becancour area (Fig. 2) that likely indicates the presence of a separate confined reservoir and
 270 may be associated with the sealing character of the fault. The fluid pressure gradient to the NW
 271 of the Champlain Fault is 10.4 kPa/m (L. Massé, personal communication).

272 The temperature gradient (Table 2) in the Becancour area is 23.5°C/km with an average
 273 surface temperature 8°C (Tran Ngoc et al., 2012).

274 With the above gradients, the minimum principal stress at the depth of the injection zone
275 around the injection well (about 1 km depth) is about 18 MPa, whereas the vertical stress is
276 about 26 MPa. Moreover, the initial reservoir pressure is about 12 MPa and initial temperature is
277 about 31 °C. Thus, a pressure build-up of 6 MPa would lead to well pressure of a magnitude
278 similar to that of the minimum principal stress. This might be relevant when considering limits on
279 the injection pressure as an injection pressure about the minimum principal stress could
280 theoretically lead to the formation of a vertical hydraulic fracture. However, the injection-
281 induced stress evolution is more complex and we also need to consider the potential for fault
282 reactivation as will be considered in the current reservoir-geomechanical model simulations.

283 Constant pressure, saturation, and temperature conditions are assumed at the top and
284 bottom boundaries of the 2D model (Fig. 3). The left and right boundaries are closed for fluid and
285 heat flow. Null displacement conditions are set normal to the left, right and bottom boundaries,
286 whereas stress is set to the top, left and right boundaries. Note though that the left and the right
287 boundaries are far away from the hydraulically bounding faults meaning that whether they are
288 simulated as open or closed boundaries, it does not have an impact on the simulation results at
289 the central part of the model. All simulations presented in this study are carried out as
290 isothermal, i.e. without taking into account the cooling effect of injected CO₂. The maximum
291 time of injection is 30 years.

292 3. RESULTS

293 The observation of fault zone rocks and estimation of fault seal capacity are first discussed
294 in order to evaluate the likely range of fault permeability that may be attributed to the
295 Champlain and the Yamaska Faults in the reservoir-geomechanical modeling of CO₂ injection in
296 the Becancour area.

297 3.1 Fault permeability

298 The vertical offset of high-angle normal faults in the St. Lawrence Lowlands is varying
299 along their strike (Fig. 1) that results in lateral change of lithological units superimposed across
300 the fault plane. For example, the vertical offset across the Saint-Cuthbert Fault progressively
301 grows toward the NE varying from 30 m at its SW tip, where limestones of the Trenton Group are
302 superimposed (Fig. 1), up to 367 m in its central segment, where the fault separates the
303 Grenvillian basement and limestones of the Trenton Group (Globensky, 1987 and references

304 therein). The along-strike variation of vertical offset of faults controls the composition of fault
305 zone rocks and the volume of shales slipped along fault planes and, consequently, the sealing
306 capacity of faults.

307 The possible range of permeability of the Yamaska and the Champlain Faults buried below
308 caprock units in the Becancour area (Fig. 1) is evaluated from (1) observations of comparative
309 faults zones exposed at the surface on the northern shore of the St. Lawrence River, (2) the
310 description of cuttings from well A027 Saint-Angele No 1 that penetrates the Yamaska Fault zone
311 (Fig. 2), and (3) 2D estimation of fault seal capacity based on shale-gouge ratio and well-log data.

312

313 3.1.1 Fault zone rocks

314 The field observations of fault zones (Fig. 1) were collected along the major normal faults
315 exposed at the surface on the northern shore of the St. Lawrence River including the Saint-
316 Cuthbert, Saint-Alban, Deschambault, Jacques Cartier, Neuville, Montmorency and Cap
317 Tourmente normal faults that belong to the same system of the SW-NE high-angle normal faults
318 as the Champlain and the Yamaska Faults.

319 The studied fault zones are generally composed of fragmented wall rocks, whose
320 composition depends on the vertical offset of faults (Fig. 1). The SW segment of the Saint-
321 Cuthbert Fault and the Saint-Alban Fault are characterized by low (<30 m) vertical offset
322 displacing argillaceous limestones of the Trenton Group. The fault rocks along these faults are
323 represented by shale-cemented calcareous breccia. The normal faults with greater vertical throw
324 separate the caprock units (Utica Shale and Lorraine Group) and the Grenvillian basement (Fig.
325 1). The Neuville (202 m) and the Montmorency (>180 m) faults, which are exposed at the
326 surface, and the Champlain (>300 m) and the Yamaska (>800 m) faults that are buried at depth,
327 belong to this group of faults.

328 The Montmorency Fault in the Quebec City area (Fig. 4a) represents the eroded analog of
329 the Yamaska and the Champlain Faults in the Becancour area (Fig. 3). The footwall of the
330 Montmorency Fault is composed of metamorphic rocks of the Grenvillian basement recovered
331 by relatively thin relic layers of limestones of the Trenton Group. The hanging wall consists of
332 limestones of the Trenton Group, Utica shales and siliciclastic rocks of the Lorraine Group. The
333 vertical offset of the Montmorency Fault is estimated to be at least 180 m if the minimum

334 thickness of the Trenton Group is taken as 100 m (Fig. 4a). However, the vertical offset is likely to
335 be greater (300-400 m) as thickness of the Trenton Group in closely located wells is varying from
336 190 m to 335 m (drilling reports for wells A257 and A175, see Appendix).

337 The fault zone of the Montmorency Fault (Fig. 4b) is filled with continuous 15-20 cm-thick
338 smears of calcareous shales dragged into the fault plane from the shale interlayers of the
339 Trenton Group in the hanging wall. The shales smears in the fault zone and in the upper part of
340 the Trenton Group are similar in composition to the overlying Utica calcareous shales. The
341 boudinated lenses of limestones are dragged in the fault zone and extended parallel to the fault
342 plane within the calcareous shale matrix (Fig. 4b). The gneisses of the footwall demonstrate
343 ductile deformations, sinistral strike-slip horizontal striation and contain zones of cataclastic
344 breccia 30-40 cm thick. The breccia is composed of angular gneissic fragments, which are solidly
345 cemented by fine-grained crushed gneiss matrix.

346 The presence of shales smeared along the fault plane as a 15-20 cm-thick continuous layer
347 is strongly supportive for the sealing behaviour of the observed segment of the Montmorency
348 Fault. This continuous shale smears have been formed in the fault segment, along which only the
349 Trenton Group is downthrown for at least 180 m, while the overlying Utica shales of the hanging
350 wall are located above the observed fault segment (Fig. 4a). One may expect that the presence
351 of continuous shale smears is even more probable for the faults with higher vertical offset, such
352 as the Champlain (300-550 m) and the Yamaska (800-1200 m) Faults (Table 3), because not only
353 the Utica shales but also the major part of the Lorraine Group are slipped along their fault planes
354 (Fig. 3).

355 The Yamaska Fault was penetrated by well A027 Sainte Angele No 1 (Fig. 2), which cut
356 through the caprock units of the Lorraine Group and the Utica Shale and the intermediate units
357 of the Trenton Group and entered granite and metamorphic rocks of the Grenvillian basement at
358 depth of 1553 m. According to the description of cuttings from the well (Farish, 1933), the
359 contact between the limestones and the metamorphic rocks is faulted. The transition zone
360 (about 3 m) is composed of dark grey calcareous shales with well-marked slickensides and calcite
361 vein. The observations of highly saline water were reported during the drilling along the faulted
362 contact between the Trenton Group and the Precambrian.

363 3.1.2 Fault seal capacity

364 Fault seal capacity for the Champlain and the Yamaska Faults is estimated along 2D
 365 vertical cross-sections (Fig. 5) using the shale gouge ratio (SGR) method (Freeman et al., 1998;
 366 Yielding et al., 1997). The SGR at a given point on a fault plane is estimated as a volume of shale
 367 in slipped interval past the point:

$$368 \quad \text{SGR} = \Sigma (V_{\text{sh}} \times \Delta z) / t \times 100\%,$$

369 where V_{sh} is the volume of shale in a given unit, Δz is the thickness of the unit, and t is the
 370 throw window. The volume of shale is calculated using natural radioactivity (GR) of rocks from
 371 well log data (Doveton, 1986):

$$372 \quad V_{\text{sh}} = (\text{GR} - \text{GR}_{\text{clean}}) / (\text{GR}_{\text{shale}} - \text{GR}_{\text{clean}}),$$

373 where GR is radioactivity of a given rock interval, GR_{clean} is the baseline of lowest
 374 radioactivity rocks and GR_{shale} corresponds to the baseline radioactivity of 'normal' shales (as
 375 opposed to uranium-rich shales). The shale volume in the lithological units decreases from 0.95
 376 at the top to 0.1 at the base of the St. Lawrence Lowlands succession (Table 3).

377 The vertical offset (throw) is increasing downward along the Champlain and the Yamaska
 378 Faults (Table 3) because continued slip has occurred along the fault planes during the
 379 sedimentation as a result of the Taconic orogeny and progressive deepening of the St. Lawrence
 380 Lowlands basin.

381 The shale gouge ratio progressively increases upward from 7% to 95% along the
 382 Champlain and the Yamaska Faults (Fig. 5) as the volume of shale in the slipped hanging wall
 383 grows toward the top of the stratigraphic succession (Table 3). The $\text{SGR} > 15\text{-}20\%$ usually
 384 characterizes faults with presence of shale smears on the fault plane and static sealing behaviour
 385 (Yielding et al., 1997). For example, the fault from the Oseberg Syd Field of the Norwegian shelf
 386 with $\text{SGR} 18\%$ seals and it is able to support a minimum cross-fault pressure difference of 0.8
 387 MPa (Freeman et al., 1998). Accordingly, the upper fault segments of the Champlain and the
 388 Yamaska Faults with $\text{SGR} > 17\text{-}21\%$ (Fig. 5) would likely have continuous shale smears and
 389 behave as a seal. Indeed, the shale smears similar in composition to the Utica calcareous shales
 390 were observed in the Yamaska fault zone in well A027 (Farish, 1933).

391 The Yamaska Fault is thus expected to have sealing behaviour along the segment with SGR
392 >17%, which is located at the same level and above the footwall reservoir sandstones of the
393 Covey Hill Formation targeted for CO₂ injection (Fig. 5b). The upper segment of the Champlain
394 Fault with SGR>21% must also be sealing (Fig. 5a). The lower segment of the Champlain Fault
395 with SGR 7-11% might be permeable but fault-orthogonal fluid flow across the lower fault
396 segment is very unlikely due to the presence of low-permeable rocks of the Grenvillian basement
397 on the opposite side of the fault plane (Fig. 5a). The sealing behaviour of the Champlain Fault in
398 the Becancour area is supported by variations in fluid pressure observed on each side of the fault
399 (Fig. 2).

400 3.2 Reservoir geomechanical coupled simulations

401 Three injection rates of 0.06 kg/s, 0.3 kg/s and 1kg/s are tested by numerical simulations
402 (Table 4) to predict fault stability during CO₂ injection in the Becancour 2D model. The absolute
403 values of the used injection rates are set lower than the full 3D field values because of the very
404 restricted width (100 m) of the 2D model along the Y axis (Fig. 3) that otherwise results in
405 unrealistically rapid fluid pressure build-up around the injection well. The pressure build-up
406 achieved for an injection rate of 0.06 kg/s in the 2D model with Y axis of 100 m is consistent with
407 the pressure build-up at 3D injection rate of 4.5 kg/s (0.15 Mt/yr.) simulated in radial model with
408 radius of 3.5 km by Tran Ngoc et al.(2012). The injection rate of 0.1-0.2 Mt/yr. is applied in pilot
409 and small-scale CCS projects (GCCSI, 2012). The injection rates of 0.3 kg/s and 1 kg/s in the 2D
410 model may be correspondingly compared with the 3D injection rates of 23 kg/s (0.8 Mt/yr.) and
411 75 kg/s (2.5 Mt/yr.), respectively (Table 4). These injection rates are compatible with CO₂
412 volumes stored in large-scale integrated CCS projects (GCCSI, 2012). It is the rate of pressure
413 build-up and the pressure magnitude relative to the in situ stress field that is most important for
414 the potential and timing of fault reactivation (Rutqvist, 2012). By varying the injection rate we
415 consider a range of pressure build-up and pressure magnitudes that might occur at the real field
416 setting when exposed to the injection.

417 Two values of fault permeability are tested: 10^{-18} m^2 for the sealing fault behaviour and 10^{-16}
418 m^2 for the permeable fault (Table 4). In first case, fault permeability is equal to the
419 permeability of the Utica shales (Table 1) that is supported by A027 well data and field
420 observations (Fig. 4b) and by the composition of the hanging wall slipped past the reservoir units
421 of the Covey Hill Formation in the footwall (Fig. 5b). In second case, fault permeability is equal to

422 the matrix permeability k_m of the reservoir sandstones (Table 1). The permeable fault behaviour
 423 is tested because in some cases, strong directional permeability contrast may exist along the
 424 fault damage zone allowing along-fault fluid circulation even if orthogonal fluid flow is closed
 425 (Agosta et al., 2012; Arch and Maltman, 1990). The higher fault permeability may also be
 426 induced as a result of brittle and dilatant deformations related to shear slip and volumetric
 427 changes of fault material under critical state when the fluid pressure approaches the minimum
 428 horizontal stress.

429 Two values of rock mass permeability are tested for the reservoir units of the Covey Hill
 430 and the Cairnside Formations (Table 4) assigned as 10-x (series 1, k_1) and 100-x (series 2, k_2)
 431 higher than respective values of matrix permeability k_m of these units (Table 1).

432 The resulting variations in several parameters (Tables 5 and 6) are analysed during the
 433 simulations as a function of changes in initial values of injection rate, fault and reservoir
 434 permeability (Table 4). We analysed the fluid pressure build-up around the injection well (Figs 6,
 435 7a), vertical surface uplift above the injection zone (Fig. 7b), effective shear strain increment (a
 436 measure of the shear strain from the start of the injection defined as the second invariant of the
 437 deviatoric strain tensor) in the injection zone and along fault zone (Figs 7d, 8-11; 14), slip along
 438 the Yamaska Fault (Fig. 7c), tensile fracturing above the injection zone (Fig. 12) and CO₂ plume
 439 growth and displacement (Fig. 13). The potential for tensile fracturing is calculated using the
 440 assumption that a tensile failure may occur in a unit as fluid pressure exceeds the minimum
 441 compressive stress, i.e., in the Becancour 2D model, the effective stress $S_{hmin}^* = S_{xx}^*$ becomes
 442 positive.

443 Series 1. Low reservoir permeability $k_1 = 10k_m$

444 Simulation 1a (injection rate 0.06 kg/s, sealing fault behaviour).

445 The fluid pressure increases around the injection well within the sedimentary succession
 446 below the caprock 1 of the Utica Shale (Fig. 6a). Most of the fluid pressure build-up occurs
 447 between the injection well and the Yamaska Fault, while the pressure increase is much less
 448 significant in the direction of the Champlain Fault (Fig. 6a). At the beginning, the fluid pressure
 449 build-up in the injection zone is higher than at the Yamaska Fault but it equalises in these areas
 450 at the end of run (Fig. 7a). The fluid pressure increase is 1.8 MPa around the well, 1.7 MPa at the

451 Yamaska fault and 0.5 MPa at the Champlain Fault after 30 years of injection (Fig. 7a, Table 5).
452 The vertical surface uplift above the injection well is 2 cm at the end of run 1a (Fig. 7b).

453 Injection-induced shear strain occurs mostly around the injection zone within the Covey
454 Hill reservoir unit propagating laterally with time (Fig. 8). The magnitude of shear strain in the
455 Yamaska fault zone remains smaller than around the well (Fig. 7d; Table 5) and no fault
456 reactivation is observed (Fig. 8). No significant shear strain occurs along the Champlain fault.

457 The effective horizontal stress S_{xx} * remains negative (i.e. compressive) within and above
458 the injection zone (Fig. 12a). The CO₂ plume is about 0.5 km wide after 30 years of injection (Fig.
459 13a; Table 5).

460 Simulation 2a (injection rate 0.3 kg/s, sealing fault behaviour).

461 The fluid pressure increases up to 8.3 MPa and 7.5 MPa around the well and in the
462 Yamaska Fault, respectively, at a simulation time approaching 30 years (Fig. 7a, Table 5). The
463 vertical displacement (uplift) of the surface above the injection well is 9 cm at the end of the run
464 (Fig. 7b).

