**QUALITY ASSURANCE PROJECT PLAN**

# A. PROJECT MANAGEMENT

## A1. TITLE AND APPROVAL SHEET

TITLE: Analysis of Environmental Hazards Related to Hydrofracturing
EPA Interagency Agreement No. DW-89-92235901-C
LBNL Interagency Agreement No. BG854806

REVISION NUMBER: 0

DATE: 12/01/2011

CONTRACT SUPPORT: Lawrence Berkeley National Laboratory

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|---|---|
| /s/ | 12/01/2011 |
| George J. Moridis, Principal Investigator | Date |

EPA APPROVALS:

| | |
|---|---|
| /s/ | 12/06/2011 |
| Stephen Kraemer, EPA Technical Research Lead for Scenario Evaluation & Modeling | Date |
| /s/ | 12/07/2011 |
| John M. Johnston, Chief, ERD Regulatory Support Branch | Date |
| /s/ | 12/06/2011 |
| James Kitchens, ERD QA Manager | Date |

**A2. TABLE OF CONTENTS**

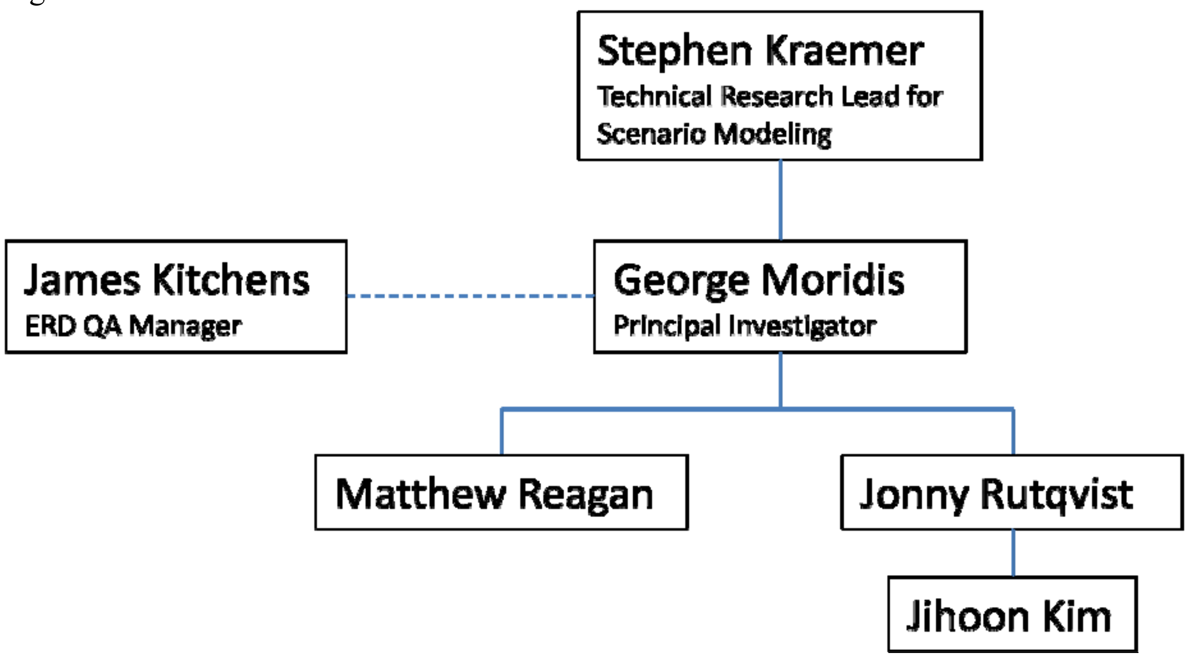
## A3. DISTRIBUTION LIST

The following individuals will be provided copies of the approved QA Project Plan. Their responsibilities are described in section A4.

Dr. George Moridis - LBNL, Berkeley, CA
Dr. Matthew Reagan - LBNL, Berkeley, CA
Dr. Jonny Rutqvist - LBNL, Berkeley, CA
Dr. Jihoon Kim - LBNL, Berkeley, CA
Dr. Peter Persoff - LBNL, Berkeley, CA
Dr. Robert Puls - EPA GWERD, Ada, OK EPA
Mr. Steve Vandegrift - EPA GWERD, Ada, OK
Dr. James W. Weaver – EPA GWERD, Ada, OK
Mr. James Kitchens – EPA ERD, Athens, GA
Dr. Stephen Kraemer - EPA ERD, Athens, GA
Dr. John M. Johnston – EPA ERD, Athens, GA
Mr. Bruce Kobelski, EPA OGWDW, Washington, DC

## A4. PROJECT / TASK ORGANIZATION

Organization Chart




Dr. George Moridis - LBNL, Berkeley, CA. Principal Investigator. Responsible for coding, TOUGH+ modeling, direction, preparation of project reports and communication with EPA;

Dr. Matthew Reagan - LBNL, Berkeley, CA. Scientist, responsible for TOUGH+, TOUGH2, and EOS9nT modeling;

Dr. Jonny Rutqvist - LBNL, Berkeley, CA Staff Scientist, responsible for coupled flow and geomechanics simulations (FLAC3D);

Dr. Jihoon Kim - LBNL, Berkeley, CA Post-doctoral research associate, responsible for coupled flow and geomechanics simulations including fracture propagation using ROCKMECH and FLAC3D;

NOTE: *Additional LBNL scientists may join the project, as dictated by evolving project needs. All scientists will be under the supervision of Dr. George Moridis, who is responsible for the overall project management.*

Dr. Peter Persoff - LBNL, Berkeley, CA QA Manager, responsible for preparation of QA project plan and self-assessment of QA compliance with this plan;

Dr. Robert Puls - EPA GWERD, Ada, OK EPA Overall Technical Research Lead on the Hydraulic Fracturing Research Program , U.S. Environmental Protection Agency, Ground Water and Ecosystems Restoration Division, Ada, OK;

Mr. James Kitchens - EPA ERD, Athens, GA EPA QA Manager, Environmental Protection Agency, Responsible for QA review/approval of the QAPP, conducting audits, and QA review/approval of the final product;

Mr. Steve Vandegrift - Ground Water and Ecosystems Restoration Division, Ada, OK, HF Program QA Manager, Environmental Protection Agency Responsible for concurrence that the QAPP meets HF Research Program requirements;

Dr. Stephen Kraemer - EPA ERD Athens, GA is the EPA Project Manager for the Hydraulic Fracturing Failure Scenarios assessment and Technical Research Lead for Scenario Evaluation and Modeling. Responsible for technical oversight, technical review of the QAPP, ensuring project goals are achieved, and review/approval of project deliverables;

Mr. Bruce Kobelski – EPA OGWDW, Washington, DC, is the EPA Project Officer over the Interagency Agreement with LBNL.

## A5. PROBLEM DEFINITION / BACKGROUND

- *Background information on the problem*

Hydrocarbon production from tight reservoirs has grown rapidly over the last few years Tight reservoirs require well and reservoir stimulation because, even with the presence of a system of natural fractures, the matrix permeability is too low to support flow at commercially viable rates without permeability enhancement. Such enhancement/stimulation is provided by a number of hydraulic fracturing (HF) methods, all of which are designed to develop a new system of artificial fractures that increase both the permeability of the system and the fracture-matrix interface area (over which reservoir fluids flow from the matrix to the permeable fractures) to provide access to larger volume of the reservoir.

This substantial increase in gas production from HF has been accompanied by controversy about the additional effects of stimulation to the subsurface beyond the confines of the tight, hydrocarbon-bearing formation. Generally speaking, the concerns are that reservoir stimulation creates significant environmental hazards via the fracturing of the overburden of reservoirs (and creating fast permeability pathways). This could result in contamination of potable groundwater resources (the main source of drinking water for a large part of the US rural population) by escaping hydrocarbons and other reservoir fluids that ascend through the subsurface.

Many concerns about hydraulic fracturing center on potential risks to drinking water resources, although other issues have been raised. In response to public concern, Congress directed the United States Environmental Protection Agency (EPA) to conduct research to examine the relationship between hydraulic fracturing and drinking water resources (USEPA, 2011a). The purpose of this modeling project is to support EPA's reports to Congress by providing credible simulations of possible failure scenarios, identifying the range of conditions under which they might be expected to occur.

This project will investigate by numerical simulation (a) the possible mechanisms of stimulation-induced overburden-failure that could lead to such upward migration of hydrocarbons, and (b) the conditions under which such catastrophic scenarios are possible. Under a separate contract, EPA is assembling a database that will include reported incidents of aquifer contamination or gas release (USEPA 2011b). If such data are available the incidents will be analyzed retrospectively.

Possible Failure Scenarios

The possible mechanisms for the upward migration of contaminants following stimulation are the following:

**A.** Failure of the well completion during stimulation because of inadequate/inappropriate design and/or weak cement. In this case, the cement around the well is the weak link and is fractured during the stimulation process, but the overburden is not (necessarily) fractured. Improper cementing and well completion can create a high-permeability pathway around the wellbore, through which contaminants can move upward (see Figure 1).

