Lawrence Berkeley National Laboratory

LBL Publications

Title

An overview of TOUGH-based geomechanics models

Permalink

<https://escholarship.org/uc/item/52n4g332>

Author

Rutqvist, J

Publication Date

2017-11-01

DOI

10.1016/j.cageo.2016.09.007

Peer reviewed

1 AN OVERVIEW OF TOUGH-BASED GEOMECHANICS MODELS

2

3

4

5 Jonny Rutqvist

6

7 *Earth Sciences Division, Lawrence Berkeley National Laboratory, MS 90-1116,*
8 *Berkeley, CA 947 20, USA*

9

10`5

11

12 Tel.: +1-510-486-5432, fax.: +1-510-486-5686

13 e-mail address: jrutqvist@lbl.gov (J. Rutqvist)

14

15

16

17 **Computers & Geosciences**

18 **Special Issue of the 2015 TOUGH Symposium**

19

20

21

22

23

24

25

26

27

28

29

30

31

32

33

34

35

36

37

38

39

40

41

42**ABSTRACT**

43

44After the initial development of the first TOUGH-based geomechanics model 15 years ago
45based on linking TOUGH2 multiphase flow simulator to the FLAC3D geomechanics
46simulator, at least 15 additional TOUGH-based geomechanics models have appeared in the
47literature. This development has been fueled by a growing demand and interest for modeling
48coupled multiphase flow and geomechanical processes related to a number of geoengineering
49applications, such as in geologic CO₂ sequestration, enhanced geothermal systems,
50unconventional hydrocarbon production, and most recently, related to reservoir stimulation
51and injection-induced seismicity. This paper provides a brief overview of these TOUGH-
52based geomechanics models, focusing on some of the most frequently applied to a diverse set
53of problems associated with geomechanics and its couplings to hydraulic, thermal and
54chemical processes.

55

56

57**Keywords:** TOUGH, modeling, fluid flow, geomechanics, THMC

58

591 INTRODUCTION

60

61A growing demand and interest for modeling coupled multiphase flow and geomechanical
62processes has resulted in the development of a growing number of models that adds
63geomechanics to the existing multiphase flow capabilities of the TOUGH family codes. This
64development started with the development of the TOUGH-FLAC simulator to meet the need
65for analyzing the effect of geomechanics on multiphase fluid flow behavior and transport
66properties around nuclear waste emplacement tunnels at the previously proposed U.S. high-
67level nuclear repository site at Yucca Mountain, Nevada ([Rutqvist et al., 2002](#); [Rutqvist and](#)
68[Tsang, 2012](#)). The TOUGH-FLAC simulator was developed as a pragmatic approach, linking
69the two existing codes, TOUGH2 and FLAC3D ([Rutqvist et al., 2002](#)). The TOUGH-FLAC
70simulator has since been adapted and applied for a wide range of geoscientific research and
71geoengineering applications, such as geologic CO₂ sequestration, enhanced geothermal
72systems, and gas production from hydrate bearing sediments ([Rutqvist \(2011\)](#) and references
73therein).

74

75Following the first development of the TOUGH-FLAC simulator, a number TOUGH-based
76geomechanical models have been and are being developed. In fact, at least 15 additional
77TOUGH-based geomechanics models of various sophistications have appeared in the
78literature. This include simulators such as TOUGH+ROCMECH ([Kim and Mordis, 2013](#)),
79TOUGH-RDCA ([Pan et al., 2014a](#)), TOUGH-CSM ([Winterfeld and Wu, 2015](#)), TOUGH-
80RBSN ([Kim et al., 2015a](#)), and many more linking TOUGH-family codes, such as TOUGH2,
81TOUGH-MP, TOUGH+, TOUGHREACT, and ITOUGH to various geomechanics models.
82For example, TOUGHREACT has been linked to geomechanics models for the analysis of

83coupled thermal, hydraulic, mechanical and chemical (THMC) processes (e.g., [Taron et al.,](#)
842009; [Zheng et al., 2014](#); [Kim et al., 2015b](#)). In recent years, additional interest and demand
85have been fueled by the need stimulate reservoirs through fracturing (e.g., for enhanced
86geothermal systems or tight gas and shale gas formations), understand the risk of leakage
87(e.g., at carbon storage sites), and to address the issue of induced seismicity.

88

89This paper provides a brief overview of the current TOUGH-based geomechanics models,
90including capabilities, applications and potential future developments. Table 1 lists and briefly
91describes 20 TOUGH-based geomechanics models that have appeared in the literature. In
92general these TOUGH-based geomechanics models differ in the assumptions about the
93mechanical behavior of porous and fractured geologic media, the numerical method used to
94perform the stress–strain calculation, the discretization scheme and how state variables and
95parameters calculated for potentially different meshes are mapped to each other, and the way
96to couple fluid flow and geomechanics. Although the TOUGH-based geomechanics models
97are developed for modeling coupled thermal-hydraulic-mechanical (THM) processes or, in
98some cases, even THMC processes, the couplings of fluid flow and geomechanics, i.e., HM
99couplings, are central to most applications and are known to be challenging to solve
100numerically depending on the specific application. Therefore, an overview of numerical
101schemes related to HM couplings schemes is devoted to the entire next section. This is
102followed by descriptions of TOUGH-FLAC, TOUGH-ROCMECH, TOUGH-RDCA,
103TOUGH-CSM, and TOUGH-RBSN, which are complementary TOUGH-based
104geomechanical models that have been most frequently applied to a diverse range of problems.
105Thereafter, other TOUGH-based geomechanics models listed in Table 1 are briefly reviewed

106before concluding the paper with some final thoughts on the current state of TOUGH-based
107geomechanics models expected future developments.

108

1092 **HM COUPLING SCHEMES**

110

111Figure 1 shows a schematic of the couplings between hydraulic and mechanical processes in a
112deformable porous media such as soil and rock ([Rutqvist and Stephansson, 2003](#)). The arrows
113indicate the couplings, which can be divided into two categories: direct (solid line arrows) and
114indirect (dashed line arrows). Direct couplings are associated with pore-volume changes and
115their instantaneous and direct effect on fluid mass balance and effective stress, whereas
116indirect couplings are occurring indirectly through changes in mechanical and hydraulic
117properties.

118

119Depending on the type of problem being solved and the porous medium properties, the
120importance of different HM couplings varies. In relatively permeable fractured hard rock, the
121indirect coupling in the form of permeability changes with stress might be most important. In
122relatively impermeable, soft and porous clay, on the other hand, direct pore-volume coupling
123may be most important. For example, when a porous deformable medium is suddenly loaded
124mechanically, the pores will be compressed and thereby squeezing the pore fluid to a higher
125pore pressure that will impact the fluid mass balance. This increase in pore-fluid pressure will
126in turn have an instantaneous effect on effective stress and volumetric strain. These are
127instantaneous two-way couplings between hydraulic and mechanical processes that can be
128challenging to resolve numerically.

129

130A number of numerical schemes have been employed for solving coupled fluid flow and
131geomechanics problems ([Minkoff et al., 2003](#); [Kim, 2010](#)). These include so-called fully
132coupled (monolithic) and sequentially coupled solution methods. In monolithic solutions, all
133the equations for fluid flow and mechanics including coupling terms are assembled into a
134large matrix system and solved simultaneously. Most of the coupled fluid flow and
135geomechanics finite element codes developed in rock and soil mechanics since the 1980s have
136employed fully coupled numerical schemes (e.g., [Noorishad et al., 1982](#)). The fully coupled
137method usually provides unconditional and convergent numerical solutions for
138mathematically well-posed problems ([Noorishad et al., 1982](#); [Rutqvist and Stephansson,](#)
139[2003](#); [Kim, 2010](#)).