465 The injection-induced shear strain (Fig. 7d) in the injection zone is the same as in the
466 Yamaska Fault until the fault is reactivated as a normal fault at 22.5 years. At this time, the
467 injection-induced pressure increase is about 7 MPa at the well and 6.5 MPa at the Yamaska fault.
468 That is, the well pressure has increased from an initial 12 MPa (at about 1 km depth) to 19 MPa,
469 which is just above the minimum principal stress magnitude. After reactivation, the shear strain
470 increases more rapidly along the fault than around the well (Fig. 7d). The Yamaska fault is initially
471 reactivated below the caprock units, within the 300 m-long fault segment that separates the
472 intermediate units (Beekmantown and Trenton Groups) in the footwall from the caprock 2
473 (Lorraine Group) in the hanging wall (Fig. 9b). During subsequent steps (Fig. 9b-d), the slip along
474 the fault propagates both upward and downward but remains below the caprock 2 units. The
475 Champlain Fault is not affected by deformation in this simulation.

476 The slip along the Yamaska Fault zone is 1 cm (Fig. 7c) and the length of the reactivated
477 segment is 600 m at 30 years (Fig. 9d). Note that in these simulations the fault reactivates
478 gradually and in a stable aseismic manner over many years of pressure build-up. This is related to
479 the perfectly plastic constitutive model applied to the fault in this case, whereas more abrupt slip
480 events could occur if using a strain-softening plastic model as in Cappa and Rutqvist (2011a).

481 Nevertheless, the timing for the initiation of fault reactivation and the total slip at the end of the
482 simulation will be similar for perfectly plastic and strain-softening models.

483 The effective minimum horizontal stress S_{xx}^* is reduced to -2 MPa in the area above the
484 injection zone due to the increase of fluid pressure but it remains negative (i.e. in compression)
485 (Fig. 12b; Table 5). Thus, even though the injection pressure has exceeded the initial minimum
486 principal stress in the injection reservoir, the effective minimum stress is still in compression and
487 hydraulic fracturing would not occur. The effective minimum stress still remains in compression
488 because the pressurization of the reservoir also results in an increase in horizontal stress within
489 the reservoir. Such local reservoir stress change along with injection or production is a well-
490 known phenomenon in oil and gas reservoir engineering and results from poro-elastic stress
491 changes that have an impact on the potential for tensile and shear failure within and around the
492 reservoir (Hawkes et al., 2005; Rutqvist, 2012; Rutqvist et al., 2008). The CO₂ plume is about 0.9
493 km wide after 30 years of injection (Fig. 13b; Table 5).

494

495 Simulation 3a (injection rate 0.3 kg/s, permeable fault behaviour).

496 The fluid pressure build-up around the injection zone and in the Yamaska Fault in run 3a is
497 the similar to that of run 2a reflecting the same injection rate (Fig. 7a, Table 5). The total
498 increase in vertical surface uplift above the injection zone is 9 cm at the end of run 3a, which is
499 also similar to run 2a (Fig. 7b; Table 5).

500 Shear strain localizes along the Yamaska fault earlier than in run 2a, at 18.2 years of
501 injection (Fig. 7c). Thus, fault reactivation is initiated at a slightly lower injection pressure
502 probably as a result of more rapid pressure diffusion into the fault. Shear slip initially localizes in
503 the 60 m-long fault segment that separates the caprock 1 (Utica Shale) in the footwall and
504 caprock 2 (Lorraine Group) in the hanging wall (Fig. 10b). After the reactivation, shear failure
505 along the Yamaska fault progresses upward and downward (Fig. 10c), eventually reaching the
506 surface (Fig. 10d). The slip along the Yamaska Fault is 4 cm at 30 years (Fig. 7c; Table 5). No shear
507 strain increase occurs along the Champlain Fault.

508 The increase in effective minimum horizontal stress S_{xx}^* in simulation 3a is the same as in
509 run 2a and it remains negative (i.e. compressive) (Table 5). The CO₂ plume is about 0.9 km wide
510 after 30 years of injection (Fig. 13b).

511 Simulation 4a (injection rate 1.0 kg/s, sealing fault behaviour).

512 The fluid pressure build-up in run 4a is higher than in the previous simulations and it
513 reaches 18.8 MPa at the well and 16 MPa at the Yamaska Fault after 17.9 years of injection (Fig.
514 7a, Table 5). The vertical surface uplift above the injection well reaches 20 cm at 17.9 years (Figs
515 7b).

516 The increase in shear strain is concentrated along the Yamaska Fault at 7.3 years (Fig. 11b),
517 signifying the initiation of fault reactivation. At this time, the pressure build-up has reached 12
518 MPa at the injection well and about 7 MPa at the Yamaska fault (Table 5). Thus, the pressure
519 build-up at the Yamaska fault leading to fault reactivation is about the same as run 2a and 3a.
520 The 7 MPa pressure build-up at the Yamaska fault represents a total pressure of about 19 MPa,
521 which is just above the minimum principal stress (about 18 MPa), whereas the total pressure at
522 the injection well (about 24 MPa) is much higher than the minimum principal stress. The shear
523 slip is initiated along the 330 m-long fault segment that separates the intermediate units
524 (Cairnside and Theresa Formations) in the footwall and the caprock 2 units (Lorraine Group) in
525 the hanging wall (Fig. 11b). The fault reactivation progressively propagates upward and
526 downward affecting the whole sedimentary succession at 17.9 years (Fig. 11c-d). The increase in
527 - shear strain grows faster along the fault than in the injection zone after the fault is reactivated
528 at 7.3 years (Fig. 7d). The slip along the Yamaska Fault is 12 cm and 17 cm after 17.9 and 30
529 years of injection, respectively (Fig. 7c; Table 5).

530 A zone of positive effective minimum horizontal stress S_{xx}^* starts to form above the
531 injection zone within the intermediate units of the Trenton Group and the Theresa Formation
532 after 10 years of injection (Fig. 12c; Table 5). At 17.9 years (Fig. 12c), the zone of positive S_{xx}^*
533 involves the area between the top of aquifer 2 (Cairnside Formation) and the base of caprock 1
534 (Utica Shale) due to strong fluid pressure build-up (Fig. 7a) localized below the caprock units. The
535 positive values of the effective horizontal stress testify for the potential of tensile fracturing in
536 the more fragile (Table 1, Young modulus) intermediate units. However, the thick part (460 m) of
537 the caprock 2 units (Lorraine Group) likely remains intact where S_{xx}^* is still negative, i.e. in
538 compression (Fig. 12c).

539 The CO₂ plume grows about 1.7 km wide after 30 years of injection (Fig. 13c). The plume
540 spreads asymmetrically, faster in the NW direction, away from the Yamaska Fault, and slower
541 toward the fault (Fig. 13c). The upward migration of the CO₂ plume is limited by the base of the
542 intermediate units (Theresa Formation).

543 Series 2. High reservoir permeability $k_2=100k_m$

544 Fluid pressure increases more homogeneously over the large area between the Champlain
545 and the Yamaska Faults in simulations 1b-4b (Fig. 6b) if compared to runs 1a-4a (Fig. 6a). High
546 rock mass permeability of the reservoir units (Table 4) results in rapid fluid propagation away
547 from the injection well and fast fluid flow dispersion in the aquifers between two reservoir-
548 bounding faults. Consequently, fluid pressure build-up in high-reservoir permeability runs 1b-4b
549 is systematically lower than in the previous simulations 1a-4a for corresponding injection rates
550 (Fig. 7a). The increase of fluid pressure in the injection zone and at the Yamaska Fault equalises
551 very rapidly, after 5-10 years of injection (Fig. 7a; Table 6). The surface vertical uplift above the
552 injection well is less significant if compared to the runs of series 1 (Fig. 7b; Table 6).

553 The Yamaska Fault is not reactivated after 30 years of injection in simulations 1b-2b with
554 sealing fault behaviour. Shear slip occurs along the 60 m-long fault segment after 27.5 years of
555 injection (Fig. 7d; Table 6) and reaches 0.5 cm at 30 years (Fig. 7c) in run 3b with injection rate
556 0.3 kg/s and permeable fault properties (Table 6). Shear failure occurs along the 330 m-long
557 segment of the Yamaska Fault at 7.8 years in run 4b at an injection rate of 1 kg/s (Figs 7d, 14a)
558 and shear slip is 10 cm at the end of run (Fig. 7c; Table 6). In both cases in which reactivation
559 occurred (3b and 4b), the reactivation occurred once the total fluid pressure at the Yamaska fault
560 reached a magnitude similar to that of the minimum principal stress.

561 The Champlain Fault remains stable in series 2 runs and it is reactivated only in run 4b with
562 high injection rate after 30 years of injection (Fig. 14d; Table 6). The fluid pressure build-up in the
563 hanging wall of the fault increases up to 16 MPa after 30 years of injection. The shear failure
564 occurs along the deep-seated 500 m-long fault segment that separates the reservoir units of the
565 Covey Hill Formation in the hanging wall and the Grenvillian basement in the footwall and
566 continues below the reservoir level (Fig. 14d). The relative displacement along the Champlain
567 Fault reaches 2.5 cm.

568 The effective minimum horizontal stress S_{xx}^* remains negative (i.e. in compression) and
569 tensile fracturing does not occur in the simulations with high reservoir permeability except in run
570 4b with high injection rate (Table 6). In this case, tensile fractures may start to form locally in the
571 intermediate unit of the most fragile (Table 1) Theresa Formation at 17.8 years. The zone of
572 positive S_{xx}^* (Fig. 12d) is much less important than in run 4a at 17.9 years (Fig. 12c). As the fluid
573 pressure increases below the caprock units, the zone of positive S_{xx}^* grows progressively in run
574 4b and involves all intermediate units (Beekmantown and Trenton Groups) and the base of

575 caprock 1 (Utica Shale) after 30 years of injection (Table 6). The S_{xx}^* remains lower in run 4b
576 (Table 6) than in run 4a (Table 5) at 30 years.

577 The CO₂ plume grows wider, up to 2 km, (Fig. 13d; Table 6) in the high-reservoir
578 permeability runs than in simulations with low reservoir permeability under the same injection
579 rate (Fig. 13c; Table 5). The vertical migration of the CO₂ plume is also more pronounced in the
580 simulations with high-reservoir permeability and low and medium injection rates (Figs 13a, b).
581 Similar to the runs of series 1, the CO₂ plume propagates asymmetrically, faster in the direction
582 opposite to the Yamaska Fault (Fig. 13b, d) as the fluid pressure build-up between the fault and
583 the injection well is more significant than toward the Champlain Fault (Fig. 6b).

584

585 4. DISCUSSION

586 The coupled reservoir-geomechanical (TOUGH-FLAC) modeling undertaken in this study
587 shows that fluid pressure build-up around the injection well and in the Yamaska fault zone
588 strongly depends on the injection rate: the higher is the injection rate, the stronger is the fluid
589 pressure build-up observed around the well and in the fault zone at the end of run (Fig. 7a,
590 Tables 5 and 6). Moreover, the simulation shows that the initiation of fault reactivation at the
591 Yamaska is strongly dependent on the pressure build-up at the fault. The increase of fluid
592 pressure in the injection zone is higher than along the Yamaska fault at the beginning of injection
593 and it equalizes at about 30 years (Fig. 7a) due to lateral fluid flow from the well to the fault. The
594 fluid pressure equilibrium is achieved faster, after 5-10 years of injection, in the simulations 1b-
595 4b with high reservoir permeability (Fig. 7a).

596 The model setting parameters applied in 2D plane strain model of the Becancour area
597 more likely characterise a lower bound of the maximum sustainable injection pressure and an
598 upper bound of possible fault slip magnitude and rupture area. As mentioned, this is because in
599 a full 3D system, there are segments of the fault away from the 2D section that would not be
600 pressurized and where the fault is not reactivated that would tend to restrict shear movements
601 along the faults. Moreover, the global permeability of the reservoir units might be higher than
602 applied in simulations 10^{-15} - 10^{-14} m² (Table 4) due to the presence of extensive natural fractures
603 that means fluid pressure build-up in the injection zone and at the faults would be lower as it is
604 supported by respective changes of ΔP_f observed in series 1 and 2 runs (Fig. 6). Additionally, the
605 width of faults is taken as 30 m and the entry pressure of fault rocks - at low value of 40 kPa to

606 test the worst case of high conductivity along fault plane. However, the field data presented
607 above suggest fault width of the Montmorency and the Yamaska faults is rather limited by 10 m
608 maximum, at least for the upper 1.5 km of depth, and their fault planes contain shale smears,
609 the rocks that generally characterized by much higher entry pressure (e.g. AL-Bazali et al., 2005).
610 If these considerations are taken into account, the risk of fault reactivation as presented in our
611 simulations is overestimated. The better constraints on CO₂-brine relative permeability and rock
612 compressibility of the intermediate and caprock units would be helpful in sensitivity analysis of
613 shear-slip risk evaluation as these parameters may affect the injection-induced fluid pressure
614 build-up (Mathias et al., 2011a).

615 Fluid pressure increase around the injection zone is asymmetrical, being higher in the area
616 between the injection zone and the Yamaska Fault than toward the more distant Champlain
617 Fault (Fig. 6). The lateral fluid flow toward the Yamaska Fault is restrained within short-distance
618 area (1.5 km) by the sealing behaviour of the fault and/or the low-permeable caprock 2 units
619 (Lorraine Group) in the hanging wall. This results in a higher fluid pressure build-up around the
620 Yamaska Fault than in the opposite direction toward the Champlain Fault (Fig. 6). Consequently,
621 the CO₂ plume grows laterally faster in the direction away from the Yamaska fault (Fig. 13),
622 toward the area with lower fluid pressure build-up.

623 Fault reactivation is controlled to a large extent by the pressure build-up at the fault which
624 in turn depends on the injection rate and the distance between fault and injection well. The
625 Yamaska Fault located closer (1.5 km) to the injection zone is reactivated more promptly than
626 more distant (4.4 km) Champlain Fault. Higher injection rate results in earlier reactivation of the
627 Yamaska Fault (Fig. 7c) due to higher fluid pressure build-up (Fig. 7a). For example, the Yamaska
628 Fault is reactivated at 7.3 years for an injection rate of 1 kg/s and only at 22.5 years when the
629 injection rate is 0.3 kg/s (Fig. 7c) in simulations of series 1. As a result, the total fault slip is more
630 significant in the simulations with earlier fault reactivation and higher injection rates (Fig. 7c).
631 The Champlain Fault is generally not reactivated; the shear failure along the fault is observed
632 (Fig. 14d) only after 30 years of injection in simulation with high injection rate (1kg/s) and high
633 permeability of reservoir units.

634 The localization of shear failure along pre-existing high-angle normal faults depends on
635 initial fault permeability. Under the sealing fault behaviour, shear slip on the Yamaska Fault
636 occurs along the fault segment located mostly below the caprock units and above the targeted

637 reservoir in the footwall (Fig. 9b-d). The fluid flow moving from the injection well to the fault
638 zone is likely trapped below the inclined sealing fault plane, where the fluid pressure build-up
639 causes the fault reactivation. When the fault is permeable, shear failure is initiated along the
640 fault segment located within the caprock 1 units of the footwall (Fig. 10b); afterward, it
641 progresses upward and downward reaching the surface (Fig. 10c-d). The fluid flow spreads from
642 the injection well toward the fault and then propagates upward along the permeable fault zone
643 being kept from across-fault lateral propagation by impermeable caprock 2 units (Lorraine
644 Group) of the hanging wall. The fluid pressure is therefore concentrating within the fault zone at
645 the level of the more rigid, brittle and thin caprock 1 unit (Utica Shale) of the footwall, where the
646 first shear slip occurs (Fig. 10b).

647 The localization of shear failure along high-angle normal faults seems to be also
648 dependent on the location of the injection zone relative to the inclined fault plane. In case of the
649 Yamaska Fault, the injected reservoir is found in the footwall of the fault plane and the shear
650 failure is initiated along the fault segment located above the targeted reservoir (Fig. 9b). In
651 contrast, when the injection is simulated in the hanging-wall reservoir (the Champlain Fault), the
652 rupture occurs along the fault segment located at the reservoir level and below it (Fig. 14d). The
653 result similar to the case of the Champlain Fault was obtained by Cappa and Rutqvist (2001a),
654 who found that the reactivation of a pre-existing high-angle normal fault occurs along the
655 segment located at the reservoir level and below it when CO₂ injection was simulated in the
656 hanging wall of the fault. The difference between the localization of reactivated fault segments
657 in two cases of the reservoir-bounding faults obtained in the present study may be explained by
658 the increase in stresses that occurred in the acute angle between the sealing fault plane and the
659 reservoir due to growing pressure build-up in the reservoir.

