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1 **AN OVERVIEW OF TOUGH-BASED GEOMECHANICS MODELS**

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42**ABSTRACT**

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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.

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

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591 INTRODUCTION

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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
68Tsang, 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).

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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 Moridis, 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,
1692013). 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.

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1863 **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 Geysers 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**

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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 Seyedi \(2010\)](#) 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 at 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-ROCMECH 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

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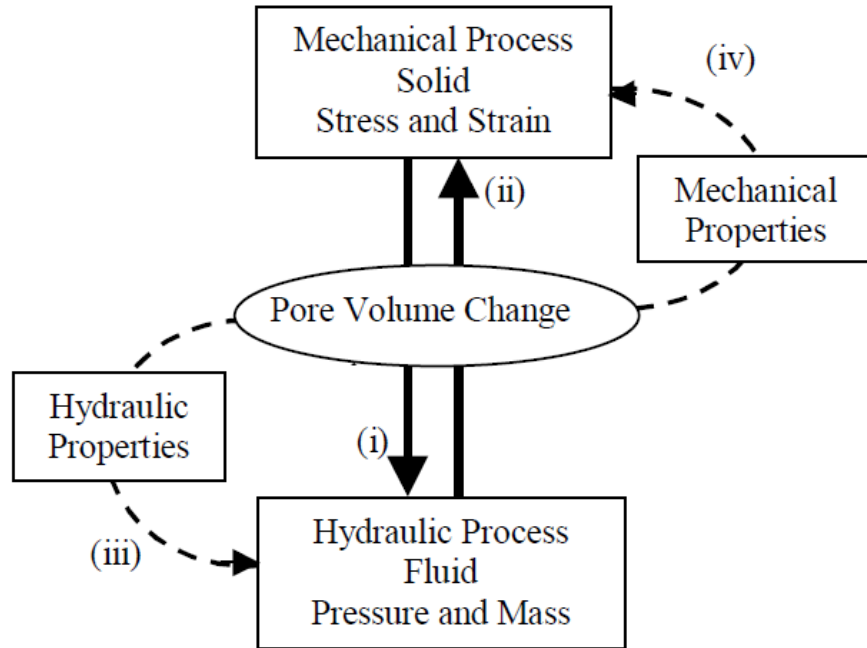
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859Figure 1. Hydromechanical couplings in geological media; (i) and (ii) are direct couplings
860through pore volume interactions, while (iii) and (iv) are indirect couplings through changes
861in material properties (Rutqvist and Stephansson, 2003).

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