140

141When linking two different codes for fluid flow and geomechanics, it is generally not possible
142to use the monolithic solution scheme. Consequently, in most TOUGH-based geomechanics
143models to date, including TOUGH-FLAC, the equations for fluid flow and geomechanics are
144solved sequentially. Sequential coupling methods might be prone to numerical instability and
145inaccuracy when solving problems involving strong direct pore-volume coupling. Analysis of
146sequential methods associated with pore-elasticity with appropriate stability properties has
147been the subject many studies ([Settari and Mourits, 1998](#); [Mainguy and Longueare, 2002](#);
148[Kim et al., 2009](#)). However, as shown by [Kim \(2010\)](#), by choosing an appropriate coupling
149scheme with so-called stress fixed iterations in the sequential scheme, the sequential solution
150becomes unconditionally stable. In a stress fixed sequential solution, flow is solved first,
151fixing the total stress field, and then geomechanics is solved from the variables obtained at the
152previous flow step. The stress fixed sequential scheme is achieved in the computation by

153calculating an appropriate porosity correction term while keeping the pore-compressibility
154non-zero and active in the reservoir simulator ([Kim et al., 2011](#)). Though the efficiency of the
155sequential, iterative schemes has been questioned ([Prevost, 2013](#)), a recent study showed that
156fixed stress split is a robust and efficient scheme for iteratively coupling poro-elastic systems
157even for highly nonlinear problems ([Mikelic et al., 2014](#)).

158

159For practical reasons, the sequential coupling method is used in all TOUGH-based
160geomechanics models except in some one-way coupled approaches and in TOUGH-CSM in
161which a monolithic solution is employed ([Winterfeld and Wu, 2015](#)). For strong pore-volume
162coupling, the various TOUGH-based geomechanics models, including TOUGH-FLAC,
163TOUGH+ROCMECH and TOUGH-CSM, have been verified against analytical solutions
164involving poro-elasticity such as solutions involving one-dimensional consolidation
165(Terzaghi) and the 2D Mandel-Cryer effects. These verifications have shown good agreement
166between numerical results and analytical solutions for both the fully coupled scheme in
167TOUGH-CSM ([Winterfeld and Wu, 2015](#)) and sequentially coupled schemes in
168TOUGH+FLAC (e.g., [Kim et al., 2012](#)) and TOUGH+ROCMECH (e.g., [Kim and Moridis,](#)
169[2013](#)). This shows that both monolithic and sequential coupling schemes can be used to solve
170problems involving strong pore-volume coupling, though the efficiency of the two schemes
171might be substantially different depending on the specific problem being solved.

172

173In the development of coupled HM numerical models, a lot of effort is usually dedicated to
174verification of algorithms related to pore-volume coupling, partly because poro-elastic
175analytical solutions for such problems exist. However, in much of the multiphase flow

176applications encountered, direct two-way pore-volume couplings may not be important, or can
177be ignored by choosing an appropriate pore-compressibility in the flow simulator. More
178common is that indirect couplings by property changes dominate. Moreover, in many cases
179one-way coupling is sufficient, for example hydraulic-to-mechanical coupling considering
180how fluid pressure gives rise to mechanical deformation and failure. In other applications,
181such as fluid-driven hydraulic fracturing propagation, very strong pore-volume coupling
182appears, especially when new fracture volume is created at the crack tip, which is very
183challenging numerically, regardless of the applied HM coupling scheme.

184

185

186 **3 TOUGH-FLAC**

187

188The TOUGH-FLAC simulator was originally developed in the late 1990s as part of the Yucca
189Mountain nuclear waste disposal project ([Rutqvist et al., 2002](#); [Rutqvist and Tsang, 2003a](#)). At
190that time TOUGH2 ([Pruess et al., 2012](#)) was the main code used for the analysis of
191unsaturated zone flow and transport of the Yucca Mountain site, but there was a need to
192analyze how flow and transport was affected by geomechanical processes ([Rutqvist and](#)
193[Tsang, 2003b](#)). The idea was then to link TOUGH2 to a geomechanics code; the FLAC3D
194code ([Itasca, 2012](#)) was selected, because it had the required geomechanics capabilities, was a
195continuum code compatible with the TOUGH2 continuum approach, and was already
196qualified and applied in the Yucca Mountain Project ([Rutqvist and Tsang, 2012](#)).

197While FLAC3D ([Itasca, 2012](#)) is a commercial code and the source code is not distributed, it
198contains a script programming capability called FISH, which makes it possible to reach and
199modify internal variables and thereby enabled the linking with the TOUGH2 code. FLAC3D
200also has the capability of implementing user defined constitutive models through C++

201programming added in a dynamic link library file ([Rutqvist, 2011](#)). Thus, despite not having
202access to the source code, FLAC3D provides sufficient flexibility for research applications
203and specialized developments to a wide range of applications. In addition, FLAC3D contains
204a large number of constitutive models, including elasto-plastic and visco-elastic (creep)
205models for solids as well as the possibility of including some discontinuities as interfaces
206between solid elements.

207As described in the previous section, TOUGH-FLAC uses sequential coupling between
208TOUGH2 and FLAC3D, whereby fluid flow variables, such as pore pressure, temperature,
209and saturation calculated by TOUGH2, are transferred to a compatible numerical grid for
210FLAC3D, which then calculates effective stresses and associated deformations, returning
211updated values for porosity, permeability, and capillary strength parameter to the flow
212simulator ([Rutqvist et al., 2002](#); [Rutqvist, 2011](#)). As described in a 2011 status paper on
213TOUGH-FLAC ([Rutqvist, 2011](#)), TOUGH-FLAC was expanded to applications, including
214geomechanical aspects of CO₂ sequestration and fault activation, geomechanical effects in gas
215production from hydrate bearing sediments, and geothermal energy production. Since 2011,
216TOUGH-FLAC applications have been further broadened along with an increasing number of
217users, including continued modeling of geomechanical aspects of CO₂ sequestration ([Cappa](#)
218and [Rutqvist, 2012](#); [Mazzoldi et al., 2012](#); [Rinaldi and Rutqvist, 2013](#); [Jeanne et al., 2014a](#);
219[Konstantinovskaya et al., 2014](#); [Rinaldi et al., 2014a, b, 2015a](#); [Figueiredo et al., 2015](#)),
220nuclear waste disposal ([Rutqvist et al., 2013](#); [2014](#)), enhanced geothermal systems ([Jeanne et](#)
221[al., 2014b-d, 2015a, b](#); [Rutqvist et al., 2015a](#); [Rinaldi et al., 2015b](#)), underground gas storage
222and compressed air energy storage ([Rutqvist et al., 2012a](#); [Kim et al., 2013](#); [Walsh et al.,](#)

2232015), and gas production from hydrate bearing formations (Kim et al., 2012; Rutqvist et al.,
2242012a).

225In the recent few years significant advancements of TOUGH-FLAC have been made,
226extending the simulations to more complex geomechanical processes, especially related to
227modeling injection-induced fault activation and induced seismicity (Rutqvist et al., 2014a;
228Rinaldi et al., 2015a), advanced constitutive models for expansive clay in nuclear waste
229isolation (Rutqvist et al., 2014b; Vilarrasa et al., 2015), and modeling of salt geomechanical
230processes coupled with temperature and multiphase flow (Blanco-Martín et al., 2015a; 2016).
231Fault activation and induced seismicity have been modeled in 3D using strain-softening (slip-
232weakening) fault friction models that enable modeling of sudden seismic slip (Rinaldi et al.,
2332015a). This includes recent 3D modeling of injection-induced fault activations associated
234with both underground CO₂ injection and during stimulation of shale-gas reservoirs (Rutqvist
235et al., 2015b; Rinaldi et al., 2015a). In some cases this has involved fully dynamic
236calculations of the fault activation and resulting ground surface motion (Rutqvist et al.,
2372014a). Implementation of more advanced fault frictional laws is underway; Urpi et al. (2016)
238present a first step in the implementation of a rate-and-state fault friction law into the
239TOUGH-FLAC framework.