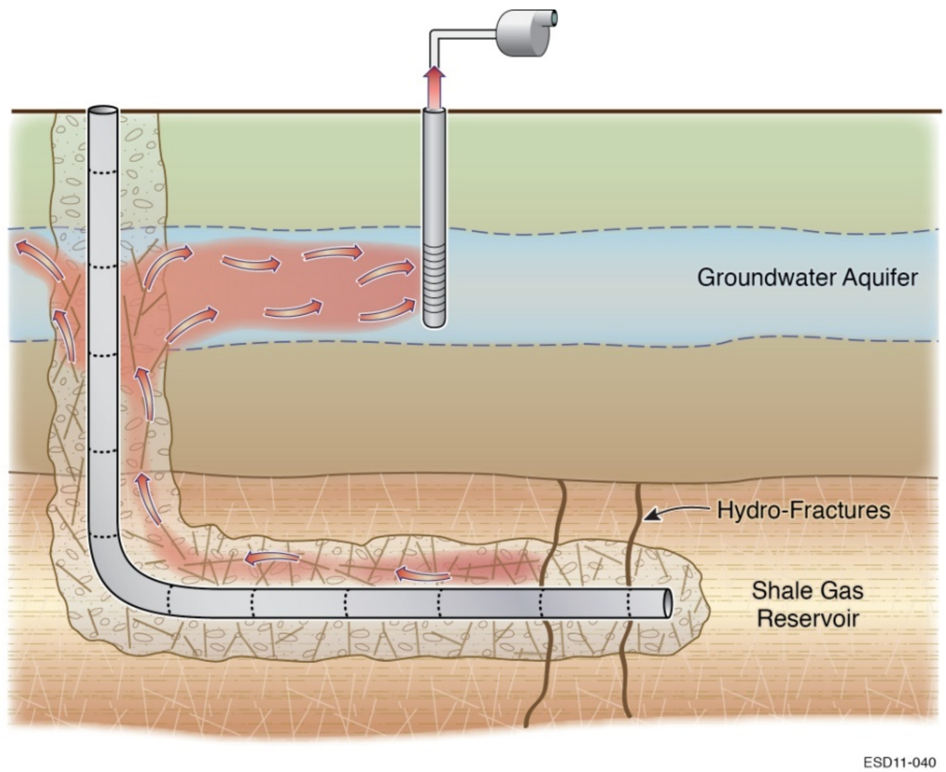



**Figure 1**. HF hypothetical failure scenario A.

**B.** Fracturing of the overburden because of inadequate design of the stimulation operation, with the resulting fractures reaching abandoned unplugged wells (or their vicinity) in conventional reservoirs. These aging wells intersect and communicate with groundwater aquifers, and inadequate or failing completions/cement can create pathways for contaminants to reach the potable groundwater resources (see Figure 2).

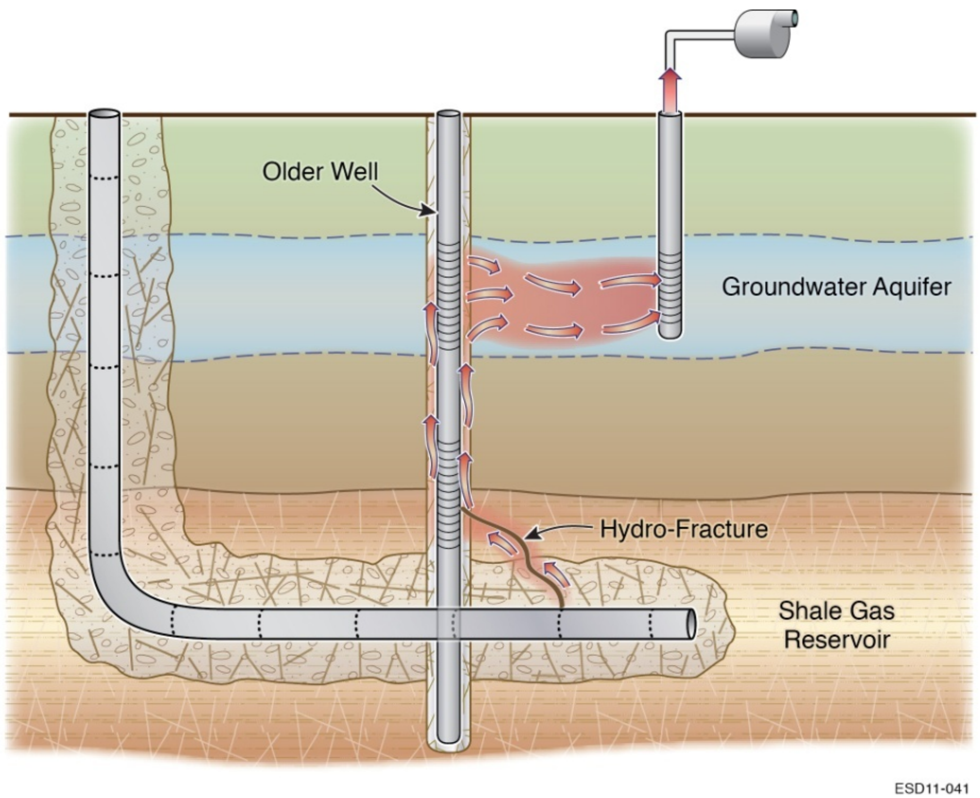



**Figure 2**. HF hypothetical failure scenario B.

**C.** Fracturing of the overburden because of inadequate design of the stimulation operation, with the resulting fractures reaching groundwater resources, or even permeable formations that communicate with (generally) shallower groundwater-bearing strata (see Figure 3).

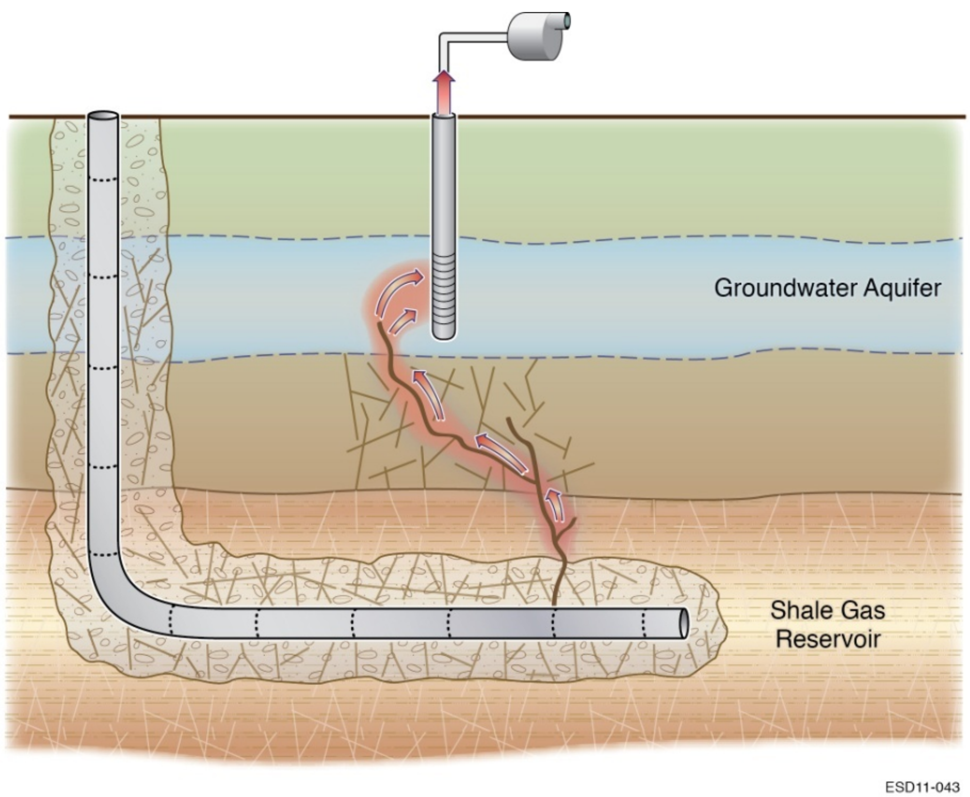



**Figure 3**. HF hypothetical failure scenario C

**D.** Induced fractures move upward and reaching groundwater resources after intercepting conventional hydrocarbon reservoirs, which may create an additional source (see Figure 4).

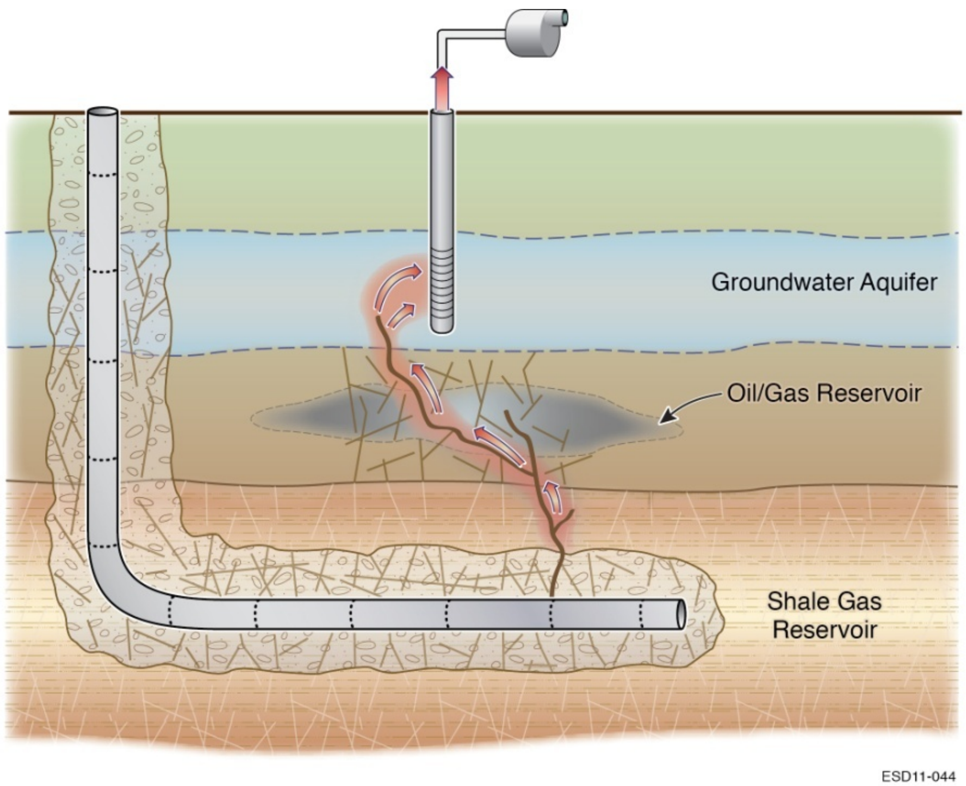



**Figure 4.** HF hypothetical failure scenario D.

**E.** Sealed/dormant fractures and faults are activated by the hydro-fracturing operation, creating pathways for upward migration of hydrocarbons and other contaminants (see Figure 5).