660 The timing of fault reactivation, length of rupture and slip rate are affected by initial fault
661 permeability. In case of the Yamaska Fault, shear slip occurs earlier, at 18.2 years, when the fault
662 is permeable (10^{-16} m^2), and later, at 22.5 years, when the fault seals (10^{-18} m^2) under the same
663 boundary conditions (Fig. 7c, runs 2a and 3a). It might be related to the length of the segment,
664 along which shear failure is initiated. When the fault is permeable, the shear deformation is
665 initiated within shorter (60 m) segment of fault plane (Fig. 10b) if compared to the case of
666 sealing fault (300 m) (Fig. 9b) (Table 5). It might take longer time to produce shear slip along a
667 longer and sealing fault segment than along a shorter and permeable fault segment. The slip

668 progresses faster along the permeable fault than along the fault with sealing behaviour. At 5.5
669 years after the fault reactivation, shear slip (Fig. 7c; Table 5) reaches 1.5 cm along the permeable
670 fault (3a) and only 0.3 cm along the sealing fault (2a).

671 The high permeability of the reservoir units (Potsdam Group) reduces the risk of fault
672 reactivation in the Becancour area due to smaller fluid pressure build-up in simulations of series
673 2 (Fig. 7a). In simulations with high-reservoir permeability, shear slip along the Yamaska Fault, if
674 occurs, happens later and over a shorter distance if compared to the simulations of series 1 (Fig.
675 7c). The Champlain Fault is reactivated in simulation with high reservoir permeability and high
676 injection rate due to faster propagation of fluid flow toward the fault and fluid pressure build-up
677 in the hanging wall. However, it is unlikely that high permeability of the reservoir units would be
678 in reality constant over the distance of 4.4 km that separates the Champlain Fault and the
679 injection well. The permeability of the reservoir units is mostly controlled by the presence of
680 natural fractures, while the matrix permeability is low (Table 1). The natural fractures do not
681 necessarily preserve the same density and orientation over the large distance, therefore the
682 reservoir permeability might be variable and reactivation of the Champlain Fault is unlikely.

683 The present study confirms the previous results of reservoir-geomechanical simulations
684 (Rutqvist et al., 2008) that the potential for shear failure along pre-existing fault is higher than
685 the potential for tensile fracturing in caprock units. In simulations 2a-3a with medium injection
686 rate, the effective minimum horizontal stress S_{xx}^* above the injection zone remains negative
687 after 30 years of injection indicating that no tensile fracturing would form (Fig. 12a-b), while the
688 Yamaska Fault is already reactivated at 18-22 years (Figs 9-10). In simulation 4a with high
689 injection rate, S_{xx}^* becomes positive after 10 years of injection (Fig. 12c) meaning possible
690 development of tensile fracturing of the intermediate units, while shear slip along the Yamaska
691 fault occurred earlier, after 7.3 years of injection (Fig. 11b).

692 Our results suggest tensile fracturing might occur in relatively more rigid and brittle
693 intermediate units (Beekmantown and Trenton Groups) starting in the most brittle rocks of the
694 Theresa Formation and the Utica Shale above the injection zone (Fig. 12c; Table 1). However, it
695 happens only after 10 years of continuous injection in the case of extremely high injection
696 pressure (much higher than the minimum principal stress at the injection reservoir) as a result of
697 high injection rate and low-reservoir permeability (run 4a, Table 5). Nevertheless, the thick (460
698 m) part of the caprock 2 unit (Lorraine Group) in this case remains intact for fracturing being

699 located within the zone of negative (i.e. compressive) effective minimum horizontal stress. The
700 risk of tensile fracturing under high injection rate is much lower if the reservoir units are
701 characterized by higher reservoir permeability (Fig. 12d). The estimation of the risk of tension
702 fracturing associated with injection-induced fluid pressure build-up likely represents the upper
703 limit of tension fracturing predictions as the sandstones of aquifers 1 and 2 may have higher
704 global permeability than applied in simulations due to the presence of natural fractures.
705 Additional measurements would be necessary to evaluate the uncertainty related to capillary
706 and entry pressure in the caprock units.

707 No tensile fracturing or fault shear slip occurs in the 2D Becancour model (Y=100 m) after
708 30 years of injection under the low-injection rate of 0.06 kg/s, which corresponds to the 3D
709 injection rate of 4.5 kg/s (0.15 Mt/yr.) in a radial model (r=3300 m), i.e. pilot or small-scale CCS
710 project. The simulation shows criterion for a sustainable (bottom-hole) injection pressure would
711 be to keep it below the magnitude of the minimum principal stress at the depth of the reservoir,
712 i.e. below 18 MPa for the depth of about 1 km as such an injection pressure would be unlikely to
713 initiate reactivation. The similar conclusion was made after the estimation of regional stress
714 magnitude (Konstantinovskaya et al., 2012). Moreover, even if reactivation is initiated the
715 simulations show that it takes years of injection and further pressure build-up to reactivate a
716 substantial rupture area that could propagate outside the injection zone and provide a leakage
717 path.

718 Finally, the surface uplift above the injection zone in the case of low-injection rate (run 1)
719 is small, varying from 1 cm to 2 cm at 30 years depending on the rock mass permeability of the
720 reservoir units (Fig. 7b; Tables 5, 6). Higher injection rates result in higher surface uplift above
721 the injection zone varying from 9 cm (runs 2-3) to 27.5 cm (run 4) after 30 years of continuous
722 injection (Fig. 7b; Tables 4, 5). In simulations with the same injection rates but higher
723 permeability of the aquifer units, the surface uplift is less pronounced (Fig. 7b; Table 6) for CO₂
724 plume propagates laterally further from the injection well along the aquifers 1 and 2 (Fig. 13d).

725 No CO₂ leakage after the fault reactivation can be expected in the Becancour area as the
726 simulations results suggest. Even under high injection rates and long-term fault reactivation
727 (runs 4a, 4b), the CO₂-saturated plume does not reach the Yamaska fault zone. The CO₂ plume
728 lateral dimensions are up to 2 km in diameter maximum (Table 6) and it is forced to migrate
729 away from the fault zone (Fig. 13) by asymmetric fluid-pressure build-up between the injection

730 well and inclined fault plane (Fig. 6). The local fracturing of intermediate and caprock 1 units that
731 started at 10 years of injection under high injection rates into the low-permeable reservoir units
732 (Fig. 12c; Table 5) seems not to allow the upward migration of CO₂ plume, which remains
733 trapped below tight intermediate units (Fig. 13c). Additionally, the caprock 2 units (Lorraine
734 Group) would have prevented its upward migration for no throughout-caprock breach has been
735 occurred in the experiments (Fig. 12). However, upward migration of brine along the Yamaska
736 Fault might be expected in case of permeable fault behaviour and/or up-to-the surface fault-
737 plane shear reactivation (runs 3a, 4a, 4b) under long-term high injection rates (Figs 10, 11, 14),
738 similar to a putative storage site in the southern North Sea (Hannis et al., 2013). An
739 understanding of brine flux along the fault as a migration pathway and environment impacts
740 would need to be demonstrated in low-probable case of continuing CO₂ injection after shear
741 failure along the Yamaska Fault.

742 Further studies would be necessary to evaluate lateral changes of fault sealing capacity
743 along the Yamaska fault to better understand the risk of fault reactivation and constrain the
744 possible timing and localization of shear failure along the fault plane within a 3D model of the
745 Becancour area. The along-strike variations in vertical offset and in orientation of fault plane
746 relative to present-day stresses may cause lateral changes in permeability and in effective
747 normal and shear stress acting on the fault plane that would influence the size of rupture area
748 and, consequently, the magnitude of induced seismicity. 3D coupled reservoir-geomechanical
749 TOUGH-FLAC modeling would be helpful to test strike-slip reactivation of the regional Yamaska
750 and Champlain Faults under the regional strike-slip stress regime. 3D modeling will also allow us
751 to obtain more realistic absolute values of injection rates that would be reasonable to apply
752 without producing fault reactivation or caprock tensile fracturing.

753 The simulations with thermal option would be necessarily to carry out to better quantify
754 temperature effects on the risk of the caprock breaching. After long-term CO₂ injection,
755 temperature cooling effects can result in local reduction in the lateral stress around the injection
756 well due to thermal contraction of the media, thus placing the overlying caprock in tensile stress
757 (Gor et al., 2013), even though the far-field area thermally equilibrates with injected cold CO₂
758 (Vilarrasa et al., 2013). Indeed, significant changes in lateral stress associated with cold sea-water
759 injection have been noted in the North Sea reservoirs (Dikken and Niko, 1987). The buoyancy-
760 driven migration of CO₂ plume above the injection zone may reinforce the cooling effect of CO₂

761 injection contributing to the risk of caprock integrity. However, it was found that in stress
762 regimes where the maximum principal stress is the vertical (as it is the case of the Becancour 2D
763 model), thermal contraction induced by liquid CO₂ injection rather mobilizes shear slip along pre-
764 existing fractures in the aquifer, while the mechanical stability of the caprock is improved
765 (Vilarrasa et al., 2013).

766 5. CONCLUSIONS

767 The permeability of high-angle normal faults affecting the Early Paleozoic sedimentary
768 succession of the St. Lawrence Lowlands basin is evaluated for the first time. The sealing capacity
769 of the Champlain and the Yamaska Faults that bound the block targeted for CO₂ injection in the
770 Becancour 2D model decreases with depth. The upper fault segments are characterized by shale
771 gouge ratio (SGR) ranging from 17-21% to 95% and they are expected to behave as a seal. The
772 lower fault segment of the Champlain Fault with SGR 7-11% might be permeable. However, the
773 across-fault fluid flow along the low-SGR fault segment would be prevented by the presence of
774 low-permeable rocks of the Grenvillian basement on the opposite side of the fault plane. The
775 sample descriptions from the well A027, which penetrated the Yamaska Fault, and field
776 observations of the Montmorency Fault confirm the fault planes with SGR > 17% are filled with
777 thick continuous smears of calcareous shales similar to the caprock 1 unit (Utica Shale).

778 The coupled reservoir-geomechanical (TOUGH-FLAC) modeling of CO₂ injection tested at
779 the Becancour 2D model confirms that injection may be carried out safely for at least 30 years
780 with no shear or tensile failure to occur in the area if low injection rates and maximum injection
781 pressure are respected. Our simulations indicate that the injection rate should be controlled
782 such that the reservoir pressure is kept below the minimum compressive stress, which is about
783 18 MPa at reservoir depth (1 km).

784 The simulation results show that the likelihood of reactivating two reservoir-bounding
785 faults (Yamaska and Champlain Faults) strongly depends on reservoir pressure at the faults,
786 which in turn depends on injection rate, hydrological properties of aquifers and the distance
787 between the faults and the injection well.

788 The fluid pressure build-up induced by injection is higher between the injection zone and
789 the inclined Yamaska Fault due to close fault location (1.5 km) and sealing behaviour of the fault
790 plane and the hanging wall. The fluid pressure increase is less significant toward the more distant

791 (4.4 km) Champlain Fault being distributed over larger area. Consequently, the CO₂ plume grows
792 asymmetrically progressing toward the NW and away from the Yamaska Fault thus reducing the
793 risk of CO₂ leakage along the fault plane.

794 Under high injection rate, the Yamaska Fault, which is located closer (1.5 km) to the
795 injection zone has a higher potential to be reactivated than the more distant (4.4 km) Champlain
796 Fault. The localization, timing, rate and length of shear slip along the Yamaska Fault depend on
797 the initial fault permeability. A more permeable fault is reactivated earlier (after 18.2 years of
798 injection) and shear failure is localized at the caprock level, within the segment (60 m) between
799 the Utica Shale and Lorraine Group, progressing subsequently toward the surface. If the fault is a
800 low permeability seal, fault slip occurs later (after 22.5 years of injection) and below the caprock
801 units, along the segment (300 m) separating the intermediate units (Beekmantown-Trenton
802 Groups) and the caprock 2 units (Lorraine Group). The shear slip progresses faster along a more
803 permeable fault than along the fault with sealing behaviour.

804 High permeability of the reservoir units (Potsdam Group) results in smaller fluid pressure
805 build-up due to more rapid fluid propagation away from the injection zone that reduces the risk
806 of fault reactivation and tensile fracturing. The fault slip along the Yamaska Fault does not occur
807 or it occurs later and the fault slip and surface uplift are less significant in simulations with high-
808 reservoir permeability compared to the low-reservoir permeability runs. The propagation of fluid
809 flow toward the Champlain Fault under the high-reservoir permeability settings triggers its
810 reactivation after 30 years of injection, but it occurs only in the case of high injection rate.

811 The fluid pressure-induced tensile fracturing occurs above the injection zone only in the
812 simulations with high injection rate, in which injection pressure becomes extremely high (much
813 higher than minimum principal stress), and it happens long after shear failure of the Yamaska
814 Fault. Tensile fractures are localized mostly within the more fragile intermediate units
815 (Beekmantown and Trenton Groups) below the caprock system. The thick (460 m) part of the
816 caprock 2 units (Lorraine Group) remains intact above the fractured zone preventing the upward
817 migration of the injected CO₂.

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1019 FIGURE CAPTIONS

1020 Fig. 1. Geological map of the St. Lawrence Lowlands modified after Globensky (1987) and
 1021 Konstantinovskaya et al. (2009; 2012). Stratigraphic units: 1, siliciclastic units of the Queenston,
 1022 Lorraine Groups and Lotbinière Formation, 2, Utica Shale, 3, carbonates of the Trenton, Black
 1023 River and Chazy Groups, 4, dolomites and sandstones of the Beekmantown Group, 5, sandstones
 1024 of the Potsdam Group; 6, thrust; 7, normal fault at surface; 8, normal fault at top of the
 1025 Grenvillian basement (after Thériault et al., 2005); 9, fault observation station. S_{Hmax} orientation
 1026 is shown after Konstantinovskaya et al. (2012a). The numbers along the normal faults indicate
 1027 vertical offset in meters, after Globensky (1987) and references therein and author's data. The
 1028 cross-sections are simplified after interpreted seismic lines from Castonguay et al. (2010);
 1029 vertical scale is given in seconds, two-way traveltime (TWT, s). Fault abbreviations: JF, Joliette;
 1030 SCF, Saint-Cuthbert; SPF, Saint-Prosper; SA, Saint-Albin; DF, Deschambault; JCF, Jacques-Cartier;
 1031 NF, Neuville; MF, Montmorency; CTF, Cap-Tormente; ChF, Champlain; YF, Yamaska; AF, Aston;
 1032 LL, Logan's Line. *TR*, Trois-Rivières; *Bc*, Becancour.

1033 Fig. 2. Time structure of the Grenvillian basement in the Becancour area, modified after Thériault
 1034 et al. (2005). Contour lines of the basement elevation are given in milliseconds, two-way
 1035 traveltime (TWT, ms). The well numbers are given after the MRNF database (see Appendix). See
 1036 Fig. 1 for the map location.

1037 Fig. 3. The 2D geological model of the Becancour area used in the reservoir-geomechanical
 1038 modeling. See Fig. 2 for the cross-section location. Note that for simplicity the normal faults in
 1039 the model are traced up to the surface; although seismic data support the continuation of faults
 1040 occurs only up to the top of the Utica Shale (see Fig. 1, cross-sections).

1041 Fig. 4 Cross-section of the Montmorency Fault (a) and photograph of the fault zone (b). The box
 1042 on the cross-section indicates the location of the photograph. See Fig. 1 for the cross-section
 1043 location.

1044 Fig. 5. The simplified 2D cross-sections used for estimation of shale-gouge ratio (SGR) for the
 1045 Champlain (a) and the Yamaska (b) Faults. Numbers along the fault planes indicate the obtained
 1046 SGR values. Tops and thickness of stratigraphic units presented in the cross-sections (Table 3) are

1047 interpreted from regional well log data, 2D model (Fig. 3) and 3D geological model of the
1048 Becancour area (Claprood et al., 2012). CH* indicates reservoir sandstones of the Covey Hill
1049 Formation (aquifer 1) targeted for CO₂ injection. See more explanation in the text.

1050 Fig. 6. Fluid pressure variations occurred in the reservoir and intermediate units after 30 years of
1051 injection in simulations with low (a) and high (b) reservoir permeability. See Table 4 for initial
1052 parameters. Abbreviations: GB, Grenvillian basement; aq, aquifer; int, intermediate; cp, caprock
1053 units; see Fig. 3 for their stratigraphic analogs.

1054 Fig. 7. Changes in fluid pressure (a), vertical surface uplift above the injection zone (b), fault slip
1055 (c) and effective shear strain increment (d) as a function of time occurred in the injection zone
1056 (well) and along the Yamaska Fault (fault zone) in simulations of series 1 (1a-4a) and series 2 (1b-
1057 4b). See Table 4 for initial and Tables 5 and 6 for resulting parameters. S_{xx}^* is effective minimum
1058 horizontal stress.