240The recent extension of the TOUGH-FLAC simulator for modeling THM processes
241associated with nuclear waste disposal in salt has been accomplished through collaboration
242between LBNL and Clausthal Technical University, Germany (Blanco-Martín et al., 2015b).
243This includes the development, implementation and application of an advanced constitutive
244model from Clausthal Technical University (the Lux/Wolters constitutive model) for THM
245induced damage, healing and sealing of salt host rocks and compaction of crushed salt

246(Blanco-Martín et al., 2016). Moreover, this involves modeling of large strain along with the
247compaction of the crushed salt backfill from a porosity of about 30% to less than 1% (Blanco-
248Martín et al., 2015a, b). Clausthal Technical University uses a different coupling scheme in
249which FLAC3D is the main code driving the simulation forward, and denotes this simulator
250FLAC-TOUGH rather than TOUGH-FLAC (Lux et al., 2014; Blanco-Martín et al., 2015b).

251Related to THM in clay, the implementation of the Barcelona Basic Model for mechanical
252behavior of unsaturated soils (Rutqvist et al., 2014b), and the Barcelona Expansive Model
253(Vilarrasa et al., 2015) for mechanical behavior of expansive soils are important additions for
254rigorous modeling of bentonite based backfill material. Moreover, the consideration of two
255structural levels, i.e., macro- and micro-structures in the expansive model, provides a link
256between mechanics and chemistry for more mechanistic modeling of THMC behavior. Two
257recent papers by Zheng et al. (2014; 2015) describe different types of chemical-mechanical
258coupling behavior in bentonite, i.e., effects of chemistry on the mechanical evolution of the
259bentonite material. In this case TOUGHREACT is linked to FLAC3D to model CM
260couplings, such as salinity effects on swelling pressure. Such chemical-mechanical coupling
261effects might be especially important when considering higher temperature disposal systems
262(Zheng et al., 2015).

263Most recently, the TOUGH-FLAC approach has been extended and applied in inverse
264modeling, by linking FLAC3D to the ITOUGH simulation–optimization code (Finsterle,
2652015) using the general structure of the TOUGH-FLAC simulator (Blanco-Martín et al.,
2662015c). The resulting simulator, ITOUGH-FLAC, provides an inverse modeling framework
267for the estimation of flow parameters, considering the system response accounting for
268geomechanical processes. Moreover, using iTOUGH2-PEST (Finsterle and Zhang, 2011) and

269TOUGH-FLAC, both flow and mechanical parameters can be estimated, including sensitivity
270analysis, uncertainty propagation and data-worth analysis. Currently, iTOUGH2-PEST with
271TOUGH-FLAC has been applied for material parameter estimation by analyzing field data at
272the In Salah CO₂ storage project. Algeria ([Rinaldi et al., 2015c](#)), and at a multi-year in situ
273heating experiment at Asse mine in Germany ([Blanco-Martín et al., 2016](#)).

274FLAC3D is a well-established code with a large user base ([Itasca, 2012](#)). It makes available
275many geomechanical constitutive models and has the flexibility to extend and implement new
276constitutive models, which is one of the most appealing features for selecting FLAC3D as the
277geomechanics code to be linked to TOUGH. One drawback with the current TOUGH-FLAC
278simulator is that it runs exclusively under Windows (because FLAC3D only runs under
279Windows), which prohibits the use ultra-large computer clusters. However, there are plans to
280port FLAC3D to Linux and to develop an [MPI](#) version in the near future (personal
281communication with Itasca, April 2016).

282

2834 **TOUGH-ROCMECH**

284
285TOUGH-ROCMECH is developed as an alternative to TOUGH-FLAC, in which the source
286code of the geomechanics part is available and therefore enabling a more efficient linking
287between multiphase flow and geomechanics, and the possibility of porting the simulator for
288computer clusters and massive parallel processing ([Kim and Moridis, 2013](#)). ROCMECH is
289an LBNL in-house developed finite element code that was tailored first for linking with
290TOUGH+ ([Kim and Moridis, 2013](#)) and later with TOUGHREACT ([Kim et al., 2015b](#)) and
291iTOUGH2 ([Finsterle, 2015](#)). Similar to TOUGH-FLAC, TOUGH-ROCMECH employs

292sequential coupling schemes, including the fixed stress split algorithms, which have been
293implemented and verified by [Kim and Moridis \(2013\)](#).

294

295The current basic ROCMECH version has the capability of modeling mechanical failure
296within solid elements through elasto-plastic Drucker-Prager or Mohr-Coulomb models. This
297has recently been extended to consider failure on multiple shear planes representing fracture
298sets of different orientation and applied for the analysis of shear stimulation related to an
299enhanced geothermal project at the Newberry Volcano, Oregon ([Smith et al., 2015](#)). A new
300multiporosity approach for poro-elasticity was also developed and implemented by [Kim et al.](#)
301[\(2012\)](#). This version of TOUGHREACT-ROCMECH has also been applied for modeling
302THMC processes for flow along fractures, considering mechanical and chemical
303(precipitation) effects on porosity and permeability ([Kim et al., 2015b](#)). These are processes
304important for the long-term sustainability of enhanced geothermal systems and for sealing of
305fractures associated with geologic containment of CO₂ and nuclear waste disposal.

306

307In a version of TOUGH+ROCMECH, capabilities for modeling 3D fracture propagation
308along a vertical pre-defined plane have been implemented. This model was applied for the
309analysis of hydraulic fracture propagation associated with stimulation of shale-gas reservoirs
310([Kim and Moridis, 2013; 2015](#)). The approach is similar to that of [Ji et al. \(2009\)](#), in which the
311fracture propagates along the boundary of the model domain through a nodal-splitting
312algorithm. [The permeability of fractured elements are increased with fracturing opening](#)
313[according to the cubic relation between flow and fracture aperture \(Rutqvist and Stephansson,](#)
314[2003\)](#). Using such an approach in the case of modeling hydraulic fracturing in tight shale, the

315 TOUGH+RealGasH2O with ROCMECH has been applied (Kim and Moridis, 2013; 2015).
316 The vertical fracturing is modeled by adding traction boundary conditions at locations where
317 nodes have been split. Moreover, once a fracture has been created adjacent to the solid
318 element, the initial single continuum element in TOUGH is changed to multiple continuum
319 for considering the local leak-off from the fracture to the surrounding porous rock.

320

321 In ROCMECH, fracturing conditions for node-splitting are based on tensile strength rather
322 than toughness. A fracturing criterion considering the effects of both effective stress normal to
323 the fracture and shear stress enables a mix-mode fracturing criterion. Using this model, Kim
324 and Moridis (2015) were able to model multiphase flow driven hydraulic fracturing and found
325 significant effects of complex two-phase flow processes, including vertical gravity
326 segregation that are processes important for estimating the fracture volume and leak-off to the
327 surrounding rock.

328

329 Ongoing developments of TOUGH-based geomechanics models linked to ROCMECH
330 includes MPI versions of both TOUGH+ROCMECH and TOUGHREACT-ROCMECH,
331 which will enable simulations of much larger problems using massive parallel processing on
332 large scale computer clusters.

333

334 **TOUGH-RDCA**

335

336Pan et al. (2014a) coupled TOUGH2 to RDCA (rock discontinuous cellular automaton), a
337code capable of simulating nonlinear and discontinuous deformation behavior, such as plastic
338yielding and the initiation, propagation and coalescence of cracks induced by changes of fluid
339pressure and temperature.

340

341RDCA uses a special displacement function to represent internal discontinuities (Pan et al.,
3422014b). A level-set method tracks the fracturing path, and a partition of unity method is used
343to improve the integral precision of fracture surface and fracture tip calculations. The
344mechanical state is evaluated by a cellular automaton updating rule. In this approach, the
345discontinuity of a crack is incorporated independently of the mesh, such that the crack can be
346arbitrarily located within an element, i.e., the method does not require any re-meshing for
347crack growth. As a result, a fixed mesh can be used in RDCA and this greatly simplifies the
348modeling procedure and its sequential integration with TOUGH2. If a fracture propagates
349through a certain element, the permeability of this element is increased according to the cubic
350law with the additional permeability of the fracture superimposed on the initial permeability
351representing the rock matrix.