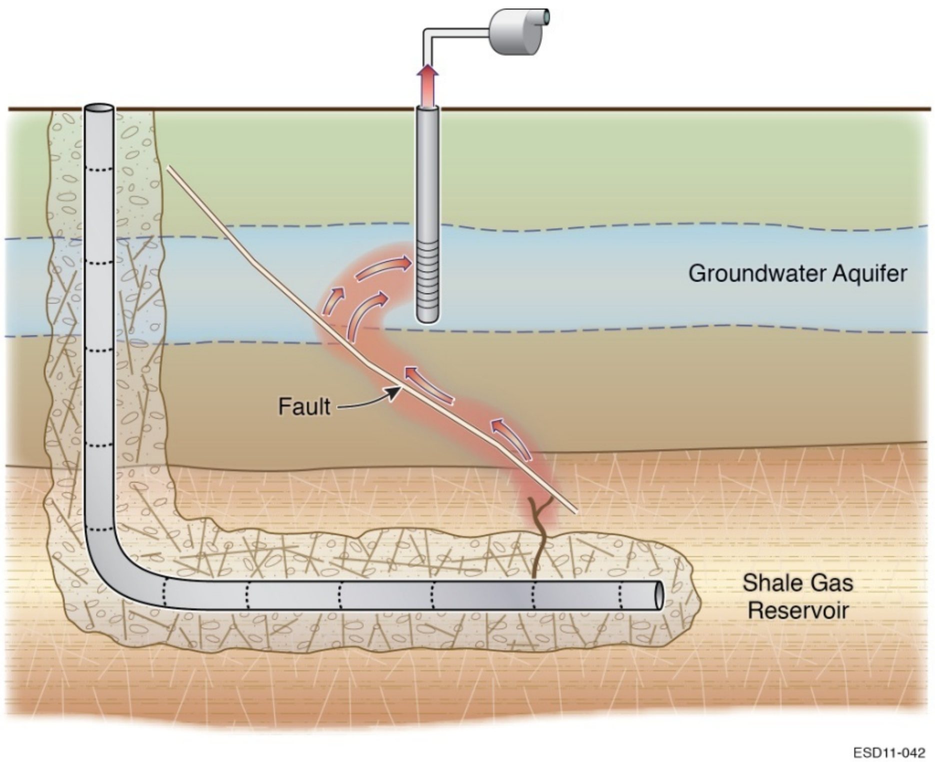



**Figure 5**. HF hypothetical failure scenario E.

- *Goals and objectives of this project that will address this problem*

This project will develop models that can be applied to proposed applications of hydraulic fracturing (HF) technology to determine the range of conditions that can lead to five types of failures identified in the problem definition. Each potential failure scenario is simulated by a separate model. The purpose of these models is to take generalized information on hydraulic fracturing operations and provide non-site specific insight into potential failure scenarios.
These models will support EPA's reports to Congress. The models are not intended to be used by operators in the design of HF projects, or by regulators in permitting decisions, but they are intended for use by either community as research tools.

The models are appropriate for their intended purpose, as they can simulate the flow and transport of gas, water, and dissolved contaminants concurrently in a fractures and porous reservoir. Full qualification of TOUGH+ software is not within the scope of this project.

- *Reasons the project is important, how it supports other existing research, programs, or regulations*

This project is important because Congress, in response to public concern, has directed the United States Environmental Protection Agency (EPA) to conduct research to examine the relationship between hydraulic fracturing and drinking water resources (USEPA, 2011a). This project will support reports that EPA is obligated to give to Congress.

HF-enhanced shale gas is a significant energy resource for the United States that must be developed in a responsible manner.

- *Reasons one model is determined to be better than another for this application*

The physical situation is too complex to be represented accurately by an analytical model. These numerical models will couple flow, transport, thermodynamics (heat flow and phase change), and geomechanics to produce realistic simulations.

The two computer codes used in this work, TOUGH+ and FLAC3D, incorporate more of the relevant physical processes than any other codes. Rutqvist (2011) reviews the subject of simulating coupled thermal-hydraulic-mechanical processes in geological media. TOUGH+ has been developed, and continues in development, because of the lack of any existing model to simulate complex processes.
The method of coupling of TOUGH+ with FLAC3D will be as reported in Rutqvist 2011, Rutqvist et al. 2009, and Rutqvist and Moridis 2009.

A brief description of TOUGH+ and FLAC3D, and their coupling, is presented in Appendix A.

- *Conflicts or uncertainties that will be resolved by this project*

Incidents of contamination of aquifers have been reported. The models will be used to investigate whether the claimed (and proposed) scenarios are possible and if so under what conditions.

## A6. PROJECT/TASK DESCRIPTION AND SCHEDULE

- *Summary of all work to be performed, products to be produced, and the schedule for Implementation*

The work is organized into nine tasks as follows:

***Task 1: Development of Data Base Related To Reported Environmental Problems***
The mathematical possibility of all the cases discussed in Tasks 3 to 7 will be constrained by the widest possible range of realistic values of properties and conditions encountered in the tight geologic systems under investigation. Thus, in this task, we propose to collect all available data (geological, reservoir, geophysical, geochemical, flow, geomechanical, type of environmental problem, extent of contamination, etc.) in cases/instances of reported problems related to stimulation operations in the US and/or Canada. We will attempt to identify cases related to all five types of geomechanical failure discussed in this proposal, and will try to make the data-base as wide as possible. This task will require extensive interaction with federal and/or state environmental protection agencies; these will provide all the available data. *The Environmental Protection Agency will be responsible for the collection and assembly of all these data, which will not be limited to their own data collection from confirmed or suspected cases of groundwater contamination by hydro-fracturing activities in shale-gas operations, but will include data collected by other agencies as well as data published in the peer-reviewed literature*. LBNL's role will be to organize the data in the database using consistent metrics, and to identify important cases that are to be fully analyzed within the context of Tasks 3 to 7. The database will be used to sharpen the focus of the investigations in Tasks 3 to 7, and to determine the limits in the conditions and parameters of systems and procedures/operations associated with environmental problems (or perceptions thereof).

Note that significant effort will be expended in Task 1 in the first 2 months from the project inception because the insights obtained here will make possible to facilitate execution of Task 2 by providing a basis for identifying and concentrating on the most likely/frequent/problematic failure mechanisms and the resulting groundwater contamination hazards.

Task Duration: From the beginning of the project to 3/31/2012

***Task 2: Preliminary Evaluation and Ranking of Failure Scenarios***
This task involves a preliminary evaluation, assessment and ranking of the various possible or potential groundwater contamination mechanisms. It will be based on (a) the analysis of the data

originating from Task 1, (b) on the evaluation of the physical likelihood of occurrence of the various failure and contamination scenarios discussed in Tasks 3 to 7, (c) on literature review, and (d) discussions with people involved in field operations of hydro-fracking. The evaluation of the latter in item (b) may involve simple mathematical scoping calculations (analytical or numerical) and assessment of limitations imposed by the geology, of the validity of assumptions, of the feasibility of conditions that are necessary for particular scenarios to occur, etc. The result of the effort in this task is to develop an initial understanding of the relative likelihood of occurrence and the corresponding contamination hazard of the various mechanisms under consideration, which would allow directing the subsequent research effort in the direction of the greatest potential impact. Note that it is entirely possible that the thorough analysis in Tasks 3 to 7 may produce results that do not agree with those from the preliminary evaluation in Task 2.

Task Duration: From 9/1/2011 to 12/01/2011

***Task 3: Analysis of Consequences of Geomechanical Wellbore Failure (Scenario A, Figure 1)***

This task focuses on the flow and geomechanics processes involved in the failure of the well completion (mainly cementing) during the stimulation process. Such a failure can allow escaping hydrocarbons to ascend through the damaged annular space around the wellbore to reach vulnerable groundwater resources. This task aims to determine (a) the well design properties, variables and conditions that can lead to such failures when exposed to the pressures that develop during stimulation operations, (b) the possible length of the failed zone along the wellbore, and the likelihood that the fractured cement can extend over long distances (if the tight formation and the groundwater are separated by considerable distances) from the stimulation point, (c) the *short*- and *long-term* environmental effect of such failure of the near-wellbore zone *during hydrocarbon production and after a well shut-down*, and (d) sensitivity to factors affecting items (a) through (c). It is expected that the limited radius of the failed zone (expected to be limited to a short radius around the wellbore) will result in a very different contamination pattern that those discussed in Tasks 5 to 7. This is expected to be focused around the wellbore, and to be generally less extensive than in the cases of Tasks 5 to 7 (especially over the long run, as production from tight systems tends to decrease very fast).