1059 Fig. 8. Changes in effective shear strain occurred around the injection zone and along the
1060 Yamaska Fault during subsequent steps of run 1a, injection rate 0.06 kg/s, sealing fault
1061 behaviour. No fault reactivation occurs in this simulation. See Table 4 for initial and Table 5 for
1062 resulting parameters. See Fig. 6 for abbreviation symbols.

1063 Fig. 9. Changes in effective shear strain occurred around the injection zone and along the
1064 Yamaska Fault during subsequent steps of run 2a, injection rate 0.3 kg/s, sealing fault behaviour.
1065 Fault slip occurs after 22.5 years of injection, within the segment separating the intermediate
1066 and caprock 2 units (b). Afterward, the shear strain increment diminishes in the injection zone
1067 and deformation localizes mostly along the fault zone (c-d), remaining within the fault segment
1068 below the caprock 2 units. See Table 4 for initial and Table 5 for resulting parameters. See Fig. 6
1069 for abbreviation symbols.

1070 Fig. 10. Changes in effective shear strain occurred around the injection zone and along the
1071 Yamaska Fault during subsequent steps of run 3a, injection rate 0.3 kg/s, permeable fault
1072 behaviour. Fault slip occurs after 18.2 years of injection (b) in the segment separating the
1073 caprock 1 and caprock 2 units. Afterward, the shear strain localizes along the fault and fault slip
1074 propagates toward the surface (c-d). See Table 4 for initial and Table 5 for resulting parameters.
1075 See Fig. 6 for abbreviation symbols.

1076 Fig. 11. Changes in effective shear strain occurred around the injection zone and along the
1077 Yamaska Fault during subsequent steps of run 4a, injection rate 1 kg/s, sealing fault behaviour.
1078 Fault slip occurs after 7.3 years of injection (b) in the segment separating the intermediate and
1079 caprock 2 units. Afterward, the shear strain localizes along the fault and fault slip propagates up
1080 the surface (c-d). See Table 4 for initial and Table 5 for resulting parameters. See Fig. 6 for
1081 abbreviation symbols.

1082 Fig. 12. The fluid-pressure induced changes in effective minimum horizontal stress S_{xx}^* occurred
1083 above the injection zone in simulations of series 1 (a-c) and 2 (d) after 30 (a-b) and 17.9-17.8 (c-
1084 d) years of injection. Negative (i.e. compressive) S_{xx}^* indicates tensile fracturing is unlikely to
1085 form (a, b); zones of positive S_{xx}^* ($P_f > S_{xx}$) correspond to the settings favorable for tensile
1086 fracturing (c, d). The large zone of positive S_{xx}^* occurs in run 4a (c) under high injection rate
1087 within the intermediate units but the thick part (460 m) of the caprock 2 units still remains
1088 intact. See Table 4 for initial and Tables 5 and 6 for resulting parameters. See Fig. 6 for
1089 abbreviation symbols.

1090 Fig. 13. Changes in liquid saturation S_L and geometry of CO₂ plume (cold colors) in the injection
1091 zone after 30 years of injection. The dotted lines indicate CO₂ plume geometry observed in runs
1092 of series 2 compared to runs of series 1 (a, b), or during the progressive steps within the same
1093 runs (c, d). Note the progressive growth of CO₂ plume away from the Yamaska Fault (c, d). See
1094 Table 4 for initial and Tables 5 and 6 for resulting parameters. See Fig. 6 for abbreviation
1095 symbols.

1096 Fig. 14. Changes in effective shear strain occurred around the injection zone and along the
1097 Champlain and the Yamaska Faults during subsequent steps of run 4b, injection rate 1 kg/s,
1098 sealing fault behaviour. The Yamaska Fault is reactivated after 7.8 years of injection (a) in the
1099 segment separating the intermediate and caprock 2 units. Afterward, the shear strain localizes
1100 along the Yamaska fault and fault slip propagates up the surface (b-d). The Champlain Fault is
1101 reactivated after 30 years of injection (d) within the segment separating the targeted reservoir
1102 units of aquifer 1 and the Grenvillian basement. See Table 4 for initial and Table 6 for resulting
1103 parameters. See Fig. 6 for abbreviation symbols.

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1106 TABLES

1107 Table 1. Main representative properties of Lower Paleozoic sedimentary units in the Becancour
1108 area.

1109 Note: The elastic properties E , ν , porosity and matrix permeability data are obtained from
1110 laboratory core analyses; λ , K , and G are calculated from E and ν , after (Zoback, 2010); ^a,
1111 determined from drill stem tests (Tran Ngoc et al., 2012); k vertical = 0.1 x k horizontal; ^b, spacing
1112 between joints. Elastic moduli for the Grenvillian basement are taken as an average granite
1113 value; for the Trenton-Black River-Chazy Groups - as equal to the Beauharnois Fm; the data on
1114 fluid-property parameters (salinity, saturation, capillary pressure and compressibility) are taken
1115 from Tran Ngoc et al. (2012).

1116 Table 2. Changes of stress/pressure and temperature with depth in the Becancour area

1117 Table 3. Estimation of seal capacity for the Champlain and the Yamaska Faults using the shale
1118 gouge ratio method (Freeman et al., 1998; Yielding et al., 1997).

1119 Note: V_{sh} , volume of shale estimated from natural radioactivity (gamma ray) well log data; Z ,
1120 depth of formation tops estimated for the Yamaska Fault as an average value from the 3D
1121 geological model of the Becancour area (Claprood et al., 2012) and for the Champlain Fault from
1122 correlation of regional well data and basement top (Fig. 3). FW, footwall, HW, hanging wall.

1123 Table 4. Initial parameters used in numerical simulations.

1124 Note: CH, Covey Hill Fm; Ca, Cairnside Fm.; k_1 , k_2 , rock mass permeability; k_m , matrix
1125 permeability.

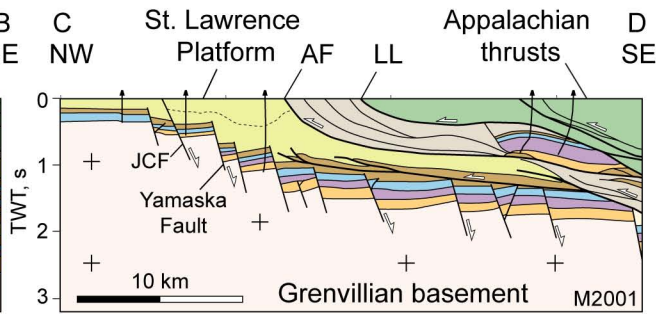
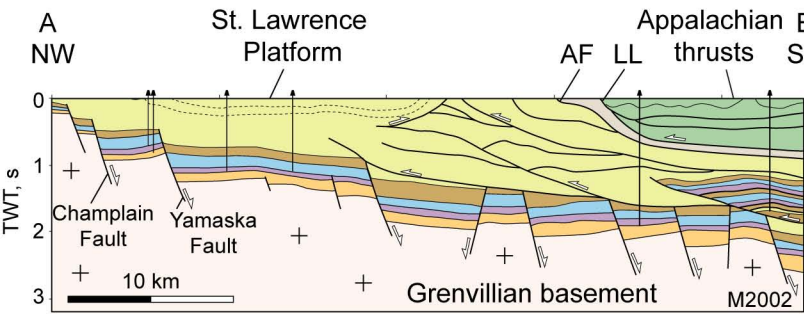
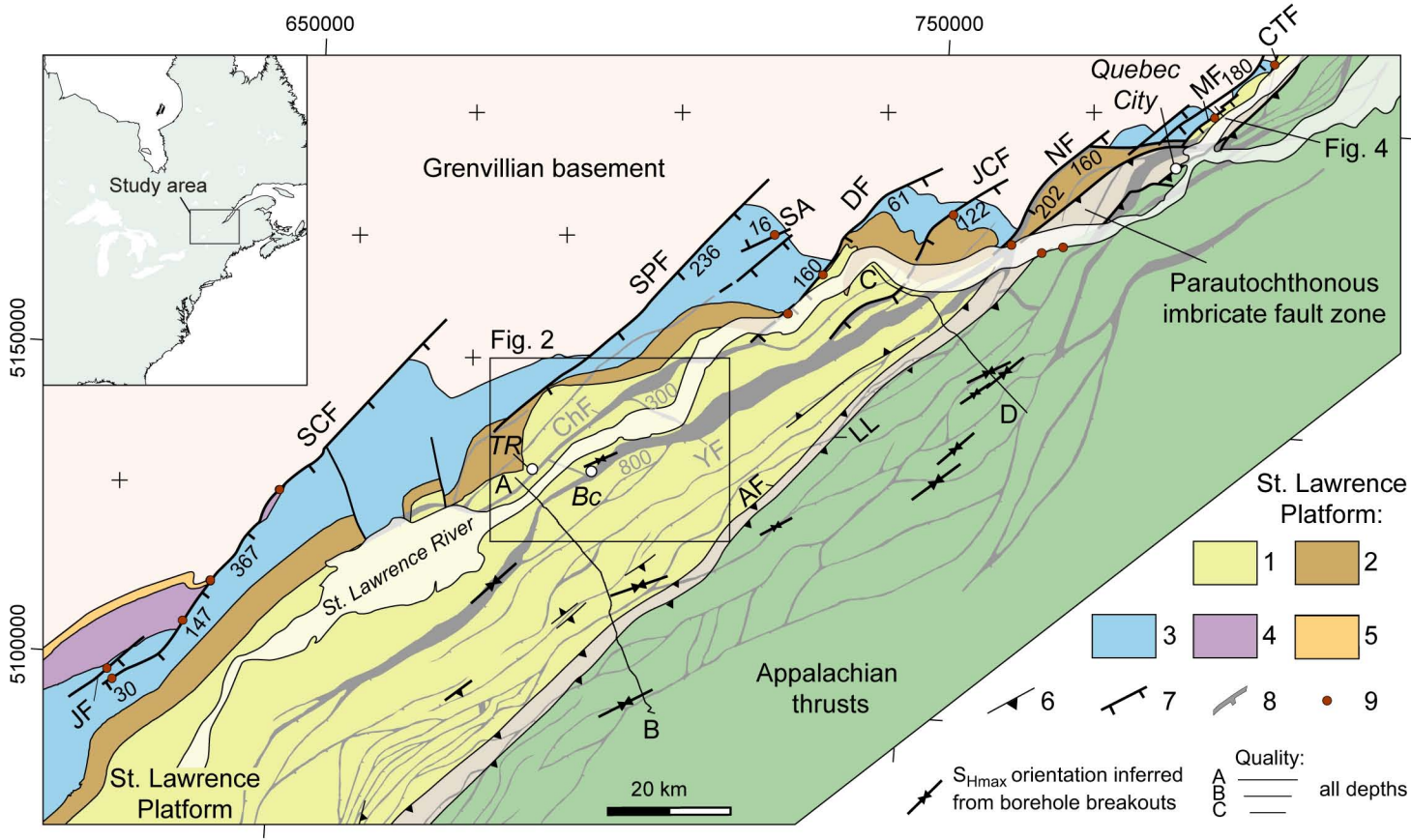
1126 Table 5. Resulting variations in fluid pressure build-up (ΔP_f), effective shear strain increment ($\Delta\gamma$),
1127 surface uplift (h), length of reactivated fault segment (L), maximum fault shear slip (d), effective
1128 minimum horizontal stress (S_{xx}^*) and CO₂ plume width (W) observed in numerical simulations 1a-
1129 4a of series 1 ($k_1 = 10k_m$) for different injection rates (IR) and fault permeability (k_f).

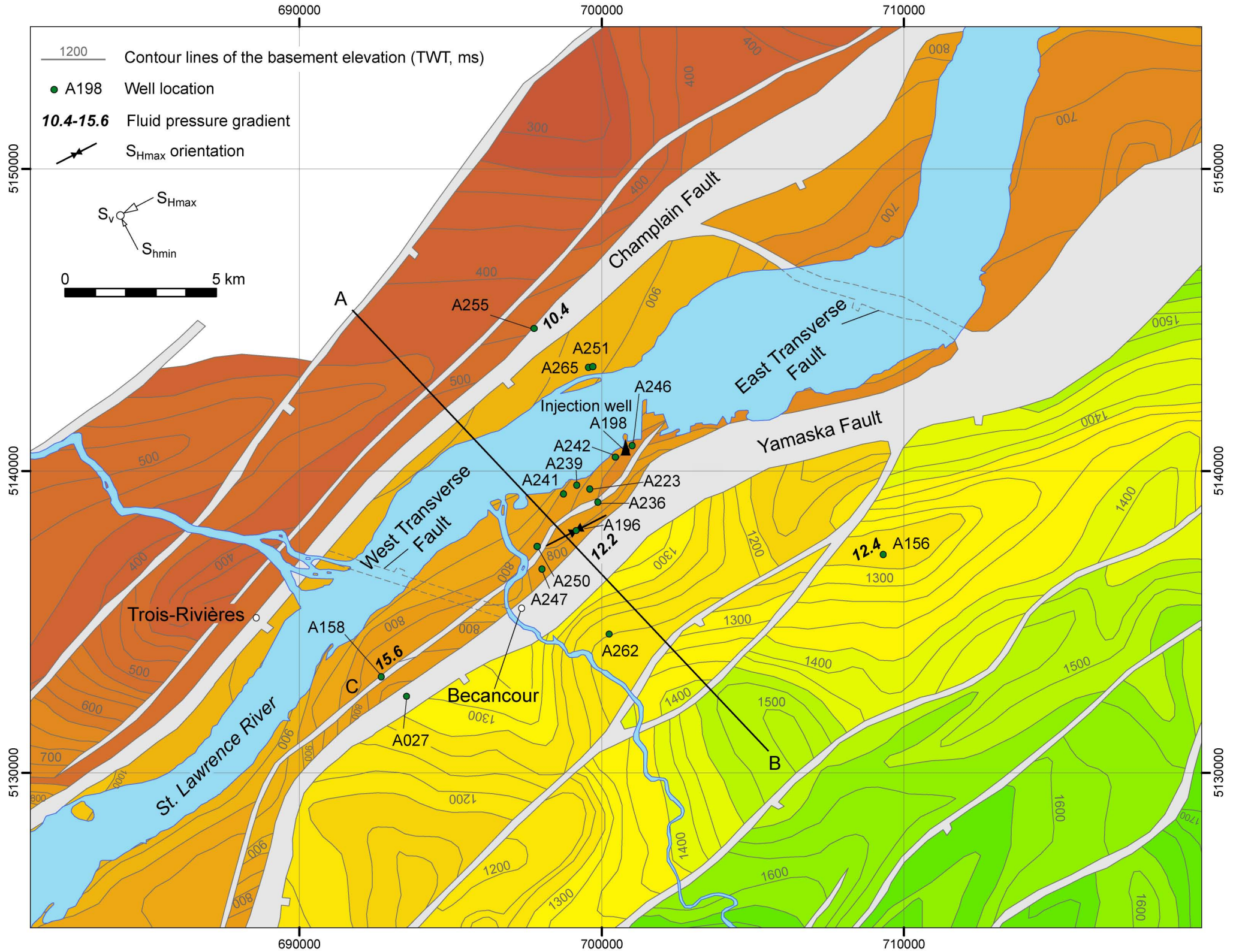
1130 Note: YF, Yamaska Fault; FW unit, footwall unit: CH, Covey Hill Fm; Ca, Cairnside Fm; th, Theresa
1131 Fm; Tr, Trenton Group; Ut, Utica Shale; Lor, Lorraine Group. See Table 4 for the rock mass k_1 and
1132 matrix k_m permeability of the reservoir units.