352

353In TOUGH-RDCA, the fracturing condition can be evaluated either by linear elastic fracture
354mechanics using fracture toughness or by a modified Mohr-Coulomb criterion. The
355toughness-based criterion includes mixed Mode I (extension) and Mode II (shear) fracture
356propagation, whereas the Mohr-Coulomb criterion is modified with a tension cut-off,
357enabling modeling of both shear and tensile failure.

358

359 TOUGH-RDCA has been verified against analytical solutions and against TOUGH-FLAC for
360 poro-elastic behavior and injection-induced ground surface uplift (Pan et al., 2013). A number
361 of simulation applications have been presented related to fluid driven fracture propagation and
362 CO₂ leakage through fractures. This includes multiple fracture propagation with intersections
363 to pre-existing fractures (Pan et al., 2014c). The code is currently limited to modeling fracture
364 propagation in 2D, whereas a 3D RDCA code is under development.

365

366 **TOUGH-CSM**

367

368 TOUGH-CSM is being developed at the Colorado School of Mines (CSM), with the ultimate
369 goal of an efficient code tailored for massive parallel processing simulations (Winterfeld and
370 Wu, 2012; 2015). The geomechanics part is accomplished by adding a mean stress equation
371 for thermo-poroelastic multi-porosity media to the standard set of governing multiphase flow
372 equations of TOUGH2-MP. In this formulation, the mean total stress is included as an
373 additional primary variable, and the coupled thermal–hydrological–mechanical system is
374 solved fully implicitly, obtaining volumetric strain and associated changes in porosity and
375 permeability. Geochemical reactions based on the TOUGHREACT code have also been
376 included in this formulation (Zhang et al., 2012; Winterfeld and Wu, 2012).

377

378 A few applications of TOUGH-CSM related CO₂ sequestration in deep sedimentary
379 formations and geothermal systems have been published (Hu et al., 2013; Winterfeld and Wu,
380 2014). In the case of CO₂ sequestration, the effect of fracturing through the caprock overlying
381 a reservoir was studied in Huang et al. (2015). Since only the mean stress was solved in the

382fully coupled simulation, some other relationships and assumptions were used to estimate the
383horizontal stress needed for evaluating the possibility of vertical fracturing through the
384caprock. The application example related to geothermal, using a version of the code denoted
385TOUGH-EGS, included simulation of ground subsidence at the Geyser geothermal field with
386comparison to the previous results obtained with TOUGH-FLAC ([Hu et al., 2015](#)).

387

388As concluded in [Hu et al. \(2015\)](#), calculations limited to mean total stress as opposed to the
389full stress tensor is a simplification that may be a shortcoming since it cannot analyze
390phenomena dependent on shear stress, such as rock failure. However, currently a new
391algorithm is being developed and tested in which the stress tensor, including all normal and
392shear stress components, are solved in a sequential manner ([Winterfeld and Wu, 2015](#)). This
393approach of calculating the stress components was verified against analytical solutions
394showing the potential of TOUGH-CSM for realistic and efficient modeling coupled
395geomechanical processes using massive parallel processing.

3967 **TOUGH-RBSN**

397

398TOUGH-RBSN is being developed at LBNL with the main goal of modeling mass transport
399through permeable media under dynamically changing hydrologic and mechanical conditions
400in 3D heterogeneous geological media ([Asahina et al., 2014](#); [Kim et al., 2015a](#)). A strong
401motivator is the potential of modeling discrete fracture propagation through heterogeneous
402geological media in 3D ([Kim et al., 2015a](#)). The simulation tool combines TOUGH2 with the
403rigid-body-spring network (RBSN) model, which enables a discrete (lattice) representation of
404elasticity, individual fractures and fracture networks in rock.

405

406 One advantage of linking TOUGH2 and RBSN resides in their common utilization of a set of
407 nodal points and properties of the corresponding Voronoi tessellation (e.g., natural neighbor
408 and volume rendering definitions). Shared use of the Voronoi tessellation facilitates every
409 stage of the analyses, including model construction and results interpretation. In such a
410 system, the discrete fractures are directly mapped onto unstructured Voronoi grids via an
411 automated geometric scheme ([Asahina et al., 2011](#)). A fracture is represented by the controlled
412 breakage of the springs (1D lattice elements) linking adjacent Voronoi cells along the fracture
413 trajectory. Fractures can propagate along Voronoi cell boundaries as THM-induced stresses
414 evolve and exceed prescribed material strength values. The fracturing process is represented
415 by the damage/breakage of the springs. A Mohr-Coulomb criterion with tension cut-off is used
416 to judge when a lattice element undergoes a fracturing event.

417

418 The RBSN code has been extensively used and validated for fracturing in concrete materials,
419 including heterogeneities such as large grain inclusions, whereas the linked TOUGH-RBSN
420 code has been verified against analytical solutions and other numerical tools for various
421 features, including poro-elasticity, swelling, and fracture deformation ([Asahina et al., 2014](#);
422 [Kim et al., 2015a](#)). Applications include validation against experimental results on desiccation
423 cracking in a fine-grained sediment (mining waste), and most recently modeling of fracture
424 propagation through a heterogeneous laboratory sample that includes pre-existing weaknesses
425 ([Kim et al., 2015a](#)).

426

427Currently a new dynamic simulation framework for RBNS is being developed. In the new
428methodology, nodal kinematic information (displacements, velocities, and accelerations) is
429calculated through the explicit time integration scheme, by which the code implementation
430with parallelization can be easily realized. The parallelization will be a requirement for being
431able to solve large-scale problems in 3D with this approach.

432

4338 **OTHER TOUGH-BASED GEOMECHANICS MODELS**

434
435In addition to TOUGH-FLAC, TOUGH-ROCMech, TOUGH-CSM, TOUGH-RDCA, and
436TOUGH-RBSN, a number of other TOUGH-based geomechanics models have been
437developed as listed in Table 1, though most of them have not been extensively applied.

438

439Some of the earlier work includes [Gosavi and Swenson \(2005\)](#) who linked TOUGH2 to the
440finite element code GeoCrack3D, and later applied it to geothermal energy applications.
441[Hurwitz et al. \(2007\)](#) linked TOUGH2 to the USGS coupled hydro-mechanical finite element
442code Biot2, named the simulator TOUGH2-Biot, and applied it to study hydro-thermal fluid
443flow and deformation in large calderas. Recently another simulator named TOUGH2Biot was
444presented ([Lei et al., 2015](#)) involving TOUGH2 linked to an in-house finite element code and
445verified against previous TOUGH-FLAC simulations of the Geysers geothermal system and
446applied to simulate CO₂ injection of a site in China.

447

448[Taron et al. \(2009\)](#) at Penn State University linked TOUGHREACT to FLAC3D, a TOUGH-
449based geomechanics model that has been applied for modeling THMC processes associated

450with geothermal systems ([Taron et al., 2009](#); [Taron and Elsworth, 2009](#); [Izada and Elsworth,](#)
4512015). For example, [Taron and Elsworth \(2009\)](#) used THMC modeling to study the evolution
452of permeability associated with mechanical, thermal, and chemical (precipitation and
453dissolution) effects. In [Izada and Elsworth \(2014; 2015\)](#), the FLAC domain was populated
454with an implicit fracture network for the analysis of injection-induced micro-seismicity during
455hydraulic stimulation.

456

457Other efforts includes [Rohmer and Seyed \(2010\)](#) who linked TOUGH2 to the French open
458source finite element mechanics code Code_Aster and simulated deep underground CO₂
459injection. [Loschetter et al. \(2012\)](#) used the TOUGH2-Code_Aster combination to model
460enhanced coalbed methane production. [Aoyagi et al. \(2013\)](#) linked TOUGH2 to FrontISRM,
461an open source finite element code in Japan, based on TOUGH-FLAC links, and
462demonstrated it by modeling a generic CO₂ injection simulation.

463

464Some of the most recent efforts include [Lee et al. \(2015\)](#) who linked TOUGH2 to UDEC,
465which is a distinct element code, enabling modeling the geomechanical behavior of fracture
466networks in 2D. [Miah et al. \(2015\)](#) presented on-going work on linking TOUGH2 with
467PyLith, which is a USGS-developed finite-element code primarily used for large-scale
468geomechanical crustal deformation and earthquake simulation (static, quasi-static and
469dynamic modes). PyLith has advanced fault frictional models that will be applied and
470benchmarked against TOUGH-FLAC implementations of rate-and-state frictional models.