Task Duration: From 11/1/2011 to 6/30/2012

***Task 4: Analysis of the Consequences of Induced Fractures Intercepting Abandoned Unplugged Wells (Scenario B, Figure 2)***

This task focuses on the flow and geomechanics processes involved during the stimulation processes, and aims to determine (a) the geologic properties and conditions that can lead to development of such limited penetration fractures, (b) the stimulation operations that can cause such fractures, (c) the extent to which the stimulation-induced fracture can reach into the overburden, (d) the *short*- and *long-term* consequences of the creation of such a fracture system into the overburden *during hydrocarbon production and after a well shut-down*, including the extent of the contaminant migration and its spread into the groundwater, and (e) sensitivity to factors affecting items (a) through (d). This study will be undertaken only if it conclusively shown that (a) such a combination of geologic and fracture scenario is possible under the range of normal operating practices and properties of the various geologic media and (b) the results of Task 1 and 2 indicate the existence of such abandoned wells among the cases of reported problems.

The two cases studied in this task both involve fractures connecting the shale stratum to conventional reservoirs with unplugged abandoned vertical wells that may be improperly completed or have failing completions, and may allow communication of fluids rising in the wellbore with the potable water aquifers they intersect. In the first case, the fractures extend across the shale stratum into a nearby depleted conventional reservoir with abandoned defective wells in the overburden or underburden (higher or lower). The energy for the lift of contaminants in this case is most likely provided by the higher pressure of the fluids in the shale (as the abandoned reservoir pressure is expected to be low) and by buoyancy, and the main contaminant reaching the groundwater is expected to be gas. In the second case, fractures extend from a deeper over-pressurized saline aquifer (underburden) through the entire thickness of the shale to an overburden (a depleted conventional petroleum reservoir with abandoned unsealed wells). The energy for the lift of contaminants in this case is most likely provided by the higher pressure of the fluids in the shale (as the abandoned reservoir pressure is expected to be low) and in the saline aquifer in addition to buoyancy, and the contaminants reaching the groundwater are expected to include gas and solutes encountered in the saline aquifer.

Task Duration: From 12/1/2011 to 7/31/2012

***Task 5: Analysis of the Consequences of Induced Fractures Reaching Groundwater Resources (Scenario C, Figure 3)***

This task focuses on the flow and geomechanics processes involved during the stimulation processes, and aims to determine (a) the geologic properties and conditions that can lead to induced fractures reaching groundwater resources, (b) the stimulation operations that can cause extensive fracturing of the overburden, (c) the extent to which the stimulation-induced fracture can reach into the overburden, (d) the *short*- and *long-term* consequences of the creation of such an unwanted extensive fracture system into the overburden *during hydrocarbon production and after a well shut-down*, including the extent of the contaminant migration and its spread into the groundwater, and (e) sensitivity to factors affecting items (a) through (d). The mathematical possibility of all these cases will be constrained by the widest possible range of realistic values of properties and conditions encountered in the tight geologic systems under investigation.

Task Duration: From 11/1/2011 to 6/30/2012

***Task 6: Analysis of Consequences of Induced Fractures Reaching Groundwater Resources After Intercepting Conventional Reservoirs (Scenario D, Figure 4)***

This task will investigate the results of stimulation-induced fractures intercepting conventional reservoirs (overlying or underlying). In a certain sense, this task is an extension of Task 1, as a fracture system extending deep into the overburden and reaching into the groundwater is a requirement for this issue to be a potential environmental problem. Obviously, the flow regime in this case is substantially different from that of Task 1 because the system highly-permeable fractures are now charged not only with the hydrocarbons that are very slowly released from the matrix of the tight system, but also from the much more permeable conventional reservoirs. Thus, fracture storage is no longer a limitation because the fractures are recharged from the permeable conventional reservoir. The activities in this task will be the same as in Task 1, but the system will now be connected to a second (and highly efficient) source. Emphasis in this task will be the estimation of the likelihood of presence of such conventional reservoirs in the vicinity of tight ones and the possibility of *a priori* identification of such conventional reservoirs by means of geophysical surveys.

Task Duration: From 11/1/2011 to 6/30/2012

***Task 7: Analysis of Consequences of Activation of Native Faults and Fractures (Scenario E, Figure 5)***

This task focuses on the flow and geomechanics processes involved in the response of native fractures and faults to the stimulation process. This task aims to determine (a) the geomechanical conditions (both in terms of system properties and stimulation practices) under which the displacement of the subsurface during stimulation is a reversible process (with the system returning to its original state after the end of stimulation), (b) the effect of displacement on the native fracture and fault aperture and permeability, (c) the *short*- and *long-term* transport effect of communication of induced fractures with native fractures and faults (in terms of the reach into the overburden) *during hydrocarbon production and after a well shut-down*, (c) the short- and long-term groundwater pollution that escaping reservoir fluids can cause under this scenario, and (d) sensitivity to factors affecting items (a) through (c).

A particular case that will be investigated in this Task is an extension of the study in Task 4, and involves the possibility of activated native faults or fractures reaching abandoned unsealed wells with failing completions in conventional reservoirs.

Task Duration: From 12/1/2011 to 7/31/2012

**NOTE: In Tasks 3 to 7, the analysis of groundwater contamination and its transport will not be limited to methane, but, as appropriate by the investigated scenario, will also include**

**salinity, normally occurring radioactive materials, and total dissolved solids (reflecting brines and contaminant-laden deeper water rising to potable water aquifers through fractures, faults, imperfectly completed wellbores, and compromised abandoned wells).**

***Task 8: Development and Implementation of a QA Program***

This task involves the development of a Quality Assurance (QA) program, and its implementation in all aspects of the various tasks of the project. Because of the extensive earlier involvement of LBNL in the evaluation studies of the Yucca Mountain High Level Radioactive Waste Repository (which required one of the most rigorous set of QA procedures meeting the Nuclear Regulatory Commission requirements), there is significant expertise in this subject. We plan to modify the LBNL QA to a level that meets the EPA requirements. A preliminary QA plan is provided as part of this submission package.

Task Duration: From project inception to 12/31/2012

***Task 9: Reporting***

This task involves the submission of (a) monthly e-mail progress reports, (b) a preliminary report on 3/1/2012, (c) an interim report on 6/1/2012, and (d) a final project report (on 9/30/2012) that describes all the activities and investigations conducted within the project. This task also includes the preparation of a minimum of two (2) manuscripts for submission to peer-reviewed journals.

Task Duration: From project inception to 12/31/2012

**Milestones**

1. 12/1/2011: Completion of a progress report
2. 3/1/2012: Completion of the initial sets of simulations of all failure scenarios (25% of total)
3. 6/1/2012: Completion of at least 80% of all simulations of all failure scenarios
4. 9/30/2012: Completion of all simulations, analyses and reports
5. 12/31/2012: Submission of manuscripts for publication.

## A7. QUALITY OBJECTIVES AND CRITERIA FOR MODEL INPUTS/OUTPUTS

- *Project data quality objectives (DQOs), performance criteria, and acceptance criteria*

Acceptance criteria. Environmental and process data will be acquired from the EPA or from the scientific literature. The quality of data acquired from the EPA will have been evaluated as part of another EPA project (USEPA 2011b). Data from both these sources will be evaluated for use on this project. Data acquired from EPA is expected to include data from representative retrospective case studies for analysis. These data will be used for input to simulations and possibly for model testing if a complete enough data set is available.

Performance criteria. The concept of target population is applied to measurements, estimates, or predictions of quantities of environmental concern (USEPA 2006, Section 4.1). In this case the predicted quantities will be the predicted spatial distributions of (a) pressure, (b) phase saturations, (c) concentrations of methane, and/or (d) concentrations of components of fracturing fluids in the groundwater horizon and in the domains under consideration. The performance criterion for these predictions will be their consistency with the input data and mathematical models embodied in the numerical models. The uncertainty of predicted values will be assessed by sensitivity studies in which input data will be varied through ranges consistent with the uncertainty of the input data.

The purpose of these models is not to duplicate field activities, but to evaluate the possibility of different failure scenarios. It is unlikely that field data will be available against which model predictions could be compared. The codes will be verified by simulation of two simplified problems by both the TOUGH+ code and the EOS9nT . The user's manual for EOS9nT (Moridis et al. 1999) provides several test problems in which numerical solutions were verified by comparison with analytical or semi-analytical solutions.

The models will be developed using two existing codes, TOUGH+ and FLAC3D. FLAC3D and the TOUGH family of codes have been verified and validated and used in nuclear waste applications with stringent quality requirements. TOUGH+ is a research code; therefore the user of the code is responsible to confirm its proper use and operation. Earlier versions of TOUGH+ are available for distribution; as distributed it is supplied with test problems that the user can run to verify proper installation. The version of TOUGH+ developed for this project will be available to EPA and ready for scrutiny by the EPA or any Federal agency. Test problems and simulation results will be provided. No user's manual will be provided, but the project reports and the code itself will provide adequate documentation for a knowledgeable user. Test problems will be run during development; input and output files and uncompiled code will be provided.

Model calibration is a process of adjusting model inputs so that predicted values match observations. Generally these models will be used to simulate the failure scenarios identified in Section A5. If sufficient information on the geological system become available that permit comparison of measured and predicted data, then model(s) will be calibrated, but it is not expected that any such data will be available.

Uncertainty and variability will be assessed by sensitivity analyses in which the important input parameters will be varied and their effects determined. All significant input data that can reasonably be expected to affect the results will be varied through a range of expected or typical values. One variable will be varied and others held constant, and results will be presented as plots of specific output values vs. varied input, other inputs having been held constant.