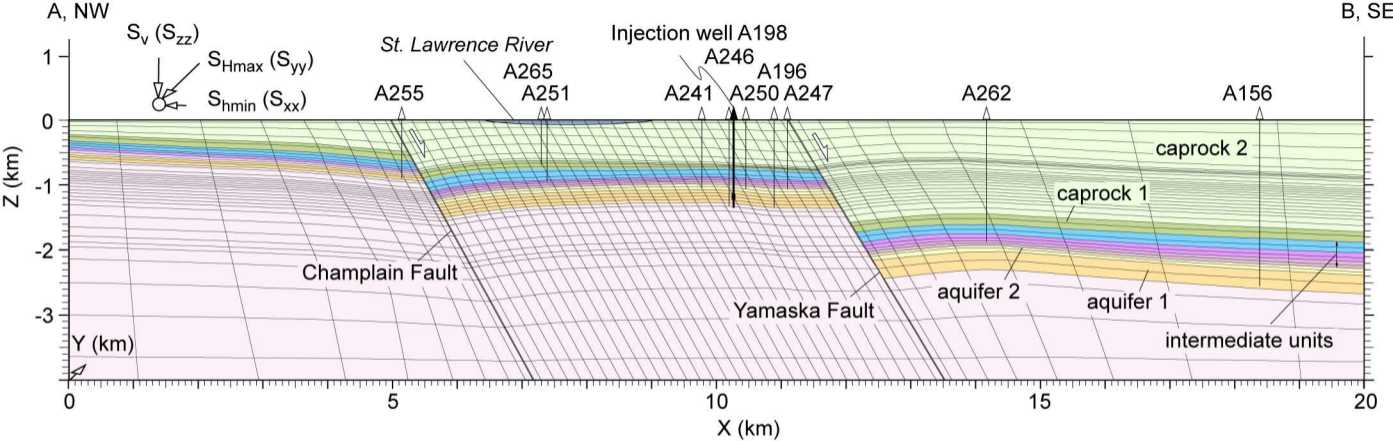
1133 Table 6. Resulting variations in fluid pressure build-up (ΔP_f), effective shear strain increment ($\Delta\gamma$),
1134 surface uplift (h), length of reactivated fault segment (L), maximum fault shear slip (d), effective
1135 minimum horizontal stress (S_{xx}^*) and CO₂ plume width (W) observed in numerical simulations 1b-
1136 4b of series 2 ($k_2 = 100k_m$) for different injection rates (IR) and fault permeability (k_f).

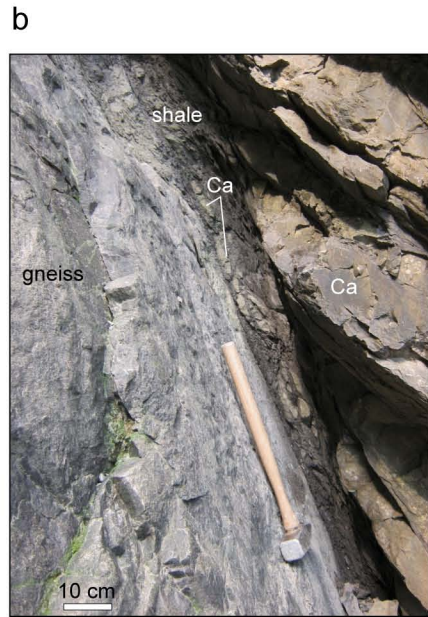
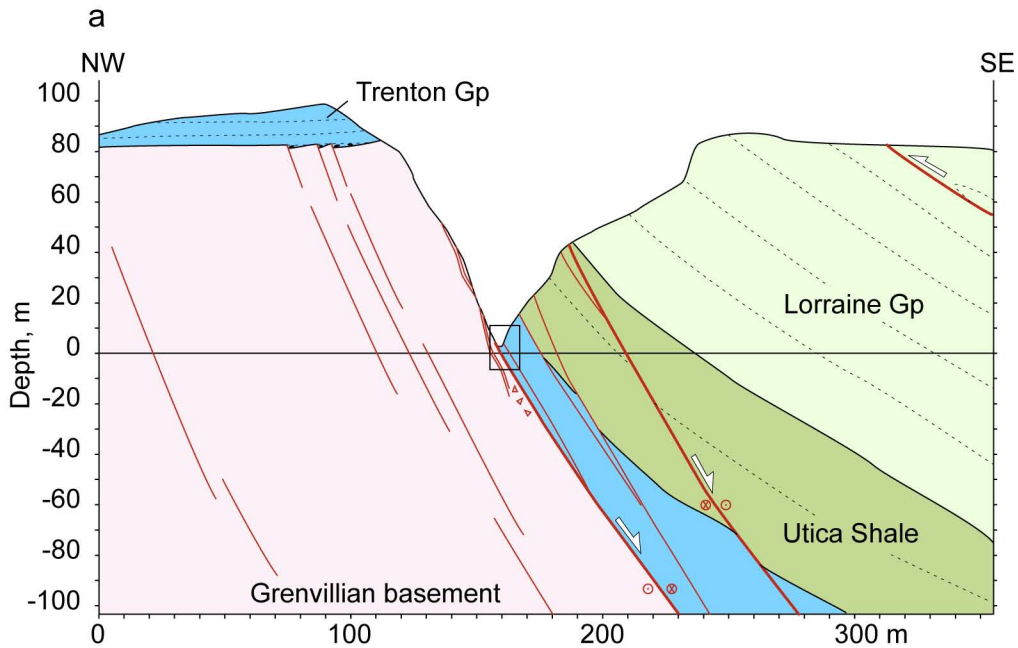
1137 Note: YF, Yamaska Fault; ^a, reactivation of the Champlain Fault; FW unit, footwall unit: GB,
1138 Grenvillian basement; CH, Covey Hill Fm; Ca, Cairnside Fm; th, Theresa Fm; Tr, Trenton Group;
1139 Ut, Utica Shale; Lor, Lorraine Group. See Table 4 for the rock mass k_2 and matrix k_m permeability
1140 of the reservoir units.

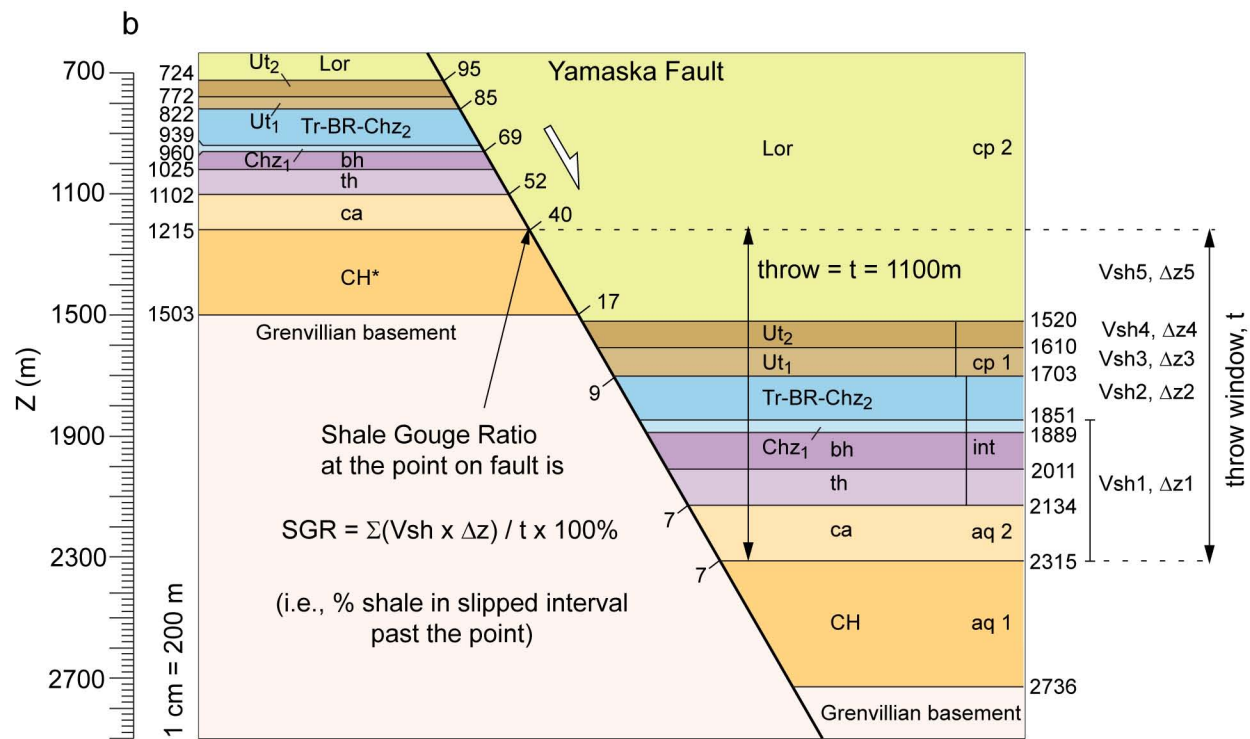
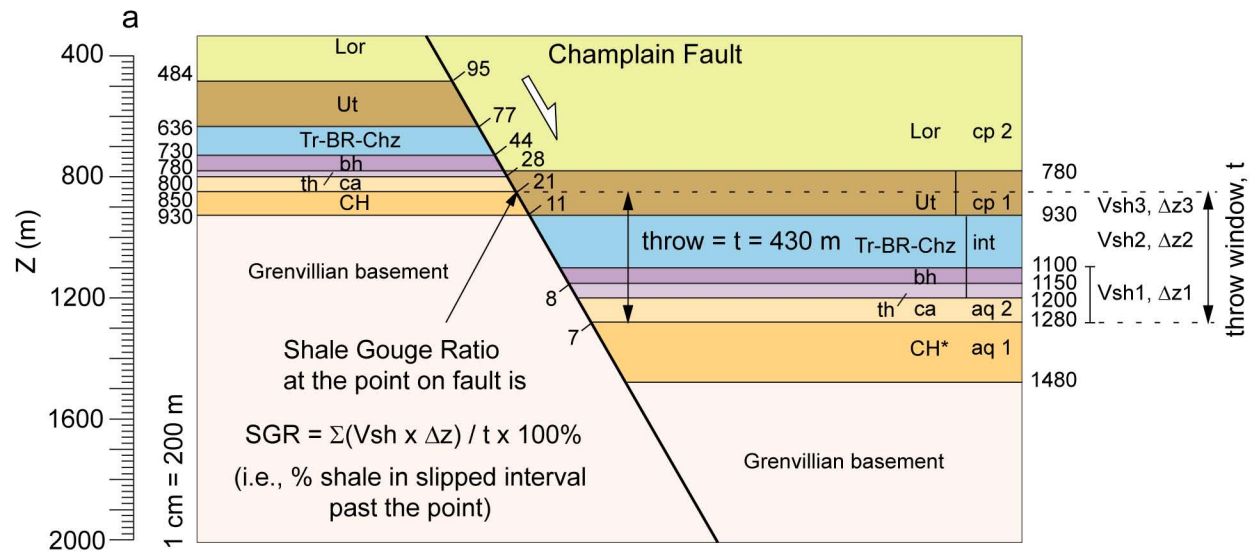
1141 Appendix. Name and location of wells in the St. Lawrence Lowlands cited in present study. See
1142 Fig. 2 for well location.





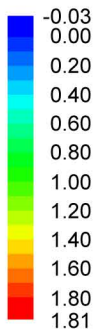






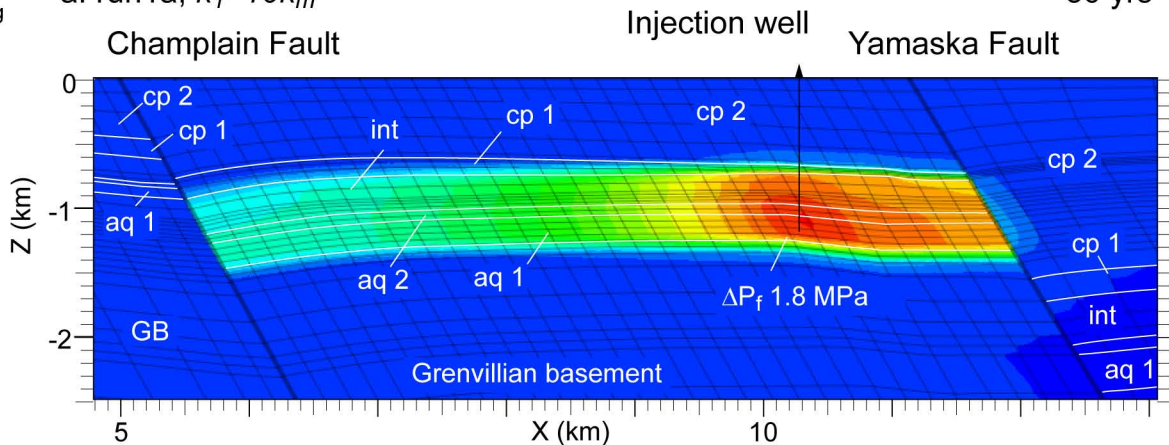
Calculated by
volumetric averaging

Fluid pressure build-up (MPa)



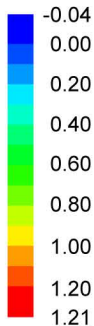
a. run1a, $k_1=10k_m$

30 yrs



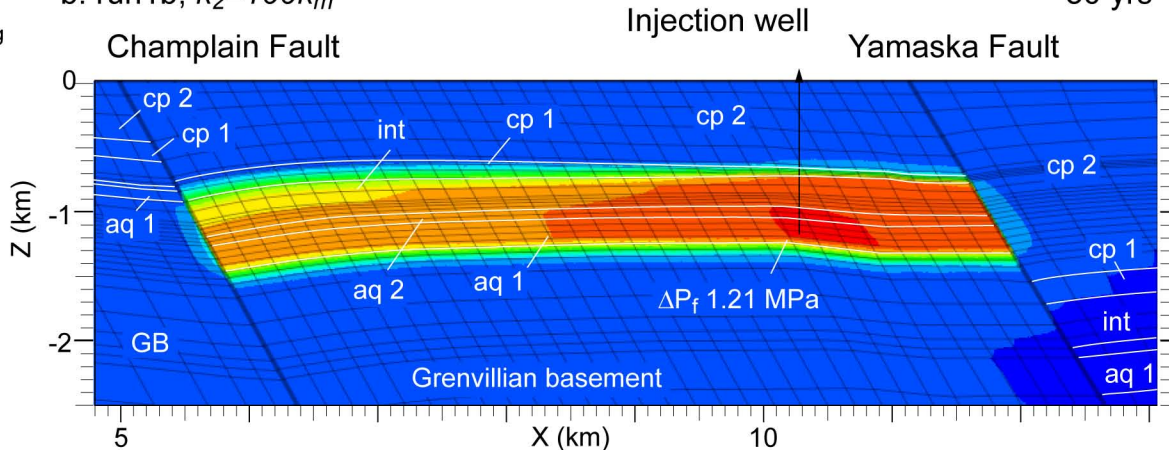
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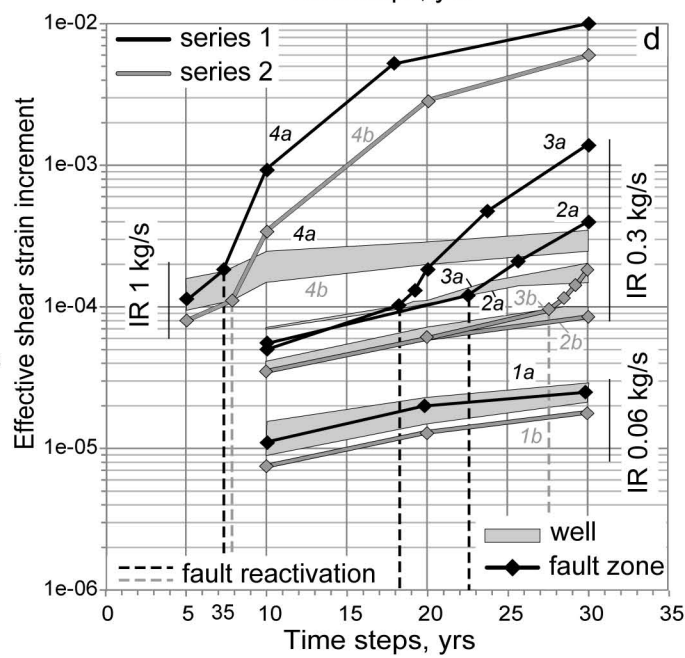
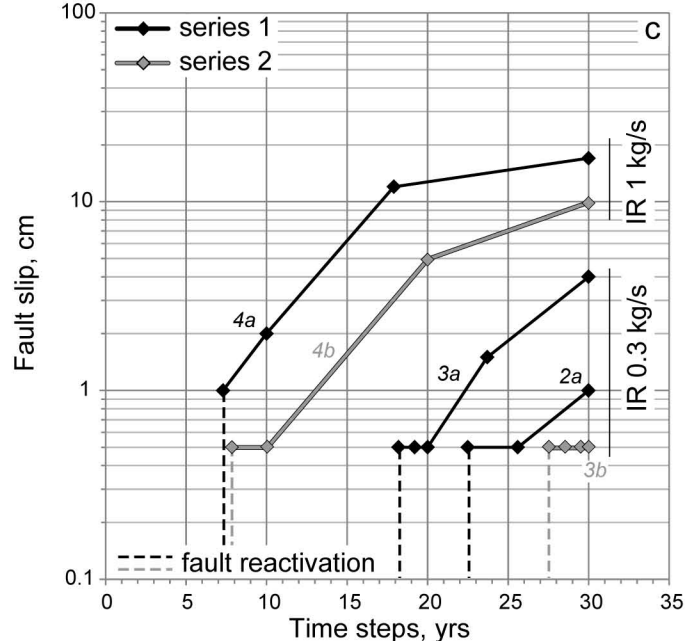
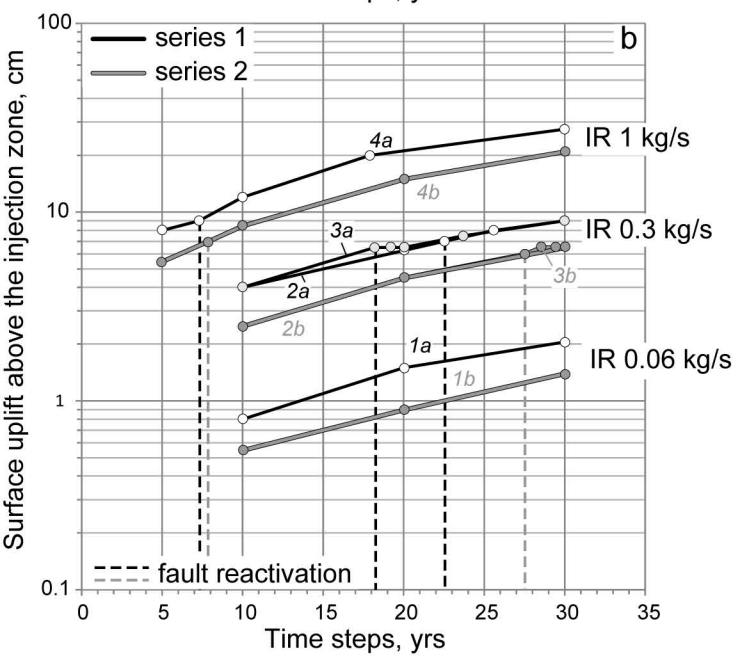
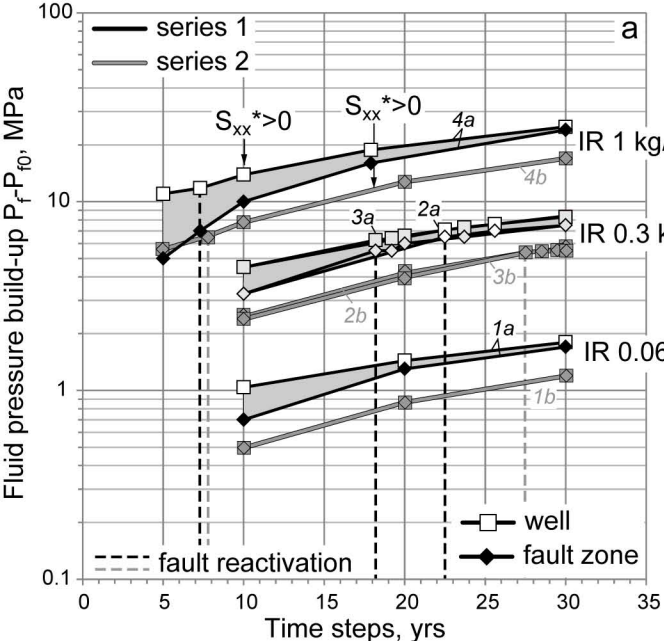
Fluid pressure build-up (MPa)