471

472Finally, simpler TOUGH-based geomechanics approaches have been developed for
473specialized applications, including [Walsh et al. \(2012\)](#) who added the effects of an external,
474vertical stress change to the porosity updates. This approach was recently applied to model
475effects of glaciation in the safety assessment of a hypothetical nuclear waste repository
476([Calder et al., 2015](#)). Another example is TOUGH2-Seed, a coupled fluid flow and
477mechanical statistical model for the study of injection-induced seismicity ([Nespolia et al.,](#)
4782015). With TOUGH2-Seed, the authors were able to model several mechanisms influencing
479each other during and after the injection phase.

480

4819 CONCLUDING REMARKS

482

483After the first development of the TOUGH-FLAC simulator 15 years ago, at least 15
484additional TOUGH-based geomechanics models have appeared in the literature (Table 1).

485

486Seven of those involve linking TOUGH2 to an in-house developed or open source finite
487element code, using sequential coupling techniques as in TOUGH-FLAC, but with access to
488the source code for the geomechanics part. One of the main motivations related to those
489developments is the access to the source code and the potential of more efficient coupling as
490well as the possibility of running the codes together on computer clusters. Among the codes
491linking TOUGH to an in-house or open source finite element code, TOUGH-ROCMCH is
492the one that has been applied most extensively to date. Most of these finite element codes are
493limited to linear poro-elasticity, although ROCMECH includes some elasto-plasticity with
494Drucker-Prager and Mohr-Coulomb constitutive models. To extend such geomechanics codes

495to more sophisticated constitutive models that are currently available in FLAC3D will require
496a substantial effort, but is feasible. TOUGH-CSM includes an unorthodox mechanical
497approach that with the current addition for calculation of the full stress tensor can be an
498efficient and useful approach for modeling large systems. TOUGH-based geomechanics
499models based on codes with access to the source code, such as TOUGH-ROCMECH and
500TOUGH-CSM, is expected to have increased user basis as more advanced constitutive
501geomechanics models and processes can be added along with their applications on large
502computer clusters.

503

504TOUGH-FLAC still remains by far the most applied TOUGH-based geomechanics model. It
505is the combination of the TOUGH2 library of fluid equations-of-states (EOS) and the
506FLAC3D library of geomechanical constitutive models that make it possible to extend
507TOUGH-FLAC to new areas of research and geo-engineering applications within a relatively
508short time. The fact that FLAC3D only runs under Windows has been viewed as a bottleneck
509since it cannot be ported to large computer clusters to reduce the computation time. However,
510the computation time is only one part of the effort. Extension into a new research area or other
511types of geological media usually involves development and implementation of new
512constitutive models, to build the mesh and populate the model with material properties,
513boundary conditions, to run the models, to interpret the results and to publish it in scientific
514journals. FLAC3D has the user interface and flexible meshing and post-processing
515capabilities that can be used to construct models for both FLAC3D and TOUGH in an
516efficient way. A [Linux](#) and [MPI](#) version of FLAC3D is planned to be developed in the next
517few years (personal communication with Itasca, April, 2016). This could be very beneficial

518for being able to run large scale problems, though there are issues on how to deal with the
519sequential coupling of codes on large-scale computer clusters.

520

521Currently there is a need for effective model simulations of fracturing and fracture
522propagation in heterogeneous geological media. The ability to model discrete fracture
523propagation in 2D has been demonstrated for TOUGH-RDCA; the fractures can propagate
524through the mesh without the need for remeshing. A 3D version of RDCA is under
525development, but this will require substantial effort and 3D fracture propagation through a 3D
526heterogeneous rock mass will be challenging. Discrete fracture propagation has also been
527demonstrated for TOUGH-ROCMECH, in 3D, but limited to a pre-defined path, such as
528vertical fracture along the boundary of the model domain. Other approaches, such as
529TOUGH-UDEC and TOUGH-PyLith, could be useful additions for modeling complex
530hydraulic stimulations and induced seismicity. TOUGH-RBSN has the potential for modeling
531complex fracturing processes in 3D in heterogeneous geological media, though more
532developments are required before it can be applied for large-scale systems. [The dependency](#)
533[of mesh orientation and size that are typically associated with hydraulic fracturing modeling](#)
534[will also have to be investigated when applying these TOUGH-based hydraulic fracturing](#)
535[models.](#)

536

537Finally, TOUGH-based geomechanics models enabling modeling of coupled THMC (through
538TOUGHREACT) as well as multi-physics joint inversion (through ITOUGH), are areas of
539active research in which significant developments and applications are expected to take place
540in the coming years. TOUGH-based geomechanics models such as TOUGH-FLAC, TOUGH-

541ROCMECH, TOUGH-CSM, TOUGH-RDCA, TOUGH-RBSN, are fully compatible to be
542extended for linking geomechanics to TOUGHREACT and ITOUGH. These TOUGH-based
543geomechanics models are complementary in terms of capabilities and application areas and
544the choice of model for a specific application will always be up to the user based on
545experience with different models, their capability and availability.

546

547**ACKNOWLEDGMENTS**

548This paper was completed with funding from the Assistant Secretary for Fossil Energy, Office
549of Natural Gas and Petroleum Technology, through the National Energy Technology
550Laboratory, and the Used Fuel Disposition Campaign, Office of Nuclear Energy, and the
551Assistant Secretary for Energy Efficiency and Renewable Energy, Geothermal Technologies
552Program, of the U.S. Department of Energy under Contract No. DE-AC02-05CH11231 with
553Lawrence Berkeley National Laboratory. The author thanks Stefan Finsterle, Chris Doughty
554and Carol Valladao at the Lawrence Berkeley National Laboratory for their review of the
555initial manuscript.

556

557

558**REFERENCES**

559

- 560Asahina, D., Bolander, J.E., 2011. Voronoi-based discretizations for fracture analysis of
561 particulate materials. *Powder Technology* 213, 92–99.
- 562Asahina, D., Houseworth, J.E., Birkholzer, J.T., Rutqvist, J., Bolander, J.E., 2014. Hydro-
563 mechanical model for wetting/drying and fracture development in geomaterials.
564 *Computers & Geosciences* 65, 13–23.
- 565Blanco-Martín, L., Rutqvist, J., Birkholzer, J.T., 2015a. Long-term modelling of the thermal-
566 hydraulic-mechanical response of a generic salt repository for heat-generating nuclear
567 waste. *Engineering Geology* 193, 198–211.
- 568Blanco-Martín, L., Wolters, R., Rutqvist, J., Lux K.-H., Birkholzer, J.T., 2015b. Comparison
569 of two simulators to investigate thermal-hydraulic-mechanical processes related to
570 nuclear waste isolation in saliniferous formations. *Computers & Geotechnics* 66, 219–
571 229.