- *Description of task that needs to be addressed and the intended uses of the output of the modeling project to achieve the task*

The task to be addressed is to determine the range of conditions that can lead to overburden failure and associated environmental degradation. The intended use of the output of the modeling project is to support EPA's report to Congress. These models may in the future be used to evaluate proposed HF projects to ensure that such unintended consequences are avoided.

- *List of requirements associated with the hardware/software configuration for those studies involving software evaluation*

FLAC3D is a commercial code and TOUGH+ is a research code. This work will be done using FORTRAN compilers and standard plotting and data analysis software, on personal computers. Calculations will be done on personal computers using codes FLAC3D version 4, TOUGH+ version 1; FORTRAN compilers will be Intel XE2011 and Intel Fortran Composer XE for Mac OS X; and TECPLOT 360, version 2011 and IGOR Pro version 6.12 will be used for visualization and analysis of data.

Conceptual model

The conceptual model is described in Moridis et al. 2010 and in Freeman et al. 2009 and 2011. The approach to fracture propagation will be similar to that in Ji et al. 2009. The key processes to be simulated in the models are fluid flow through porous media, fractures, and faults; desorption of gas from shale, tensile failure of rock, transport advection, dispersion, dissolution of gas in water, heat flow.

Characteristics of the physical system are the stratigraphy, properties of various rock layers (e.g., porosity, permeability, mineral and chemical analysis of rock). The characteristics of the physical system change as a result of HF, and these changes must be incorporated in the models. Typical simulations will cover geographic area up to a few $km^2$, and run for simulated times up to five years.

The final project report will explicitly state and justify all assumptions used to the models. These are also discussed in Moridis et al, 2010, and in Freeman et al. 2009 and 2011. Two assumptions that are specific to this work are: Flow of gas from the shale matrix to fractures is not described by the Darcy models because (I) the desorption gas from shale follows a non-linear isotherm and (ii) pore sizes are small compared to the mean free path of gas molecules (Knudsen flow). Flow of gas within induced fractures is also not described by the Darcy model but by the Forchheimer model because of inertial effects.

Moridis et al. (2010) describe the approach to be used to model flow in shale-gas reservoirs. A similar technical approach has been chosen for the present work. This approach is justified by the fact that it is an extension of methods that have been successfully used for simulations of flow in tight gas reservoirs . Fracture flow will be simulated using a dual-permeability scheme, in which fracture and matrix flow are represented by interacting continua. The matrix will be simulated using a Multiple Interacting Continua (MINC) scheme, with stress-dependent porosity and permeability.

Code verification.

The logic and structure of the codes will be documented in the code itself using comment lines, and in the final report. The logic and structure of FLAC3D and TOUGH+ have been described in their respective user's manuals (Itasca, 2009, Moridis et al. 2008).
No other software or model is exists that can be used to simulate the complex processes in the failure scenarios described in Section A5. To verify that the TOUGH+ code is correctly simulating the mathematical model, a simplified problem will be simulated with both TOUGH+ and with EOS9nT (Moridis et al. 1998), or, where possible, to an analytical solution. EOS9nT has been qualified for use in the contaminant transport studies in support of the license application for the High-Level Nuclear Waste Repository in the unsaturated zone of Yucca Mountain, Nevada. Representative results of these simulations can be found in Moridis et al. (2003), Moridis and Seol (2006a;b) and Seol and Moridis (2006). Moridis et al. (1998) is the user's manual for EOS9nT and contains several test problems demonstrating agreement with analytical and semi-analytical solutions, and Bechtel SAIC Corporation, (2004) provides traceability the software qualification for the Yucca Mountain License Application.

Two simplified problems will be run, using TOUGH+ and either EOS9nT (or an analytical or semi-analytical solution), using the same grid and boundary and initial conditions. The criterion for acceptance will be that all simulated output problem, (pressures, temperatures, saturations, and concentrations) agree within 2% for all places and times in the simulation domain.

FLAC3D is a commercial code and a user's manual, which includes several verification problems with comparison with analytical solutions, is available (Itasca 2009). The code

TOUGH+ is a research code and no user's manual will be prepared. Documentation will be adequate to allow a qualified person to reproduce the work or to run new problems, but a final user's manual will not be prepared. TOUGH+ is a research code; therefore the user of the code is responsible to confirm its proper use. As distributed it is with supplied with test problems that the user can run to verify proper installation and operation. Note that the TOUGH family of codes has been extensively documented (Moridis et al. 2008, Zhang et al. 2008) and much of that documentation is also relevant to TOUGH+.

Input data required for these simulations will be obtained from the EPA (collected as part of another project, USEPA 2011b) or obtained from the technical literature. Input data include:

- site stratigraphy
- rock properties (grain density, intrinsic matrix permeability, permeability of natural fracture network, matrix and fracture porosity, fracture spacing and aperture)
- initial conditions (fracture and matric saturation, pressures)
- gas composition
- pore water composition
- gas adsorption isotherm
- thermal conductivity and specific heat of rocks
- parameters for van Genuchten model of relative permeability
- fracturing pressure
- number of stages
- injected volumes
- pressure evolution during injection
- volumes of fracturing fluid recovered.

This list is not necessarily exhaustive.

It is not expected that all these data have been, or can be, measured in the field. For data not available from measurements, values will be taken from the scientific literature or assumed and justified based upon values in the literature. Uncertainty of input data will be justified based upon values in the literature.

Uncertainty of simulation results will be determined by sensitivity studies in which input values will be varied through the range of their uncertainty.

## A8. SPECIAL TRAINING REQUIREMENTS/CERTIFICATION

- *Types of required training and certification needed by the project team*

The required qualifications of the members of the project team are

- ✓ Advanced degree in appropriate field of engineering
- ✓ Experience in analysis of similar hydrologic and rock-mechanics problems through use of numerical models
- ✓ Record of peer- reviewed publications.

Qualification will be assured by reference to the records of LBNL's HR department and by reference to publications cited in the resumés of team members,

No special training is necessary other than to the QA requirements of this project

## A9. DOCUMENTS AND RECORDS

To ensure that all personnel identified in Section A3 have the current version of the QAPP, e-mail will be used to distribute electronic copies of the QAPP and record acknowledgment of receipt.

The product of this work will be development of the models for the failure scenarios described in Section A. This work will be documented in

- An LBNL report describing the method and approach, and presenting representative simulations. This report will provide guidance sufficient for a qualified person to reproduce the work, but no user's manual for TOUGH+ will be produced. A User's manual for FLAC3D already exists (Itasca, 2009). The codes will be available for license through LBNL.

- Manuscript(s) submitted to peer-reviewed scientific journals

The following documents will be stored electronically on LBNL computers assigned to the researchers:

- computer codes created in the course of development of the models, including test problems for code verification and validation.
- final computer code(s)and input and output files used to generate results.
- records documenting planning and communication between LBNL and EPA or other interested parties
- records documenting in-house review of final report and external peer review of manuscripts submitted for publication.

Researchers will use hard-copy scientific notebooks to record day-to-day activities and decisions.

All documentation shall provide enough detail to allow for reconstruction of the project activities. Documentation practices shall conform to ORD PPM 13.2, "Paper laboratory Records."

All records will be delivered in electronic format to EPA (including scans of hard copy records such as notebooks) at the end of the project for archiving. The record package will include a directory to facilitate location of particular records.

- *Description of information to be included in reports*

The final project report will contain the following elements:

- ✓ Background and description of the problem
- ✓ Development of mathematical representation of processes
- ✓ Development of numerical models to simulate processes
- ✓ Simulation of representative examples of failure scenarios
- ✓ Discussion of simulation results
- ✓ Conclusions and recommendations

*Proper document control and distribution procedures*

- *Details on document storage*
- *Backup plan for records stored electronically*

Work will be done on personal computers and backed up automatically on separate hard drives. Copies will be maintained of all work documents, including codes, input files, and output files necessary for a qualified individual to reproduce the work. Work for this project will be stored separate from work on other projects in a special directory or on a dedicated ESD server.

- *Description of the change control process (who approves changes, etc.)*
  Any change to this QAPP will be approved by the Principal Investigator, EPA Technical Lead and EPA QA Manager. The revised QAPP will be distributed to all participants identified in Section A3.
- *Length of retention periods for each record*
  All records will be delivered in electronic format to EPA (including scans of hard copy records such as notebooks) at the end of the project for archiving. The record package will include a directory to facilitate location of particular records. Records will be retained by EPA for a length of time to be determined by the EPA.
- *Data assessment reports, interim project progress reports*
  Interim project progress reports will be submitted to EPA as requested by the EPA project manager. Some of these reports may support EPA's report to Congress.
- *Model science formulation report, peer review reports*
  The model science formulation will be documented in the final project report and in manuscript(s) submitted to peer-reviewed scientific journals.

## B. MEASUREMENT AND DATA ACQUISITION

### B1. SAMPLING PROCESS DESIGN
This project includes no sampling. This section is not applicable.

### B2. SAMPLING METHODS
This project includes no sampling. This section is not applicable.

### B3. SAMPLE HANDLING AND CUSTODY
This project includes no sampling. This section is not applicable.

### B4. ANALYTICAL METHODS
This project includes no analysis of samples. This section is not applicable.

### B5. QUALITY CONTROL
This project includes no direct measurement or data acquisition. This section is not applicable.

### B6. INSTRUMENT/EQUIPMENT TESTING, INSPECTION, AND MAINTENANCE
This project will use no measurement or test equipment. This section is not applicable.

### B7. INSTRUMENT/EQUIPMENT CALIBRATION
This project includes no measurement or test equipment. This section is not applicable.