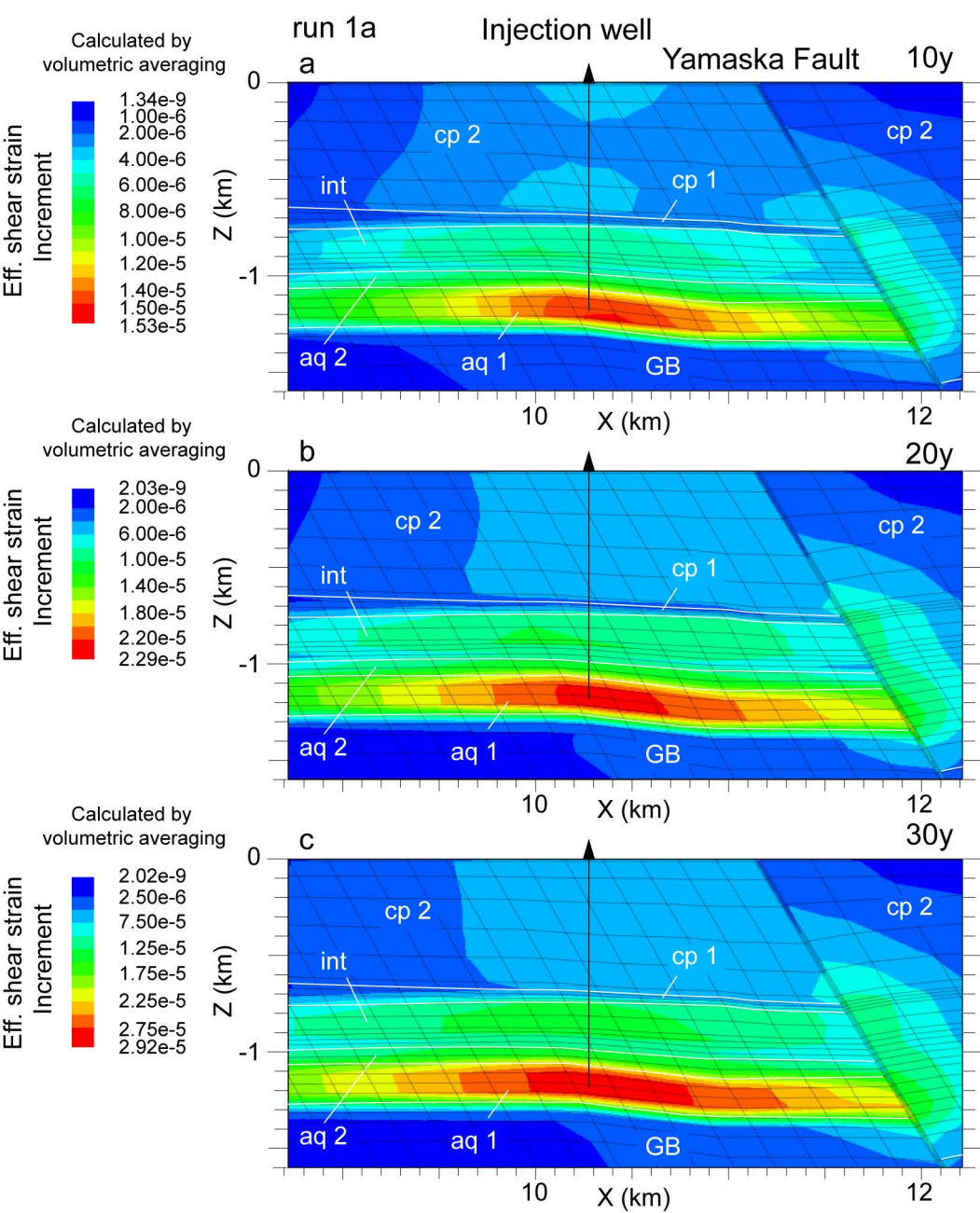


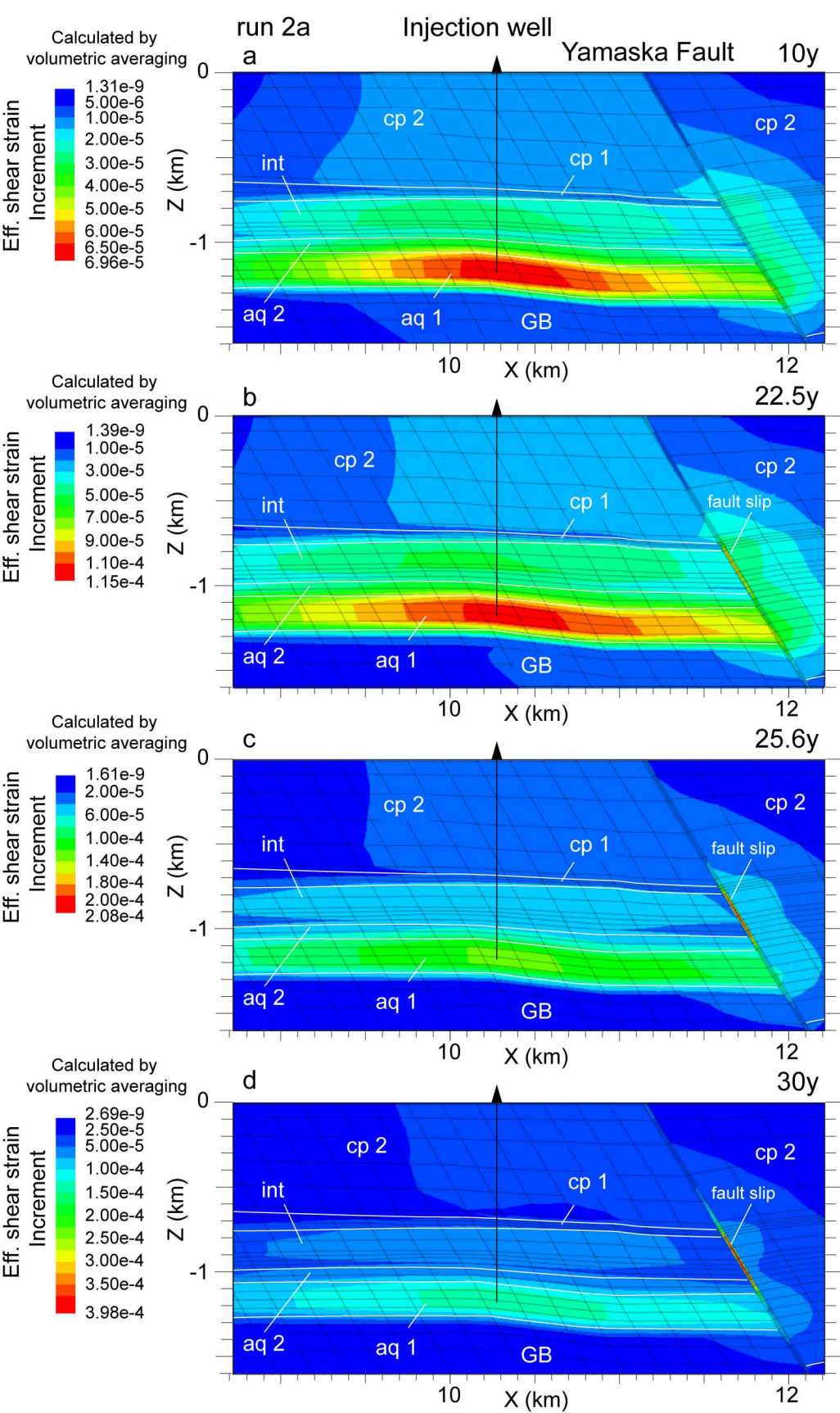
b. run1b, $k_2=100k_m$

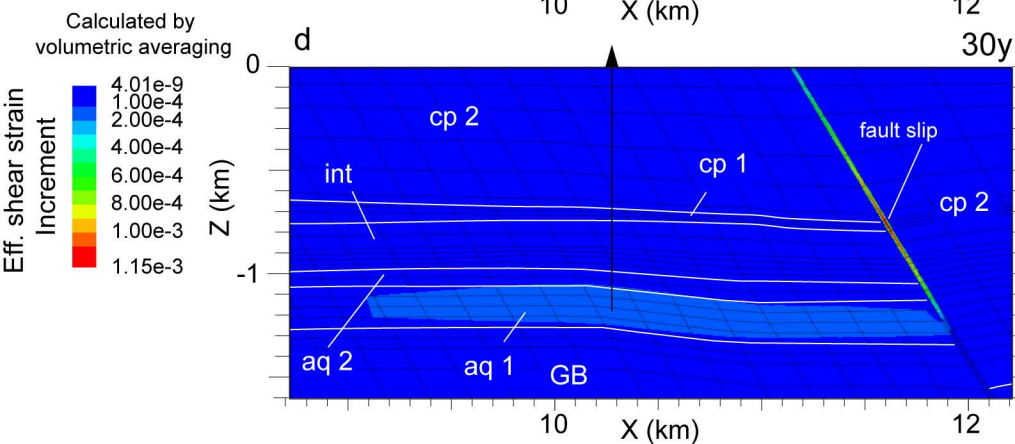
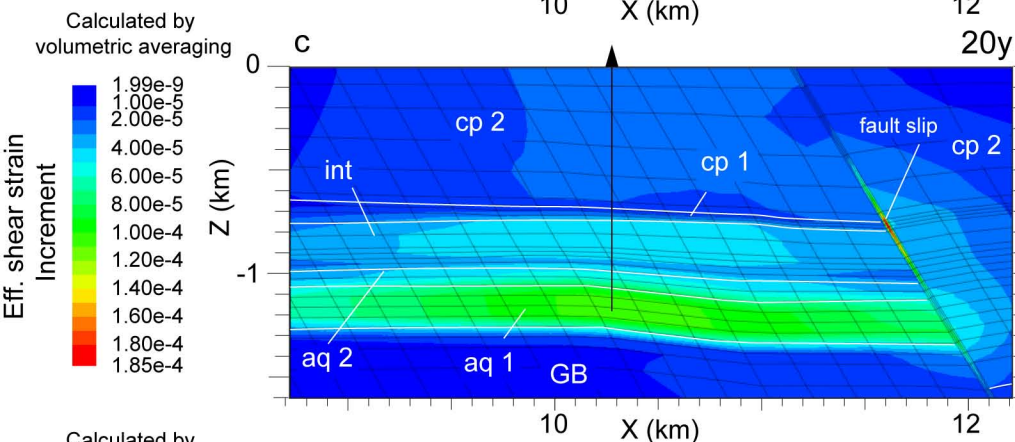
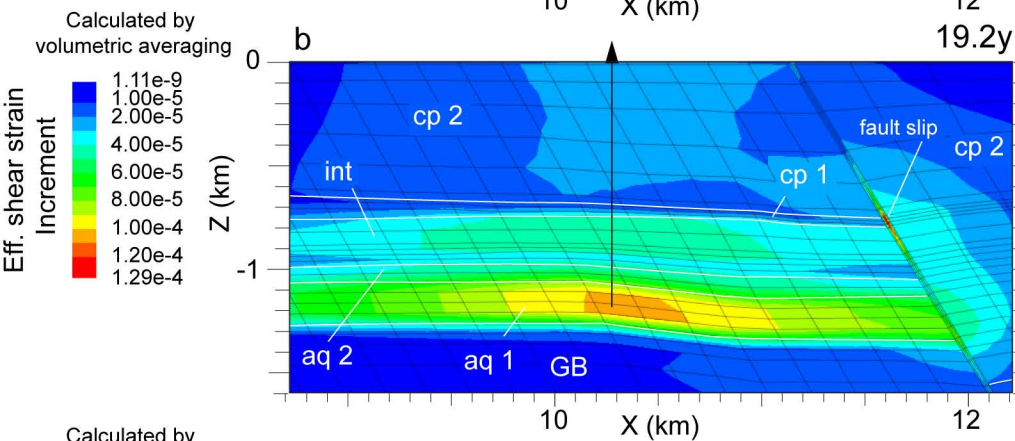
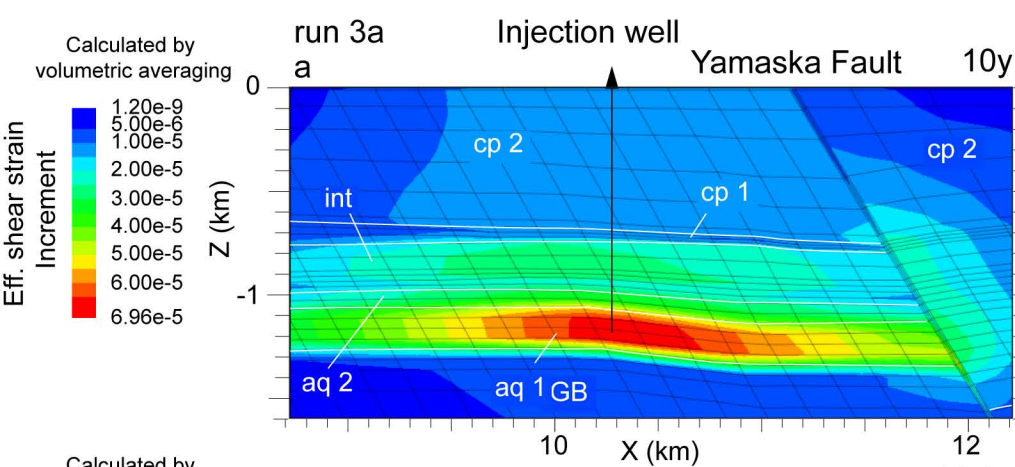
30 yrs