572 Blanco-Martín, L., Rutqvist, J., Doughty, C., Zhang, Y., Oldenburg C., 2015c. iTOUGH-
 573 FLAC modeling of thermal-hydraulic-mechanical processes related to steam-assisted
 574 heavy oil recovery from diatomite. Proceedings of the TOUGH Symposium 2015,
 575 Lawrence Berkeley National Laboratory, Berkeley, California.
 576 Blanco-Martín, L., Wolters, R., Rutqvist, J., Lux, K.-H., Birkholzer, J.T., 2016. Thermal–
 577 hydraulic–mechanical modeling of a large-scale heater test to investigate rock salt and
 578 crushed salt behavior under repository conditions for heat-generating nuclear waste.
 579 Computers & Geotechnics 77, 120–133.
 580 Calder, N., Avis, J., Kremer, E., Walsh, R., 2015. Application of 1D hydromechanical
 581 coupling in TOUGH2 to a deep geological repository glaciation scenario. Proceedings of
 582 the TOUGH Symposium 2015, Lawrence Berkeley National Laboratory, Berkeley,
 583 California.
 584 Cappa, F., Rutqvist, J., 2012. Seismic rupture and ground accelerations induced by CO₂
 585 injection in the shallow crust. Geophysical Journal International 190, 1784–1789.
 586 Figueiredo, B., Tsang, C.F., Rutqvist, J., Bensabat, J., Niemi, A., 2015. Coupled hydro-
 587 mechanical processes and fault reactivation induced by CO₂ Injection in a three-layer
 588 storage formation. International Journal of Greenhouse Gas Control 39, 432–448.
 589 Finsterle, S., 2015. What's new in iTOUGH2?. Proceedings of the TOUGH Symposium 2015,
 590 Lawrence Berkeley National Laboratory, Berkeley, California.
 591 Finsterle, S., Zhang, Y., 2011. Solving iTOUGH2 simulation and optimization problems using
 592 the PEST protocol. Environmental Modelling and Software 26, 959–968.
 593 Gosavi, S., Swenson, D., 2005. Architecture for a coupled code for multiphase fluid flow, heat
 594 transfer and deformation in porous rock, Proceedings of the Thirtieth Workshop on
 595 Geothermal Reservoir Engineering Stanford University, Stanford, California, January 31-
 596 February 2, 2005.
 597 Hu, L., Winterfeld, P.H., Fakcharoenphol, P., Wu, Y.-S., 2013. A novel fully-coupled flow and
 598 geomechanics model in enhanced geothermal reservoirs. Journal of Petroleum Science
 599 and Engineering 107, 1–11.
 600 Huang, Z.-Q., Winterfeld, P.H., Xiong, Y., Wu, Y.-S., Yao, J., 2015. Parallel simulation of
 601 fully-coupled thermal-hydro-mechanical processes in CO₂ leakage through fluid-driven
 602 fracture zones. International Journal of Greenhouse Gas Control 34, 39–51.
 603 Hurwitz, S., Christiansen, L.B., Hsieh, P.A., 2007. Hydrothermal fluid flow and deformation
 604 in large calderas: inferences from numerical simulations. Journal of Geophysical
 605 Research 112, B02206.
 606 Itasca, 2012. FLAC3D V5.0, Fast Lagrangian Analysis of Continua in 3 Dimensions, User's
 607 Guide. Itasca Consulting Group, Minneapolis, Minnesota.
 608 Izadia, G., Elsworth, D., 2014. Reservoir stimulation and induced seismicity: Roles of fluid
 609 pressure and thermal transients on reactivated fractured networks. Geothermics 51, 368–
 610 379.
 611 Izadia, G., Elsworth, D., 2015. The influence of thermal-hydraulic-mechanical- and chemical
 612 effects on the evolution of permeability, seismicity and heat production in geothermal
 613 reservoirs. Geothermics 53, 385–395.
 614 Jeanne, P., Guglielmi, Y., Cappa, F., Rinaldi, A.P., Rutqvist, J., 2014a. The effects of lateral
 615 property variations on fault-zone reactivation by fluid pressurization: application to CO₂
 616 pressurization effects within major and undetected fault zones. Journal of Structural
 617 Geology 62, 97-108.

618 Jeanne, P., Rutqvist, J., Dobson, P.F., Walters, M., Hartline, C., Garcia, J., 2014b. The impacts
 619 of mechanical stress transfers caused by hydromechanical and thermal processes on fault
 620 stability during hydraulic stimulation in a deep geothermal reservoir. *International*
 621 *Journal of Rock Mechanics & Mining Sciences* 72, 149–163.

622 Jeanne, P., Rutqvist, J., Vasco, D., Garcia, J., Dobson, P.F., Walters, M., Hartline, C., Borgia
 623 A., 2014c. A 3D hydrogeological and geomechanical model of an Enhanced Geothermal
 624 System at The Geysers, California. *Geothermics* 51, 240–252.

625 Jeanne, P., Rutqvist, J., Hartline, C., Garcia, J., Dobson, P.F., Walters, M., 2014d. Reservoir
 626 structure and properties from geomechanical modeling and microseismicity analyses
 627 associated with an enhanced geothermal system at The Geysers, California. *Geothermics*
 628 51, 460–469.

629 Jeanne, P., Rutqvist, J., Rinaldi, A.P., Dobson, P.F., Walters, M., Hartline, C., Garcia, J.,
 630 2015a. Seismic and aseismic deformations and impact on reservoir permeability: The
 631 case of EGS stimulation at The Geysers, California, USA. *Journal of Geophysical*
 632 *Research Solid Earth* 120, 7863–7882.

633 Jeanne, P., Rutqvist, J., Dobson, P.F., Garcia, J., Walters, M., Hartline, C., Borgia, A., 2015b.
 634 Geomechanical simulation of the stress tensor rotation caused by injection of cold water
 635 in a deep geothermal reservoir. *Journal of Geophysical Research Solid Earth* 120, 8422–
 636 8438.

637 Ji, L., Settari, A., Sullivan, R.B., 2009. A novel hydraulic fracturing model fully coupled with
 638 geomechanics and reservoir simulation. *SPE Journal* 14, 423–430.

639 Kim, J., 2010. Sequential methods for coupled geomechanics and multiphase flow. Ph.D.
 640 Thesis, Department of Energy Resources Engineering, Stanford University, California,
 641 264 pp.

642 Kim, J., Moridis, G.J., 2013. Development of the T+M coupled flow–geomechanical
 643 simulator to describe fracture propagation and coupled flow–thermal–geomechanical
 644 processes in tight/shale gas systems. *Computers & Geosciences* 60, 184–198.

645 Kim, J., Moridis, G.J., 2015. Numerical analysis of fracture propagation during hydraulic
 646 fracturing operations in shale gas systems. *International Journal of Rock Mechanics &*
 647 *Mining Sciences* 76, 127–137.

648 Kim, J., Tchelepi, H.A., Juanes, R., 2009. Stability, accuracy and efficiency of sequential
 649 methods for coupled flow and geomechanics. In: *SPE reservoir simulation symposium*,
 650 2009 [Paper 119084].

651 Kim, J., Tchelepi, H.A., Juanes, R., 2011. Stability and convergence of sequential methods
 652 for coupled flow and geomechanics: fixed-stress and fixed-strain splits. *Computer*
 653 *Methods in Applied Mechanics and Engineering* 200, 1591–1606.

654 Kim, J., Moridis, G.J., Yang, J., Rutqvist, J., 2012. Numerical studies on two-way coupled
 655 fluid flow and geomechanics in hydrate deposits, Society of Petroleum Engineers. SPE-
 656 141304-PA, *SPE Journal* 17, 485–501.

657 Kim, J., Sonnenthal, E., Rutqvist, J., 2012. A modeling and sequential numerical algorithms of
 658 coupled fluid/heat flow and geomechanics for multiple porosity materials. *International*
 659 *Journal of Numerical Methods in Engineering* 92, 425–456.

660 Kim, H.-M., Rutqvist, J., Jeong, J.-H., Choi, B.-H., Ryu, D.-W., Song, W.-K., 2013.
 661 Characterizing excavation damaged zone and stability of pressurized lined rock caverns
 662 for underground compressed air energy storage. *Rock Mechanics and Rock Engineering*
 663 46, 1113–1124.

664 Kim, K., Rutqvist, J., Nakagawa, S., Houseworth, J., Birkholzer, J., 2015a. Simulation of
665 fluid-driven fracturing within discrete fracture networks using
666 TOUGH-RBSN. Proceedings of the TOUGH Symposium 2015, Lawrence Berkeley
667 National Laboratory, Berkeley, California.

668 Kim, J., Sonnenthal, E., Rutqvist, J., 2015b. A sequential implicit algorithm for chemo-thermo-
669 poro-mechanics for fractured geothermal reservoir. Computers & Geosciences 76, 59–71.

670 Konstantinovskaya, E., Rutqvist, J., Malo, M., 2014. CO₂ storage and potential fault
671 instability in the St. Lawrence Lowlands sedimentary basin (Quebec, Canada): Insights
672 from coupled reservoir-geomechanical modeling. International Journal of Greenhouse
673 Gas Control 22, 88–110.