### B8. INSPECTION/ACCEPTANCE OF SUPPLIES AND CONSUMABLES
This project will use no supplies or consumables. This section is not applicable.

### B9. NON-DIRECT MEASUREMENTS (DATA ACQUISITION REQUIREMENTS)

EPA is acquiring data, including new measurements, in another project (USEPA 2011b). Input data for the models will be acquired from the EPA and from scientific literature. This project will not use any measuring or test equipment.

### B10. DATA MANAGEMENT AND HARDWARE/SOFTWARE CONFIGURATION

The following data (including computer codes and input and output files) will be managed by this project:

DATA

Environmental and process data will be acquired from the EPA or from the scientific literature. The quality of data from the EPA will have been evaluated as part of another EPA project(USEPA 2011b). Data from both these sources will be accepted as accurate for use on this project. Accurate transcription of these data into input files will be verified by line-by-line hand checking (direct comparison of input files with the source data).

SOFTWARE

Code verification

Code verification is discussed in Section A7.

Version control

Each modification of the software need not be archived, but each version that will be documented in the project reports and considered for release will be assigned a unique version number and archived.

## C. ASSESSMENT AND OVERSIGHT

## C1. ASSESSMENTS AND RESPONSE ACTIONS

### Plans for science and product peer review

The final project report to EPA, and LBNL reports(s) will be peer reviewed as a matter of LBNL policy (LBNL 2008). Manuscript(s) will be submitted to peer-reviewed journals and presented at technical conferences.

### Audit

A Technical Systems Audit will be conducted on site by the EPA Quality Assurance Manager, early enough in the project (expected early in 2012) to allow for identification and correction of any issues that may affect data quality. Detailed checklists, based on the procedures and requirements specified in this QAPP will be prepared and used during the audit.

## C2. REPORTS TO MANAGEMENT

Monthly progress reports and a final report will be submitted to EPA. Interim reports will be submitted to EPA as part of the March 2012 milestone, or upon request from the EPA Technical Lead for use as input to EPA's reports to Congress.

# D. DATA VALIDATION AND USABILITY

Environmental and process data will be acquired from the EPA or from the scientific literature. The quality of data from the EPA will have been evaluated as part of another EPA project (EPA 2011b). Data from both these sources will be evaluated for use on this project.

Attributes to be considered for acceptance will include whether the data were collected (i) using standard methods, (ii) according to approved procedures, and (iii) under a QA program. It is to be expected that available data may not be sufficient to meet the input requirements of the models; in such cases reasonable values will be assumed and justified.

## D.2 Validation methods

Model components such as theory and mathematical and numerical procedures will be validated by technical review. To a great extent, the theory and mathematical and numerical procedures used in these codes have already been validated by technical review, peer review, and acceptance by the scientific community.

Outputs of simulations are not guarantees but are reasonable expectations, based upon the quality of input data, and uncertainty estimated from sensitivity of outputs to uncertainty of inputs. Limitations on the use of outputs of simulations will be discussed in the reports.

## D.3 Reconciliation with User Requirements

The project interim and final reports will describe and justify any deviations from this plan, and will include discussion of results, and will discuss limitations of the use of output data for users of the report.

**REFERENCES**

Bechtel-SAIC Corporation, 2004. *Radionuclide Transport Models Under Ambient Conditions*, MDL-NBS-HS-000008, REV 02, available on line at www,osti.gov/bridge/servlets/purl/841251-9mVrM7/841251.pdf

Freeman C.M., Moridis, G.J.; Ilk, D.; Blasingame, T.A 2009. SPE 124961. A Numerical Study of Performance for Tight Gas and Shale Gas Reservoir Systems. Presented at the 2009 SPE Annual Technical Conference and Exhibition held in New Orleans, Louisiana, USA, October 4-7, 2009

Freeman C.M., Moridis, G.J.; Ilk, D.; Blasingame, T.A 2010 SPE 131583. A Numerical Study of Transport and Storage Effects for Tight Gas and Shale Gas Reservoir Systems. Presented at the 2010 SPE International Oil & Gas Conference and Exhibition held in Beijing, China, June 8-10, 2010.

Freeman, C.M.; Moridis, G.J.; Blasingame, T.A 2011. A Numerical Study of Microscale Flow Behavior in Tight Gas and Shale Gas Reservoir Systems. Transport in Porous Media 90: 253-268 (doi: 10.1007/s11242-011-9761-6).

Itasca, 2009. FLAC$^{3D}$, Fast Lagrangian Analysis of Continua in 3 Dimensions, Version 4.0. Minneapolis, Minnesota, Itasca Consulting Group, 438pp.

Ji, L., Settari, A., and Sullivan, R.B. 2009. A Novel Hydraulic Fracturing Model Fully Coupled With Geomechanics and Reservoir Simulation. SPE Journal 14 (3): 423-430.

LBNL 2008. Operating and Quality Management Plan Pub-3111, Rev. 10.

Freeman, C.M. 2010. SPE 139250. Analysis of Mechanisms of Flow in Fractured Tight-Gas and Shale-Gas Reservoirs.

Moridis, G.J.; Wu, Y.S.; Pruess, K. 1998. EOS9nT: A TOUGH Module for the Simulation of Flow and Solute/Colloid Transport. LBNL report LBNL-41639.

Moridis, G.J.; Kowalsky, M.B.; Pruess, K. 2008. TOUGH+Hydrate v1.0 User's Manual: A Code for the Simulation of System Behavior in Hydrate-Bearing Geologic Media. LBNL Report LBNL-149E.

Moridis, G.J., Q. Hu, Y.-S. Wu, and G.S. Bodvarsson, Preliminary 3D Site-Scale Studies of Radioactive Colloid Transport in the Unsaturated Zone at Selected Yucca Mountain Locations, Journal of Contaminant Hydrology, 60, 25-286, 2003 (LBNL-45876).

Moridis, G.J., and Y. Seol, Three-Dimensional Radionuclide Transport Through the Unsaturated Zone of the Yucca Mountain Site: 1. Nonsorbing $TcO_4^-$ Solutes, LBNL-60639 (2006a) - In review, Transport in Porous Media.

Moridis, G.J., and Y. Seol, Three-Dimensional Radionuclide Transport Through the Unsaturated Zone of the Yucca Mountain Site: 3. Colloids, LBNL-60641 (2006b) - In review, Transport in Porous Media.

Rutqvist J., Moridis G.J., Grover T., and Collett T. (2009) Geomechanical response of permafrost-associated hydrate deposits to depressurization-induced gas production. Journal of Petroleum Science and Engineering 67 (2009) 1-12.

Rutqvist, J.; Moridis, G.J. 2009. Numerical Studies on the Geomechanical Stability of Hydrate-Bearing Sediments, SPE Journal, June 2009, 267-282.

Rutqvist, J. 2011 . Status of The TOUGH-FLAC Simulator And Recent Applications Related to Coupled Fluid Flow and Crustal Deformations . Computers & Geosciences 37, (6) 739-750. (LBNL Report LBNL-4210E).

Seol, Y., and Moridis, G.J., Three-Dimensional Radionuclide Transport Through the Unsaturated Zone of the Yucca Mountain Site: 2. Sorbing Solutes, LBNL-60640 (2006) - In review, Transport in Porous Media.

USEPA, 2011a *Draft Plan to Study the Potential Impacts of Hydraulic Fracturing on Drinking Water Resources,* Office of Research and Development, U.S. Environmental Protection Agency, EPA/600/D-11/001, February 7, 2011. Available online at: http://water.epa.gov/type/groundwater/uic/class2/hydraulicfracturing/index.cfm

USEPA 2011b Data Collection/Mining for Hydraulic Fracturing Case studies. Work assignment WA-HF-2-10, Technical directive 7HF101HF, QA Id no. G-15952, Contract # EP-C-08-034.

USEPA 2006 Guidance on Systematic Planning Using the Data Quality Objectives Process EPA QA/G-4.

Zhang, Keni; Yu-Shu Wu; Karsten Pruess 2008 User's Guide for TOUGH2-MP - A Massively Parallel Version of the TOUGH2 Cod. LBNL Report LBNL-315E

**APPENDIX A. Description of Software Codes TOUGH+ and FLAC3D, adapted from Moridis (2011) and Rutqvist (2011).**

TOUGH

The acronym "TOUGH" stands for "**T**ransport Of **U**nsaturated **G**roundwater and **H**eat" and reflects the original geothermal focus of the code, which has over the years expanded into a family of multi-dimensional, multi-component models that are designed for the simulation of the coupled transport of fluids and heat in porous and/or fractured geologic media.

Since its first release in 1987 by a team of researchers at the Lawrence Berkeley National Laboratory headed by Karsten Pruess, the TOUGH family has been enriched by a large number of modules that describe a variety of important Equations-Of-State (EOS, involving various mass components) and has evolved to include several derivatives and descendants (e.g., EOS modules for multi-component volatile organic compounds; decay chains of multiple radionuclides, gas hydrates, and supercritical CO2; modules for coupled multi-phase flow and reactive transport, and coupled thermo-hydrologic-mechanical processes; inverse modeling for parameter estimation, sensitivity analysis, and uncertainty quantification; parallelization for multi-core PCs, workstation clusters, supercomputers, etc.). The TOUGH family of codes is currently used to address a wide spectrum of problems, which includes applications to geothermal reservoir engineering, nuclear waste disposal in geologic formations, geologic carbon sequestration, gas hydrate research, vadose zone hydrology, environmental remediation, oil and gas reservoir engineering, and other coupled mass transport and energy transfer problems in complex subsurface geologic settings. The international TOUGH user community currently numbers almost 400 organizations (research laboratories, government agencies, private companies, universities, etc.) in over 40 countries.