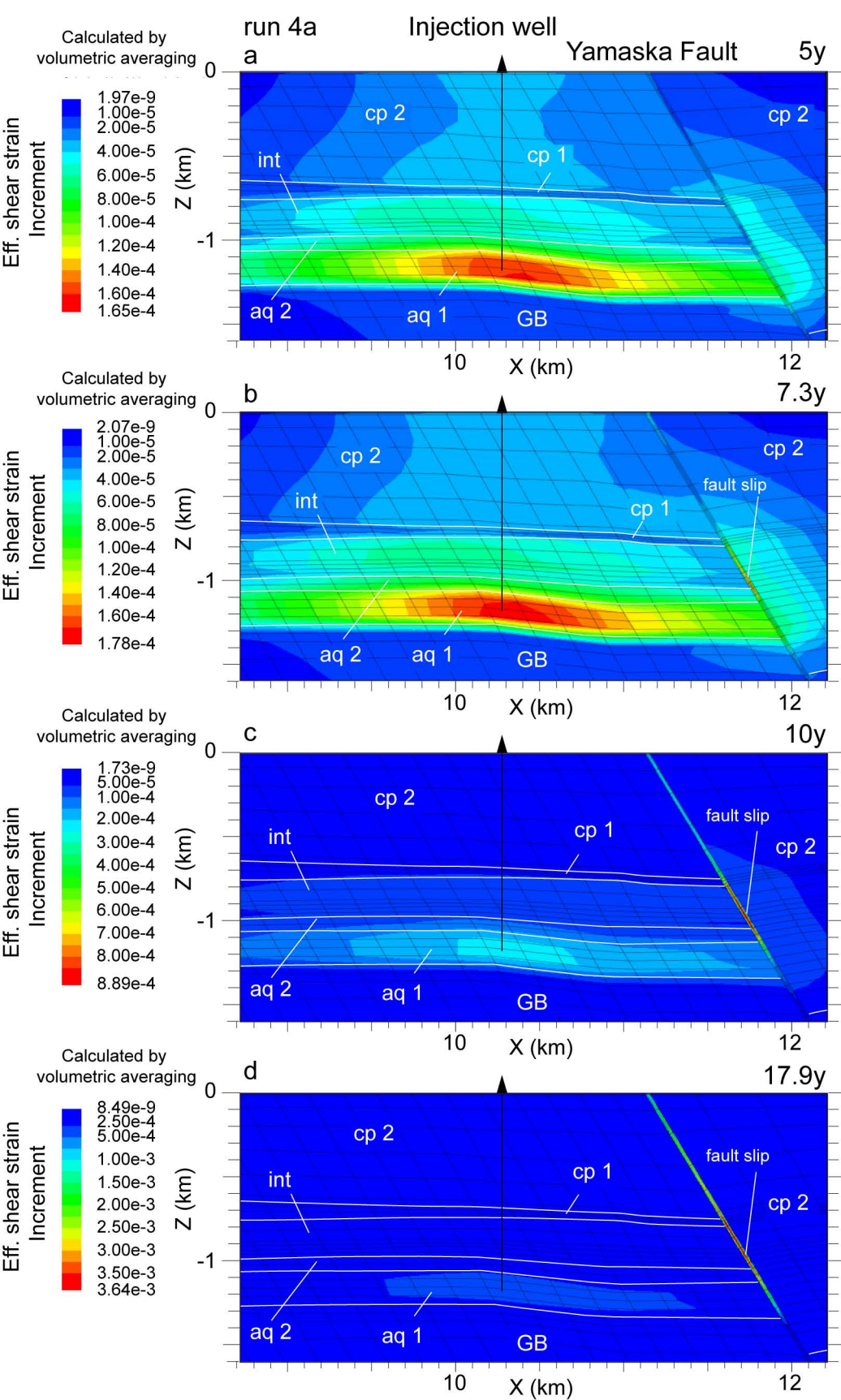


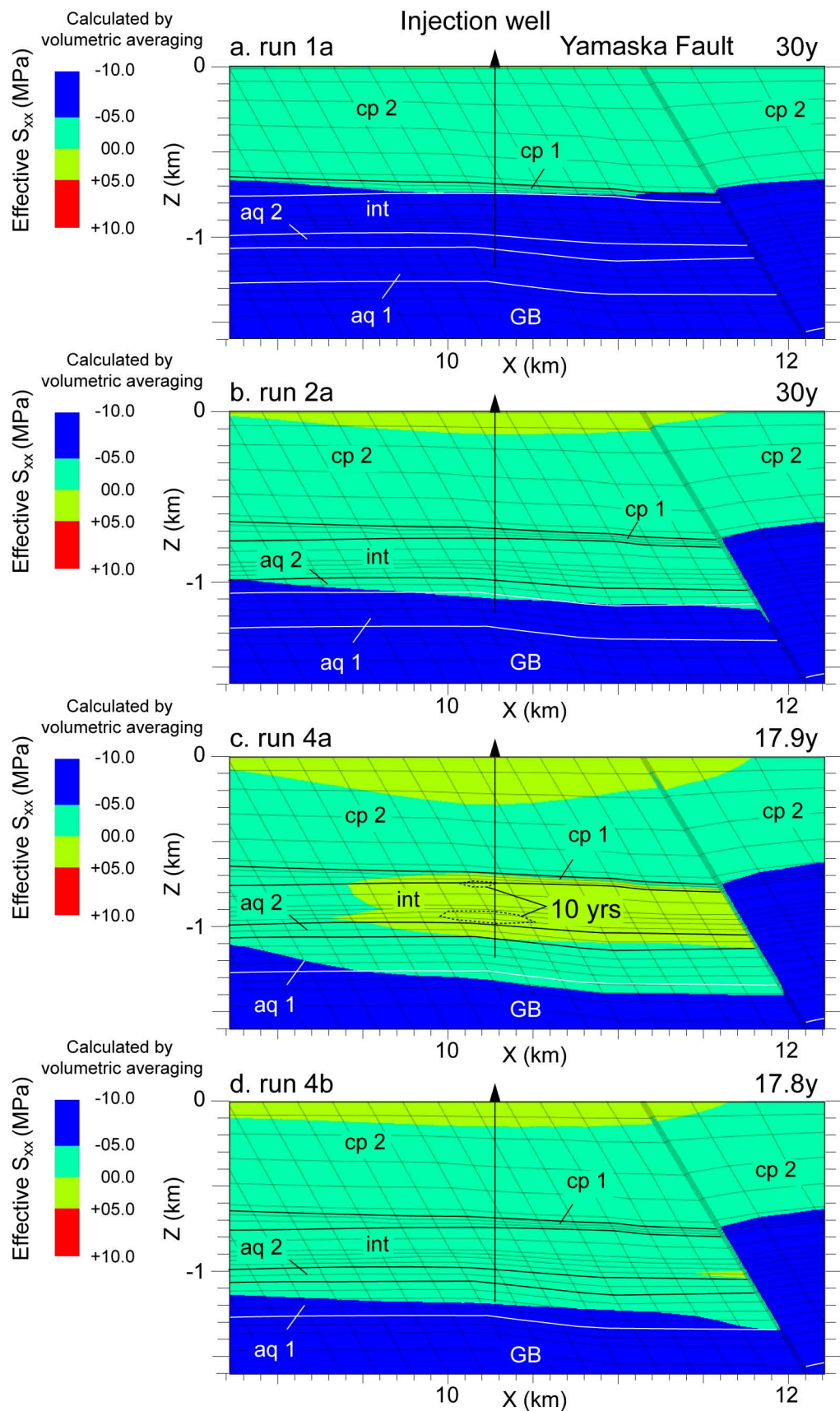


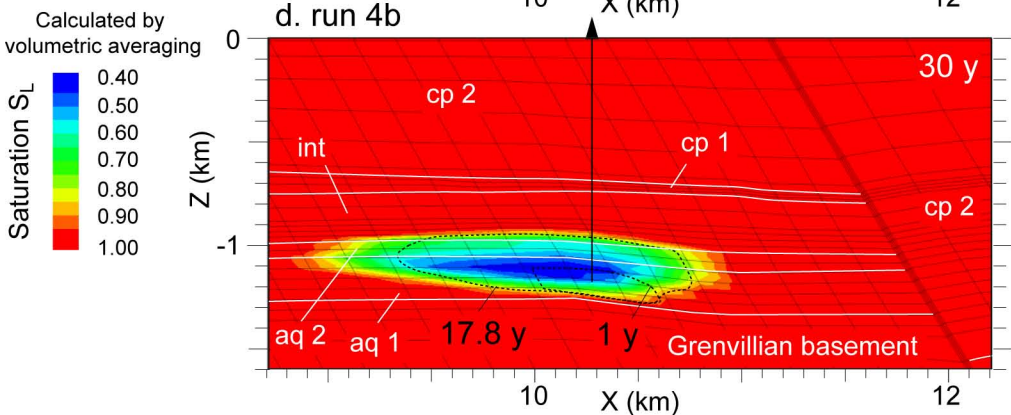
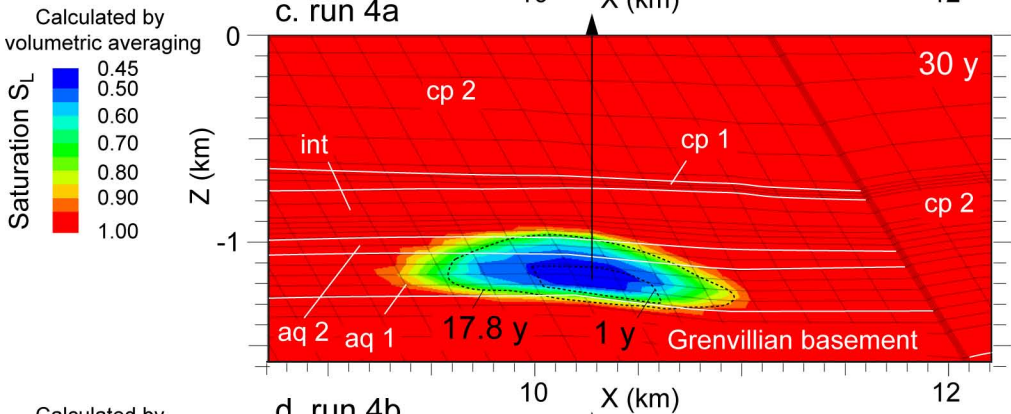
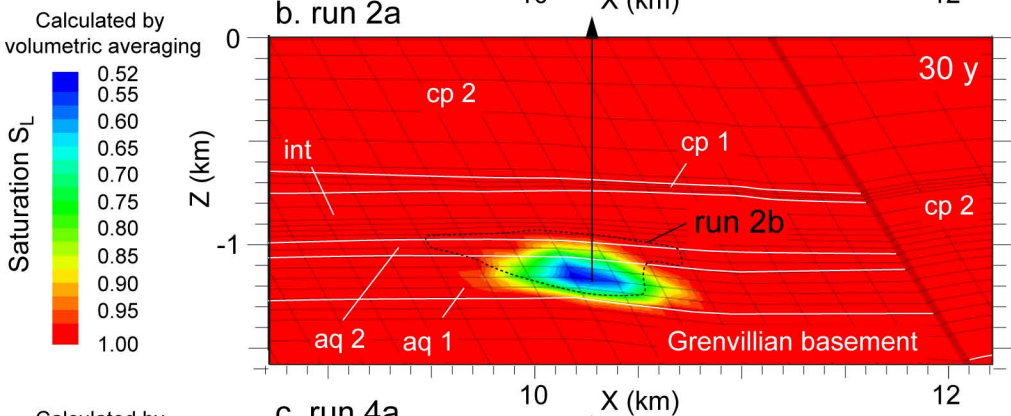
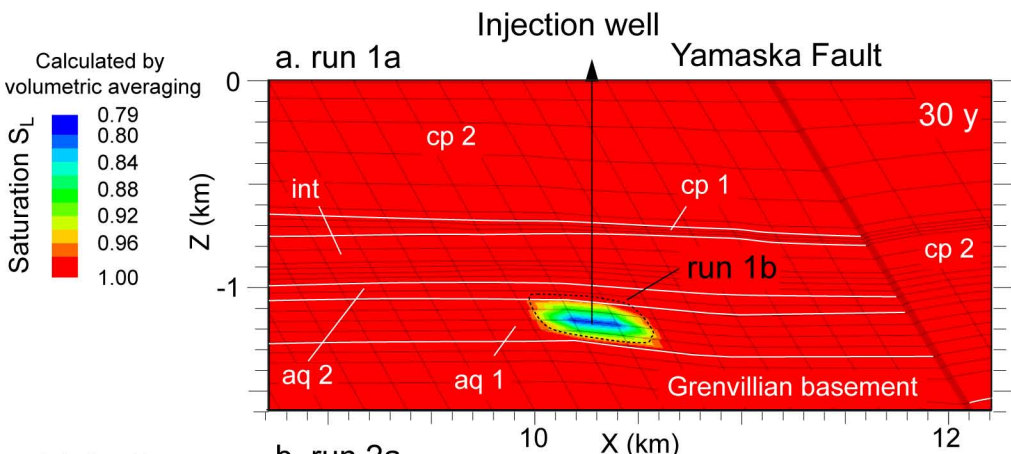












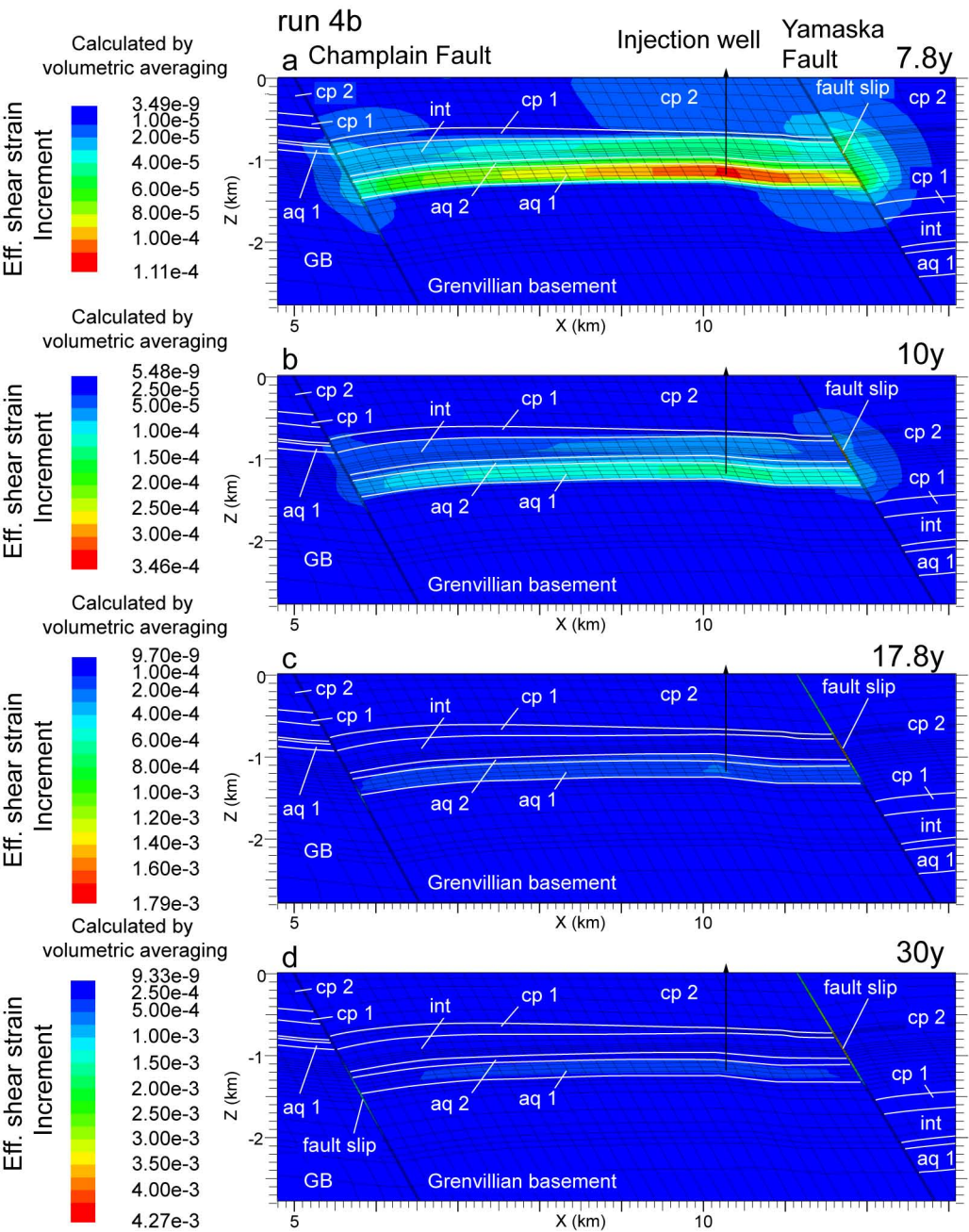


Table 1. Main representative properties of Lower Paleozoic sedimentary units in the Becancour area.