674 Lee, J., Min, K.-B., Rutqvist, J., 2015. TOUGH-UDEC simulator for the coupled multiphase
675 fluid flow, heat transfer, deformation in fracture porous media. Proceedings of 13th
676 Congress of the ISRM, Montreal, Quebec, Canada, May 10 - 13, 2015.

677 Lei, H., Xu, T.F., Jin, G., 2015. TOUGH2Biot – A simulator for coupled thermal–
678 hydrodynamic–mechanical processes in subsurface flow systems: Application to CO₂
679 geological storage and geothermal development. Computers & Geosciences 77, 8–19.

680 Loschetter, A., Smai, F., Sy, S., Burnol, A., Leynet, A., Lafortune, S., Thoraval, A., 2012.
681 Simulation of CO₂ storage in coal seams: coupling of TOUGH2 with the solver for
682 mechanics Code_Aster, Proceedings of the TOUGH Symposium 2012, Lawrence
683 Berkeley National Laboratory, Berkeley, California.

684 Lux, K.-H., Rutenberg, M., Seeska, R., Düsterloh, U., 2014. Kopplung der Software codes
685 FLAC3D und TOUGH2 in Verbindung mit in situ-, laborativen und numerischen
686 Untersuchungen zum thermisch-hydraulisch-mechanisch gekoppelten Verhalten von
687 Tongestein unter Endlagerbedingungen. TU Clausthal; 2014 [Final Rep BMWi-Proj
688 02E11041].

689 Mainguy, M., Longuemare, P., 2002. Coupling fluid flow and rock mechanics: Formulations
690 of the partial coupling between reservoir and geomechanics simulators. Oil & Gas
691 Science and Technology – Rev IFP 57, 355–367.

692 Mazzoldi, A., Rinaldi, A.P., Borgia, A., Rutqvist, J., 2012. Induced seismicity within geologic
693 carbon sequestration projects: Maximum earthquake magnitude and leakage potential.
694 International Journal of Greenhouse Gas Control 10, 434–442.

695 Miah, M., Blanco-Martín, L., Foxall, W., Rutqvist, J., Rinaldi, A.P., Mullen, C., 2015.
696 Development of a hydro-geomechanical model to simulate coupled fluid flow and
697 reservoir geomechanics, Proceedings of the TOUGH Symposium 2015, Lawrence
698 Berkeley National Laboratory, Berkeley, California.

699 Mikelic, A., Wang, B., Wheeler, M.F., 2014. Numerical convergence study of iterative
700 coupling for coupled flow and geomechanics. Computers & Geosciences 18, 325–341.

701 Minkoff, S.E., Stone, C.M., Bryant, S., Peszynska, M., Wheeler, M.F., 2003. Coupled fluid
702 flow and geomechanical deformation modeling, Journal of Petroleum Sciences and
703 Engineering 38, 37–56.

704 Nespolia, M., Rinaldi, A.P., Wiemer, S., 2015. TOUGH2-SEED: A coupled fluid flow and
705 mechanical statistical model for the study of injection-induced seismicity. Proceedings of
706 the TOUGH Symposium 2015, Lawrence Berkeley National Laboratory, Berkeley,
707 California.

708 Noorishad, J, Ayatollahi, M.S., Witherspoon, P.A., 1982. A finite element method for coupled
709 stress and fluid flow analysis of fractured rocks. *International Journal of Rock Mechanics*
710 *and Mining Sciences* 19, 185–193.

711 Pan, P.-Z., Rutqvist, J., Feng, X.-T., Yan, F., 2013. Modeling of caprock discontinuous
712 fracturing during CO₂ injection into a deep brine aquifer. *International Journal of*
713 *Greenhouse Gas Control* 19, 559–575.

714 Pan, P.-Z., Rutqvist, J., Feng, X.-T., Yan, F., 2014a. An approach for modeling rock
715 discontinuous mechanical behavior under multiphase fluid flow conditions. *Rock*
716 *Mechanics and Rock Engineering*, 47, 589–603.

717 Pan, P.-Z., Rutqvist, J., Feng, X.-T., Yan, F., Jiang, Q., 2014b. A discontinuous cellular
718 automaton method for modeling rock fracture propagation and coalescence under fluid
719 pressurization without remeshing. *Rock Mechanics and Rock Engineering* 47, 2183–
720 2198.

721 Pan, P.-Z., Rutqvist, J., Feng, X.-T., Feng, Yan, F., 2014c. TOUGH–RDCA modeling of
722 multiple fracture interactions in caprock during CO₂ injection into a deep brine aquifer.
723 *Computers & Geosciences* 65, 24–36.

724 Prevost, J.H., 2013. One-way versus two-way coupling in reservoir-geomechanical models.
725 in *Poromechanics V: Proceedings of the Fifth Biot Conference on Poromechanics*,
726 Vienna, Austria, July 10-12, 2013.

727 Pruess, K., Oldenburg, C., Moridis, G., 2012. TOUGH2 user's guide, version 2.1, LBNL-
728 43134 (revised), Lawrence Berkeley National Laboratory, Berkeley, California

729 Rinaldi, A.P., Vilarrasa, V., Rutqvist, J., Cappa, F., 2015a. Fault reactivation during CO₂
730 sequestration: Effects of well orientation on seismicity and leakage. *Greenhouse Gas*
731 *Sciences and Technology* 5, 1–12.

732 Rinaldi, A.P., Rutqvist, J., Sonnenthal, E.L., Cladouhos, T.T., 2015b. Coupled THM modeling
733 of hydroshearing stimulation in tight fractured volcanic rock. *Transport in Porous Media*
734 108, 131–150.

735 Rinaldi, A.P., Rutqvist, J., Finsterle, S., Liu, H.-H., 2015c. Inverse modeling of coupled fluid
736 flow and geomechanics with iTOUGH-PEST and TOUGH-FLAC: Application to In
737 Salah CO₂ storage site. *Proceedings of the TOUGH Symposium 2015*, Lawrence
738 Berkeley National Laboratory, Berkeley, California.

739 Rinaldi, A.P., Jeanne, P., Rutqvist, J., Cappa, F., Guglielmi, Y., 2014a. Effects of fault-zone
740 architecture on earthquake magnitude and gas leakage related to CO₂ injection in a
741 multilayered sedimentary system. *Greenhouse Gases: Science and Technology* 4, 99-120.

742 Rinaldi, A.P., Rutqvist, J., Cappa, F., 2014b. Geomechanical effects on CO₂ leakage through
743 fault zones during large-scale underground injection. *International Journal of Greenhouse*
744 *Gas Control* 20, 117–131.

745 Rinaldi, A.P., Rutqvist, J., 2013. Modeling of deep fracture zone opening and transient ground
746 surface uplift at KB-502 CO₂ injection well, In Salah, Algeria. *International Journal of*
747 *Greenhouse Gas Control* 12, 155–167.

748 Rohmer, J., Seyedi, D.M., 2010. Coupled large scale hydromechanical modelling for caprock
749 failure risk assessment of CO₂ storage in deep saline aquifers. *Oil & Gas Science and*
750 *Technology – Rev IFP* 65, 503–517.

751 Rutqvist, J., 2011. Status of the TOUGH-FLAC simulator and recent applications related to
752 coupled fluid flow and crustal deformations. *Computers & Geosciences*, 37, 739–750.

753Rutqvist, J., Stephansson, O., 2003. The role of hydromechanical coupling in fractured rock
 754 engineering. *Hydrogeology Journal* 11, 7–40.

755Rutqvist, J., Tsang, C.-F., 2002. A study of caprock hydromechanical changes associated with
 756 CO₂ injection into a brine aquifer. *Environmental Geology* 42, 296–305.

757Rutqvist, J., Tsang, C.-F., 2003a. TOUGH-FLAC: A numerical simulator for analysis of
 758 coupled thermal-hydrologic-mechanical processes in fractured and porous geological
 759 media under multi-phase flow conditions. *Proceedings of the TOUGH symposium 2003*,
 760 Lawrence Berkeley National Laboratory, Berkeley, May 12–14.