Approximately 200 researchers and engineers from a dozen countries attended the 2009 TOUGH Symposium. The 108 papers presented by international researchers and research groups at the Symposium covered a wide range of topics, including:

- Coupled process modeling (thermal, hydrological, chemical, mechanical, biological) in porous and fractured geologic media
- Hydrocarbon recovery
- Geologic CO2 storage/sequestration
- Methane hydrate dissociation and gas recovery
- Performance assessment of nuclear waste repositories
- Geothermal reservoir studies
- Vadose zone hydrology
- Fate and transport of volatile organic compounds
- Reactive transport modeling for environmental remediation
- Design and analysis of laboratory and field experiments

• Automatic model calibration and uncertainty analysis
• Code verification and validation
• Enhanced process capabilities and user features
• Numerical methods, grid generation, and parallel computing

**TOUGH+-FLAC STRUCTURE**

The following description of the TOUGH-FLAC structure incorporates the most recent code developments, specifically linking $FLAC^{3D}$ to the newly released TOUGH+ code (Rutqvist and Moridis, 2008, 2009). In this approach, the two constituent codes—TOUGH+ and $FLAC^{3D}$—are linked through a coupled thermal-hydrological-mechanical (THM) model (Figure 1). Depending on the specific problem at hand and the specific porous medium (e.g., fractured rock, unsaturated clay, or hydrate-bearing sediments), a number of coupling functions have been developed.

In Figure 1, the data exchanges between TOUGH+ and $FLAC^{3D}$ are illustrated with arrows going through the central THM model. The arrow on the right-hand side of Figure 1 shows the transmission of the effective stress $\sigma'$ and strain $\varepsilon$ (computed in $FLAC^{3D}$) to TOUGH for calculation of the updated porosity $\varphi$ and the corresponding porosity change $\Delta\varphi$. This mechanically induced $\Delta\varphi$ has an immediate effect on fluid flow behavior. For example, if a change in $\sigma'$ and $\varepsilon$ causes $\varphi$ to decrease, the pore pressure is expected to rise, especially if the permeability is low.

For a porous deformable medium, two models for mechanically induced porosity changes are implemented in the most recent version linking $FLAC^{3D}$ to TOUGH+ :
(i) A poroelastic model (based on the approach proposed by Settari and Mourits, 1998) that considers macroscopic stress/strain changes and grain deformability
(ii) An empirical model (proposed by Rutqvist and Tsang, 2002) that describes a nonlinear change in porosity as a function of the effective mean stress

The $\Delta\varphi$ computed from either of these models is used to estimate changes in $k$ by means of empirical equations. The updated $\varphi$ and k values are in turn used to estimate changes in the hydraulic and wettability properties of the porous medium (i.e., aqueous- and gas-phase relative permeabilities *krA* and *krG*, and capillary pressure *Pc*) by employing appropriate scaling equations. Currently, the capillary pressure is scaled with permeability and porosity according to a function by Leverett (1941).

For fractured media, a similar exponential empirical model has been applied to correct permeability for changes in the three-dimensional stress field (e.g., Rutqvist et al., 2002, 2008a). The fractured-media model accounts for anisotropic changes in permeability assuming three orthogonal sets of fractures such as at Yucca Mountain, Nevada (Rutqvist et al. 2008a, Rutqvist and Tsang, 2003b).

The arrow on the left side of Figure 1 depicts the flow of data obtained from TOUGH+ (or TOUGH2) (namely pressure *P*, temperature *T*, and phase saturations $S\beta$) to FLAC3D for processing and estimates their impact on the effective stress $\alpha\Delta P\beta$ ($\alpha$ being Biot's effective stress parameter), as well as on thermal and swelling strains ($\varepsilon T$ and $\varepsilon sw$, respectively). Capabilities for modeling of moisture swelling and geomechanical behavior of unsaturated soil have recently been implemented into TOUGH-FLAC (see Rutqvist et al., 2010a). In this model, the swelling can either be introduced as a function of phase saturation or as a function of suction (or capillary pressure, *Pc*), using the Barcelona Basic Model for elastoplastic behavior of unsaturated soils (Rutqvist et al., 2010a).

Additionally, changes in *P*, *T*, and $S\beta$ may also result in changes in other mechanical properties listed in Figure 1. These include bulk modulus *K*, shear modulus *G*, cohesion *C*, and coefficient of internal friction $\mu$. For example, in the case of hydrate-bearing sediment, geomechanical properties change as a function of solid-phase saturations, i.e., hydrate and ice saturations (Rutqvist and Moridis, 2009). In the case of unsaturated soil, the bulk modulus and friction angle are functions of suction (Rutqvist et al., 2010a).

In the current TOUGH-FLAC modeling approach, FLAC3D is invoked from TOUGH+ (or TOUGH2) using a system call. This is different from the earliest version, in which TOUGH2 multiphase flow simulation was invoked from FLAC3D. Invoking the quasistatic mechanical calculation from the multiphase flow simulation enables tighter and more rigorous coupling and improved efficiency. For example, it is now possible to invoke $FLAC^{3D}$ in each Newton iteration and when calculating the Jacobian in TOUGH+. Coupling to the $FLAC^{3D}$ code is still made possible through the use of the $FLAC^{3D}$ FISH programming capability, which enables access to internal $FLAC^{3D}$ arrays and parameters. However, the Itasca Consulting Group (which develops and maintains FLAC3D) has provided new FISH variables for a more efficient transfer of TOUGH parameter directly to the $FLAC^{3D}$ grid-elements, avoiding the previous, tedious interpolation between TOUGH mid-element nodes and $FLAC^{3D}$ corner nodes.

In the new TOUGH+ version, three coupling schemes are available:
(i) Jacobian: This is the highest level of iterative coupling, in which all the geomechanical and flow parameters are continuously updated (in every Newtonian iteration of every time step), and their changes are accounted for in the computation of the Jacobian matrix.
(ii) Iterative: In this scheme, the geomechanical and flow parameters are corrected at the end of each Newtonian iteration of each time step, and the contribution of their changes between Newtonian iterations is not accounted for in the computation of the Jacobian matrix.
(iii) Time-step: This represents the weakest coupling option and involves correction of the geomechanical and flow parameters once in (i.e., at the end of) each time step. As in the iterative scheme, the parameter changes do not contribute to the computation of the Jacobian matrix.

The full Jacobian option is a sequentially implicit scheme, whereas the iterative and the time-step coupling options are sequentially explicit schemes. The full Jacobian scheme is necessary for problems in which pore-volume (direct) couplings dominate, i.e., when a mechanically induced $\Delta\varphi$ gives rise to a relatively strong and rapid change in pore pressure, and where it is necessary to rigorously preserve the fluid mass and heat balances. In problems when the so-called property changes (indirect) couplings dominate, iterative or time-step coupling schemes are sufficient. It is well known that there could be serous stability issues in problems where pore-volume coupling dominates, such as when a low permeability porous medium is mechanically squeezed by an external force. However, as it turns out, the coupling of a TOUGH and $FLAC^{3D}$ is equivalent to the coupling of a finite volume reservoir simulator to a finite element geomechanical simulator, which, according to recent work by Kim (2010), corresponds to a mixed formulation that is stable in space. Moreover, by choosing an appropriate coupling scheme with so-called stress fixed iterations in the sequential scheme, the solution becomes unconditionally stable (Kim, 2010). Work is under way to study numerical stability issues in TOUGH-FLAC when pore-volume coupling dominates. However, in the overwhelming number of multiphase flow applications encountered, the pore-volume coupling does not dominate, whereas one-way coupled, or problems in which property changes dominate, are the most common.

## RUNNING A TOUGH-FLAC SIMULATION

To run a TOUGH-FLAC simulation, the user needs a license for TOUGH+ (or TOUGH2) and $FLAC^{3D}$, as well as access to routines for linking the two simulators. A TOUGH-FLAC simulation is typically developed according to the steps in Figure 2. The user first develops numerical grids for the two codes that should have the same geometry and element numbering. The user then typically runs a TOUGH simulation test to make sure that the TOUGH code can execute the specific problem setup without consideration of the mechanical coupling. This may include an initially steady-state TOUGH simulation to establish initial conditions, including vertical gradients of pressure and temperature. Typical input parameters for the TOUGH simulation include grain density, porosity, permeability, thermal conductivity, specific heat, relative permeability and water retention curves, as well as hydraulic and thermal boundary conditions (e.g., fixed fluid pressure and temperature). Similarly, a $FLAC^{3D}$ simulation may be conducted to assure correct input of (for example) mechanical boundary conditions and to establish initial equilibrium stress gradients. Typical input parameters for the $FLAC^{3D}$ simulation include bulk density, elastic parameters (bulk- and shear-modulus), strength parameters (e.g., cohesion and friction angle), as well as mechanical boundary conditions (e.g., fixed displacement or stress).

After initial runs with TOUGH and $FLAC^{3D}$, the linked TOUGH-FLAC simulation is set up. This involves preparing a binary file called FLAC3D.sav that should contain the geomechanical model, as well as essential FLAC3D FISH routines that handle the links between $FLAC^{3D}$ and TOUGH+ (or TOUGH2). The simulation is initiated by starting a TOUGH+ (or TOUGH2) simulation with the geomechanical option activated. The first time FLAC3D is invoked, it restores information and the initial mechanical state from the FLAC3D.SAV binary file. FLAC3D then reads initial pressure and temperature as defined in TOUGH+ (or TOUGH2), runs to mechanical equilibrium, and then saves the new mechanical state to the FLAC3D.SAV binary file. This procedure of restoring, running to a new mechanical equilibrium, and saving to the binary file is repeated every time the FLAC$^{3D}$ mechanical calculation is invoked. The TOUGH-FLAC simulation runs seamlessly without need for user interference and produces required outputs for simulation times defined in the TOUGH input file.