Model	Base	Aquifer 1	Aquifer 2	Intermediate units			Caprock 1	Caprock 2	Fault zone
Property	Grenvillian Basement	Covey Hill Fm	Cairnside Fm	Theresa Fm	Beauharnois Fm	Trenton-Black River-Chazy Gps	Utica Shale	Lorraine Gp	Rock fill/Joint
Lithology	granite	sandstone	sandstone	sandstone	dolomite	limestone	Ca shale	siltstone	Ca shale
Thickness in injection well (m)		195	90	40	34	153	47	694	10 ^b
Netpay thickness in injection well (m)		188	63	4	0	0,5			
Young's modulus, E (GPa)	60	27,56	43,69	53,97	49,28	49,28	42,28	28,71	42,28
Poisson's ratio, ν (-)	0,25	0,022	0,26	0,29	0,23	0,23	0,29	0,32	0,29
Bulk modulus, K (GPa)		16,35	29,84	42,84	30,88	30,88	33,38	26,58	
Shear modulus, G (GPa)		11,30	17,39	20,92	19,97	19,97	16,30	10,87	
Lame's constant λ , (GPa)		8,81	18,25	28,89	17,57	17,57	22,51	19,33	
Rock density, ρ_s (kg/m ³)	2665	2583	2593	2670	2754	2695	2665	2571	2665
Biot's coefficient, α (-)	1	1	1	1	1	1	1	1	
Friction angle, φ (°)									25
Dilation angle, ψ (°)									0
Cohesion, Pa									5E+05
Porosity, ϕ (-)	0,07	0,06	0,04	0,05	0,07	0,09	0,07	0,05	0,07
Matrix permeability, k_m (m ²)		2,6E-16	1,1E-16	1,2E-16	2,3E-16	1,6E-16	1E-18	1E-18	
Rock mass permeability ^a , k_1 (m ²)=10 k_m	1E-18	2,6E-15	1,56E-15	1,2E-16	2,3E-16	1,6E-16	1E-18	1E-18	1e-18 or
Rock mass permeability ^a , k_2 (m ²)=100 k_m	1E-18	2,6E-14	1,56E-14	1,2E-16	2,3E-16	1,6E-16	1E-18	1E-18	1e-16
Salinity (g/l)	n/a	109	242	157	150	179	n/a	n/a	n/a
Residual gas (CO ₂) saturation (-)	0,214	0,262	0,214	0,214	0,214	0,214	0,214	0,214	0,214
Residual liquid saturation (-)	0,33	0,273	0,33	0,33	0,33	0,33	0,33	0,33	0,33
Saturated liquid saturation (-)	1	1	1	1	1	1	1	1	1
Entry pressure P_0 (kPa)	40,00	44,10	40,00	40,00	40,00	40,00	40,00	40,00	40,00
Exponent m (-)	0,55	0,5582	0,621	0,55	0,55	0,55	0,55	0,55	0,55
α (1/Pa)	2,00E-05	2,268E-05	2,00E-05	2,00E-05	2,00E-05	2,00E-05	2,00E-05	2,00E-05	2,00E-05
Capillary pressure, max, kPa	200000	200000	200000	200000	200000	200000	200000	200000	200000
Compressibility, 1/Pa	1.861e-9	1.939e-9	3,96E-09	1.861e-9	1.861e-9	1.861e-9	1.861e-9	1.861e-9	1.861e-9

Note: The elastic properties E, ν , porosity and matrix permeability data are obtained from laboratory core analyses; λ , K, and G are calculated from E and ν , after (Zoback, 2010); ^a, determined from drill stem tests (Tran Ngoc et al., 2012); $k_{vertical} = 0.1 \times k_{horizontal}$; ^b, spacing between joints. Elastic moduli for the Grenvillian basement are taken as an average granite value; for the Trenton-Black River-Chazy Groups - as equal to the Beauharnois Fm; the data on fluid-property parameters (salinity, saturation, capillary pressure, entry pressure and compressibility) are taken from Tran Ngoc et al. (2012).

Table 2. Changes of stress/pressure and temperature with depth in the Becancour area

Average S_{Hmax} orientation	N59°E
Minimum horizontal stress $\Delta S_{hmin} = \Delta S_{xx}$ (MPa/km)	18
Maximum horizontal stress $\Delta S_{Hmax} = \Delta S_{yy}$ (MPa/km)	40
Vertical stress $\Delta S_v = \Delta S_{zz}$ (MPa/km)	25,6
Fluid pressure ΔP_{f0} (MPa/km)	12,17
Surface temperature T_0 (°C)	8
Temperature gradient ΔT (°C)	23,5

Table 3. Estimation of seal capacity for the Champlain and the Yamaska Faults using the shale gouge ratio method (Freeman et al., 1998; Yielding et al., 1997)

a. Champlain Fault

Hydrology	Lithological unit	Footwall		Hanging wall		V_{sh}	Fault throw (m)	SGR (%)			
		Z (m)	ΔZ (m)	Z (m)	ΔZ (m)			FW	HW		
Caprock 2	Lorraine Gp	0	484	0	780	0,95					
Caprock 1	Upper Utica Shale	484	152	780	150	0,6	296	95	sealing behaviour		permeable?
Interm. units	Trenton-Black River-Chazy Gps	636	94	930	170	0,14	294	77			
	Beekmantown Gp - Beauharnois Fm	730	50	1100	50	0,1	370	44			
	Beekmantown Gp - Theresa Fm	780	20	1150	50	0,1	370	32		8	
Aquifer 2	Potsdam Gp - Cairnside Fm	800	50	1200	80	0,1	400	28		8	
Aquifer 1	Potsdam Gp - Covey Hill Fm	850	80	1280	200	0,1	430	21		7	
	Grenvillian basement	930	N/A	1480	N/A	N/A	550	11			

b. Yamaska Fault

Hydrology	Lithological unit	Footwall		Hanging wall		V_{sh}	Fault throw (m)	SGR (%)			
		Z (m)	ΔZ (m)	Z (m)	ΔZ (m)			FW	HW		
Caprock 2	Lorraine Gp	0	724	0	1520	0,95					
Caprock 1	Upper Utica Shale	724	48	1520	88	0,6	796	95	sealing behaviour		permeable?
	Lower Utica Shale	772	51	1610	83	0,44	838	91			
Intermed. units	Trenton-Black River-Upper Chazy Gps	822	117	1703	148	0,14	881	85		9	
	Lower Chazy Gp	939	23	1851	34	0,1	912	73			
	Beekmantown Gp - Beauharnois Fm	960	63	1889	109	0,1	929	69			
	Beekmantown Gp - Theresa Fm	1025	72	2011	122	0,1	986	60			
Aquifer 2	Potsdam Gp - Cairnside Fm	1102	107	2134	171	0,1	1032	52		7	
Aquifer 1	Potsdam Gp - Covey Hill Fm	1215	291	2315	404	0,1	1100	40	7		
	Grenvillian basement	1503	N/A	2736	N/A	N/A	1233	17			

Note: V_{sh} , volume of shale estimated from natural radioactivity (gamma ray) well log data; Z, depth of formation tops estimated for the Yamaska Fault as an average value from the 3D geological model of the Becancour area (Claprood et al., 2012) and for the Champlain Fault from correlation of regional well data and basement top (Fig. 3). FW, footwall, HW, hanging wall.

Table 4. Initial parameters used in numerical simulations

Series #	run #	Injection rate	Fault permeability	Reservoir permeability			Corresponding 3D injection rate (r=3.5 km)	
				Aquifer 1 CH	Aquifer 2 Ca		kg/s	Mt/yr.
		kg/s	m ²	m ²	m ²			
Series 1	1a	0,06	1E-18	2,60E-15	1,56E-15	$k_1 = 10 k_m$	4,5	0,15
	2a	0,3	1E-18				23	0,8
	3a		1E-16				75	2,5
	4a	1	1E-18					
Series 2	1b	0,06	1E-18	2,60E-14	1,56E-14	$k_2 = 100 k_m$	4,5	0,15
	2b	0,3	1E-18				23	0,8
	3b		1E-16				75	2,5
	4b	1	1E-18					

Note: CH, Covey Hill Fm; Ca, Cairnside Fm; k_1, k_2 , rock mass permeability; k_m , matrix permeability (see Table 1).

Table 5. Resulting variations in fluid pressure build-up (ΔP_f), effective shear strain increment ($\Delta \gamma$), surface uplift (h), length of reactivated fault segment (L), fault shear slip (d), effective minimum horizontal stress (S_{xx}^*) and CO₂ plume width (W) observed in numerical simulations 1a-4a of series 1 ($k_1 = 10k_m$) for different injection rates (IR) and fault permeability (k_f).

run #	Initial parameters			Resulting data										
	IR	k_f	time step	$\Delta P_f = P_f - P_{f0}$		$\Delta \gamma$		h	Yamaska Fault		S_{xx}^*		W	
				well	YF zone	well	YF zone		reactivated segment	d	MPa	unit		
kg/s	m ²	yrs	MPa	MPa			cm	L (m)	FW unit	cm	MPa	unit	km	
1a	0,06	1E-18	10	1,04	0,7	1,55E-05	1,10E-05	0,8						
			20	1,44	1,3	2,30E-05	2,00E-05	1,5						
			30	1,8	1,7	2,90E-05	2,50E-05	2,05	no			negative		0,5
2a	0,3	1E-18	10	4,5	3,25	7,00E-05	5,50E-05	4						
			22,5	7,1	6,5	1,20E-04	1,20E-04	7	300	th-Tr	0,5			
			25,6	7,6	7	1,40E-04	2,07E-04	8	400	Ca-Tr	0,5			
3a	0,3	1E-16	10	4,5	3,25	6,99E-05	5,00E-05	4						
			18,2	6,26	5,5	1,02E-04	1,02E-04	6,5	60	Ut	0,5			
			19,2	6,4	5,5	1,10E-04	1,29E-04	6,5	180	Tr-Ut	0,5			
			20	6,6	6	1,10E-04	1,85E-04	6,5	500	th-Lor	0,5			
			23,7	7,3	6,5	1,50E-04	4,70E-04	7,5	830	Ca-Lor	1,5			
4a	1	1E-18	5	11	5	1,60E-04	1,10E-04	8						
			7,3	11,8	7	1,80E-04	1,80E-04	9	330	Ca-Tr	1			
			10	13,9	10	2,50E-04	9,40E-04	12	450	Ca-Ut	2	(+2)	th, Tr	
			17,9	18,8	16	2,80E-04	5,20E-03	20	700	Ca-Lor	12			1,3
			30	24,9	24	3,50E-04	1,00E-02	27,5	1400	CH-Lor	17	(+4)	Ca-Ut	1,7

Note: YF, Yamaska Fault; FW unit, footwall unit: CH, Covey Hill Fm; Ca, Cairnside Fm; th, Theresa Fm; Tr, Trenton Gp; Ut, Utica Shale; Lor, Lorraine Gp. See Table 4 for the rock mass k_1 and matrix k_m permeability of the reservoir units.

Table 6. Resulting variations in fluid pressure build-up (ΔP_f), effective shear strain increment ($\Delta\gamma$), surface uplift (h), length of reactivated fault segment (L), fault shear slip (d), effective minimum horizontal stress (S_{xx}^*) and CO₂ plume width (W) observed in numerical simulations 1b-4b of series 2 ($k_2 = 100k_m$) for different injection rates (IR) and fault permeability (k_f).

run #	Initial parameters			Resulting data										
	IR	k_f	time step	$\Delta P_f = P_f \cdot P_{f0}$		$\Delta\gamma$		h	Yamaska Fault			S_{xx}^*		W
				well	YF zone	well	YF zone		reactivated segment		d	MPa	unit	
kg/s	m ²	yrs	MPa	MPa			cm	L (m)	FW unit	cm	MPa	unit	km	
1b	0,06	1E-18	10	0,51	0,5	8,80E-06	7,50E-06	0,55						
			20	0,87	0,87	1,50E-05	1,30E-05	0,9						
			30	1,21	1,2	2,13E-05	1,80E-05	1,4	no			negative	0,5	
2b	0,3	1E-18	10	2,5	2,4	4,10E-05	3,50E-05	2,5						
			20	4,25	4,25	7,20E-05	6,00E-05	4,5						
			30	5,8	5,8	9,90E-05	8,50E-05	6,5	no			negative	1,2	
3b	0,3	1E-16	10	2,47	2,4	4,10E-05	3,50E-05	2,5						
			20	4,2	4	7,10E-05	6,00E-05	4,5						
			27,5	5,4	5,4	9,40E-05	9,40E-05	6	60	Ut	0,5			
			28,5	5,5	5,5	1,00E-04	1,14E-04	6,5	180	Tr-Ut	0,5			
			29,5	5,6	5,5	1,00E-04	1,54E-04	6,5	500	th-Lor	0,5			
			30	5,7	5,5	1,00E-04	1,83E-04	6,5	700	Ca-Lor	0,5	negative	1,2	
4b	1	1E-18	5	5,6	5,6	9,50E-05	8,00E-05	5,5						
			7,8	6,6	6,6	1,11E-04	1,10E-04	7	330	Ca-Tr	0,5			
			10	7,8	7,8	1,50E-04	3,47E-04	8,5	450	Ca-Ut	0,5			
			17,8	11,7	11,7	2,00E-04	1,79E-03	13,7	800	Ca-Lor	5	(+0,4)	th	
			20	12,75	12,75	2,00E-04	2,90E-03	15	1200	CH-Lor	5			
			30	17	17	2,50E-04	6,00E-03	21	500 ^a /1400	GB ^a /CH-Lor	10	(+2,8)	th-Ut	2

Note: YF, Yamaska Fault; ^a, reactivation of the Champlain Fault; FW unit, footwall unit: GB, Grenvillian basement; CH, Covey Hill Fm; Ca, Cairnside Fm; th, Theresa Fm; Tr, Trenton Gp; Ut, Utica Shale; Lor, Lorraine Gp. See Table 4 for the rock mass k_2 and matrix k_m permeability of the reservoir units.

Appendix. Name and location of wells in the St. Lawrence Lowlands cited in present study. See Fig. 2 for well location.

NN	Well no.	Well Name	Year	Location (UTM NAD83 z18)		Elevation	End depth
				X	Y	mKB	mKB
1	A027	Canadian Seaboard. Sainte-Angèle No 1	1933	693564,84	5132519,55	25,60	1603,25
2	A156	Husky, Gentilly No 1	1971	709333,23	5137234,43	41,75	2612,14
3	A158	Husky Bruyères No 1	1971	692730,38	5133160,72	34,53	1390,50
4	A175	SOQUIP et al., Les Saules No 1	1975	779535,52	5191473,39	49,14	975,66
5	A196	SOQUIP Petrofina Bécancour 1	1981	699140,79	5138042,62	12,85	1228,00
6	A198	SOQUIP Petrofina, Bécancour No 2	1981	700814,50	5140665,43	11,78	1265,00
7	A223	Intermont. Bécancour No 1	1992	699612,00	5139396,00	11,26	850,70
8	A236	Junex. Bécancour No 2	2002	699874,99	5138967,52	10,10	930,00
9	A239	Junex. Bécancour No 3	2003	699174,51	5139533,47	7,25	935,50
10	A241	Junex. Bécancour No 4	2003	698745,33	5139237,59	8,20	1054,00
11	A242	Junex. Bécancour No 5	2003	700446,31	5140457,08	7,91	981,36
12	A246	Junex. Bécancour No 6	2004	701027,30	5140831,13	8,35	1002,18
13	A247	Junex. Bécancour No 7	2004	698042,90	5136740,50	9,40	1069,23
14	A250	Junex. Bécancour No 8	2006	697878,26	5137501,40	7,20	1048,00
15	A251	Junex, Champlain No 1	2006	699650,95	5143492,47	8,41	958,00
16	A255	Junex, Champlain No 2	2007	697763,02	5144709,86	22,79	930,00
17	A257	Junex Saint-Augustin-de-Desmaures No 1	2008	769981,51	5184176,63	74,43	837,00
18	A262	Junex, Bécancour No 8	2008	700265,33	5134581,73	34,65	1902,71
19	A265	Canadian Forest Oil, Champlain No 1-H	2008	699572,42	5143424,57	7,85	1482,00