761Rutqvist, J., Tsang, C.-F., 2003b. Analysis of thermal-hydrologic-mechanical behavior near an
 762 emplacement drift at Yucca Mountain. *Journal of Contaminant Hydrology* 62–63, 637–
 763 652.

764Rutqvist, J., Tsang, C.-F., 2012. Multiphysics processes in partially saturated fractured rock:
 765 Experiments and models from Yucca Mountain. *Reviews of Geophysics* 50, RG3006,
 766 2012.

767Rutqvist, J., Wu, Y.-S., Tsang, C.-F., Bodvarsson, G., 2002. A Modeling Approach for
 768 Analysis of Coupled Multiphase Fluid Flow, Heat Transfer, and Deformation in Fractured
 769 Porous Rock. *International Journal Rock Mechanics & Mining Sciences* 39, 429–442.

770Rutqvist, J., Kim, H.-M., Ryu, D.-W., Synn, J.-H., Song, W.-K., 2012a. Modeling of coupled
 771 thermodynamic and geomechanical performance of underground compressed air energy
 772 storage in lined rock caverns. *International Journal of Rock Mechanics & Mining*
 773 *Sciences* 52, 71–81.

774Rutqvist, J., Moridis, G.J., Grover, T., Silpngarm, S., Collett, T.S., Holdich, S.A., 2012a.
 775 Coupled multiphase fluid flow and wellbore stability analysis associated with gas
 776 production from oceanic hydrate-bearing sediments. *Journal of Petroleum Science and*
 777 *Engineering* 92–93, 65–81.

778Rutqvist, J., Leung, C., Hoch, A., Wang, Y., Wang, Z., 2013. Linked multicontinuum and
 779 crack tensor approach for modeling of coupled geomechanics, fluid flow and transport in
 780 fractured rock. *International Journal of Rock Mechanics and Geotechnical Engineering* 5,
 781 18–31.

782Rutqvist, J., Cappa, F., Rinaldi, A.P., Godano, M., 2014a. Modeling of induced seismicity and
 783 ground vibrations associated with geologic CO₂ storage, and assessing their effects on
 784 surface structures and human perception. *International Journal of Greenhouse Gas*
 785 *Control* 24, 64–77.

786Rutqvist, J., Zheng, L., Chen, F., Liu, H.-H., Birkholzer J., 2014b. Modeling of Coupled
 787 Thermo-Hydro-Mechanical Processes with Links to Geochemistry Associated with
 788 Bentonite-Backfilled Repository Tunnels in Clay Formations. *Rock Mechanics and Rock*
 789 *Engineering* 47, 167–186.

790Rutqvist, J., Dobson, P.F., Garcia, J., Hartline, C., Jeanne, P., Oldenburg, C.M., Vasco D.W.,
 791 Walters, M., 2015a. The northwest Geysers EGS demonstration project, California: Pre-
 792 stimulation modeling and interpretation of the stimulation. *Mathematical Geosciences* 47,
 793 3–26.

794Rutqvist, J., Rinaldi, A.P., Cappa, F., Moridis, G.J., 2015b. Modeling of fault activation and
 795 seismicity by injection directly into a fault zone associated with hydraulic fracturing of
 796 shale-gas reservoirs. *Journal of Petroleum Science and Engineering* 127, 377–386.

797Settari, A., Mourits, F., 1998. A coupled reservoir and geomechanical simulation system,
 798 *Society of Petroleum Engineers Journal* 3, 219–226.

799 Smith, T., Sonnenthal, E., Cladouhos, T., 2015. Thermal-hydrological-mechanical modelling
 800 of shear stimulation at Newberry Volcano, Oregon. Proceedings of the 49th US Rock
 801 Mechanics/Geomechanics Symposium, San Francisco, CA, USA, 28 June- 1 July 2015.
 802 American Rock Mechanics Association ARMA, Paper No. 15-680.
 803 Taron, J., Elsworth, D., 2009. Thermal–hydrologic–mechanical–chemical processes in the
 804 evolution of engineered geothermal reservoirs. *International Journal of Rock Mechanics
 805 & Mining Sciences* 46, 855–864.
 806 Taron, J., Elsworth, D., Min, K.B., 2009. Numerical simulation of thermal–hydrologic–
 807 mechanical–chemical processes in deformable, fractured porous media. *International
 808 Journal of Rock Mechanics & Mining Sciences* 46, 842–854.
 809 Urpi, L., Rinaldi, A.P., Rutqvist, J., Cappa, F., Spiers, C.J., 2016. Dynamic simulation of CO₂-
 810 injection-induced fault rupture with 1 slip-rate dependent friction coefficient.
 811 *Geomechanics for the Energy and Environment* (accepted April 28, 2016).
 812 Vilarasa, V., Rutqvist, J., Blanco-Martín, L., Birkholzer, J., 2015. Use of a dual structure
 813 constitutive model for predicting the long-term behavior of an expansive clay buffer in a
 814 nuclear waste repository. *ASCE's International Journal of Geomechanics* D4015005.
 815 .
 816 Walsh, R., Calder, N., Avis, J., 2012. A Simple Implementation of 1D Hydromechanical
 817 Coupling In TOUGH2, Proceedings of the TOUGH Symposium 2012, Lawrence
 818 Berkeley National Laboratory, Berkeley, California.
 819 Walsh, R., Nasir, O., Calder, N., Sterling, S., Avis J., 2015. Combining TOUGH2 and
 820 FLAC3D to solve problems in underground natural gas storage. Proceedings of the
 821 TOUGH Symposium 2015, Lawrence Berkeley National Laboratory, Berkeley,
 822 California.
 823 Winterfeld, P.H., Wu, Y.-S., 2012. Development of an advanced thermal-hydrological-
 824 mechanical model for CO₂ storage in porous and fractured saline aquifers. Proceedings of
 825 the TOUGH Symposium 2012, Lawrence Berkeley National Laboratory, Berkeley,
 826 California, 2012.
 827 Winterfeld, P. H., Wu, Y.-S., 2014. Simulation of CO₂ sequestration in brine aquifers with
 828 geomechanical coupling. In *Computational Models for CO₂ Sequestration and
 829 Compressed Air Energy Storage*, edited by J. Bundschuh and R. Al-Khoury, Chapter 8,
 830 CRC Press, New York, NY, 2014.
 831 Winterfeld, P.H., Wu, Y.-S., 2015. A coupled flow and geomechanics simulator for CO₂
 832 storage in fracture reservoirs. Proceedings of the TOUGH Symposium 2015, Lawrence
 833 Berkeley National Laboratory, Berkeley, California.
 834 Zhang, R., Yin, X., Winterfeld, P.H., Wu, Y.-S., 2012. A fully coupled model of
 835 nonisothermal multiphase flow, geomechanics, and chemistry during CO₂ sequestration
 836 in brine aquifers. Proceedings of the TOUGH Symposium 2012. Lawrence Berkeley
 837 National Laboratory, California.
 838 Zheng, L., Rutqvist, J., Liu, H.-H., Birkholzer, J.T., Sonnenthal E., 2014. Model evaluation of
 839 geochemically induced swelling/shrinkage in argillaceous formations for nuclear waste
 840 disposal. *Applied Clay Science* 97–98, 24–32.
 841 Zheng, L., Rutqvist, J., Birkholzer, J.T., Liu, H.H., 2015. On the impact of temperatures up to
 842 200°C in clay repositories with bentonite engineer barrier systems: a study with coupled
 843 thermal, hydrological, chemical, and mechanical modeling. *Engineering Geology* 197,
 844 278–295.

845
846
847

848
849
850
851
852
853

854
855
856
857
858

859Figure 1. Hydromechanical couplings in geological media; (i) and (ii) are direct couplings
860through pore volume interactions, while (iii) and (iv) are indirect couplings through changes
861in material properties ([Rutqvist and Stephansson, 2003](#)).

862
863
864
865
866
867
868
869
870