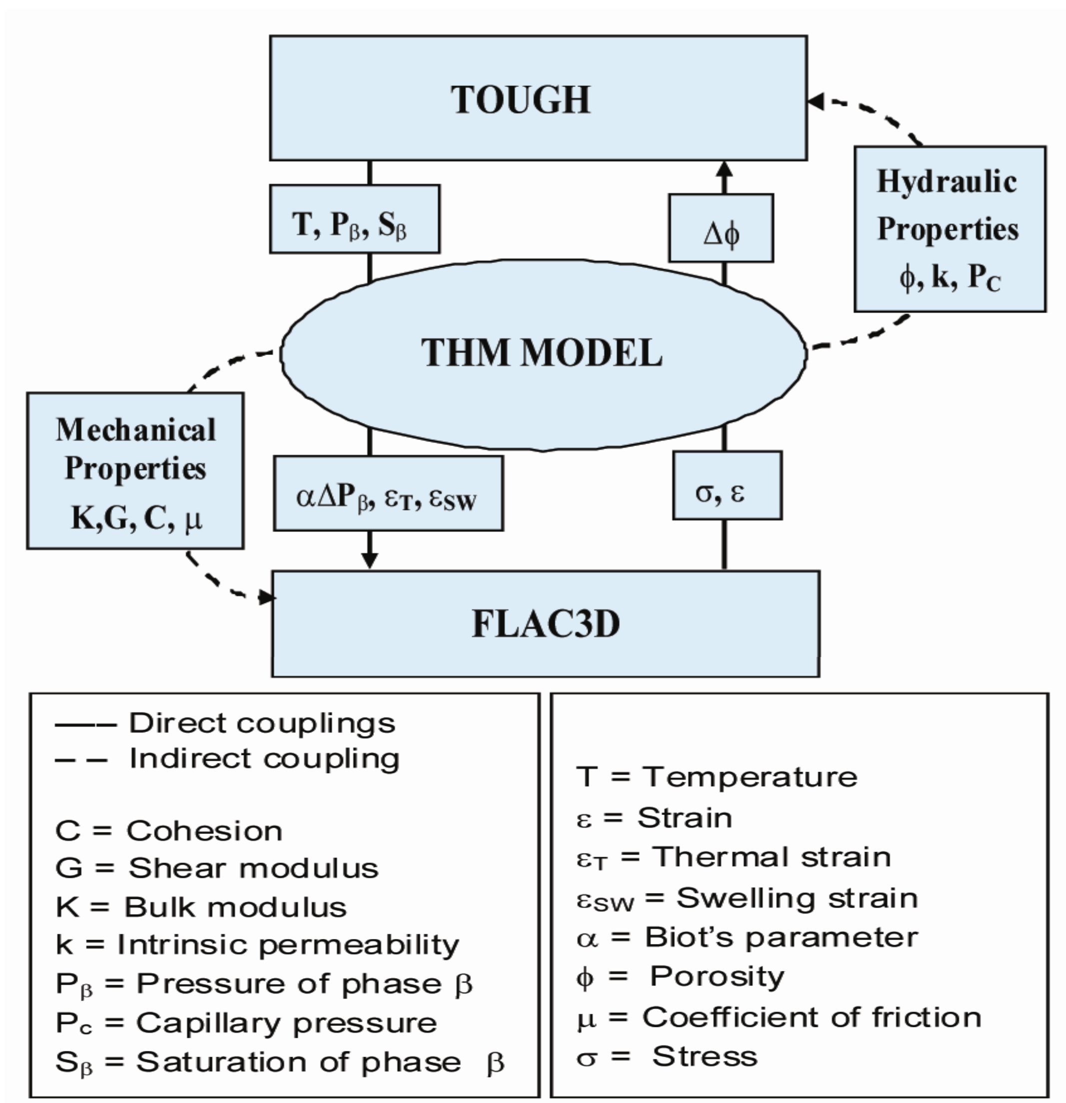



Figure 1. Schematic of linking TOUGH+ with FLAC3D for a coupled THM simulation.

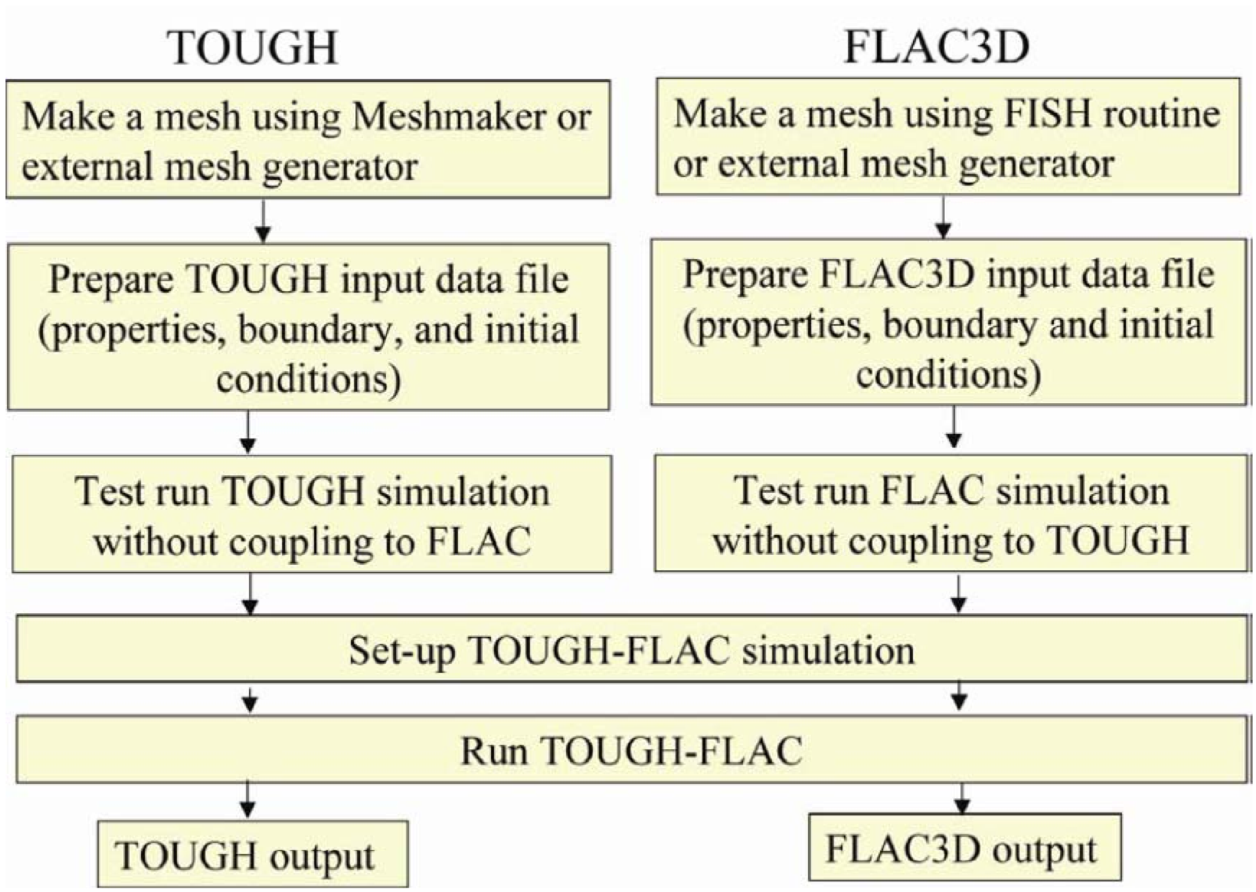



Figure 2. Steps for developing a coupled TOUGH-FLAC simulation of a particular problem.

**References cited in Appendix A.**

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

Leverett, M.C., 1941. Capillary behavior in porous media. Trans, AIME, 142, 341–358.

Rutqvist, J., Freifeld, B., Min, K.-B., Elsworth, D., Tsang, Y., 2008a. Analysis of thermally induced changes in fractured rock permeability during eight years of heating and cooling at the Yucca Mountain Drift Scale Test. International Journal of Rock Mechanics and Mining Sciences 45, 1373–1389.

Rutqvist, J., Ijiri, Y., Yamamoto, H., 2010a. Implementing the Barcelona Basic Model into TOUGH-FLAC for analysis of geomechanical behavior of unsaturated soils. (Submitted).

Rutqvist, J., Moridis, G.J., 2009. Numerical Studies on the Geomechanical Stability of Hydrate-Bearing Sediments. Society of Petroleum Engineers (SPE) Journal 14, 267–282, SPE-126129.

Rutqvist, J., Moridis, G., 2008. Development of a Numerical Simulator for Analyzing the Geomechanical Performance of Hydrate-Bearing Sediments. In: Proceedings of the 42nd U.S. Rock Mechanics Symposium, San Francisco, California, USA, June 29-July 2, 2008, American Rock Mechanics Association, ARMA, Paper No. 139.

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

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

Rutqvist, J., Wu, Y.-S., Tsang, C.-F., Bodvarsson, G., 2002. A modeling approach for analysis of coupled multiphase fluid flow, heat transfer, and deformation in fractured porous rock. International Journal of Rock Mechanics and Mining Sciences 39, 429-442.

Settari, A., Mourits, F.M., 1998. A Coupled reservoir and Geomechanical Simulation System. Society of Petroleum Engineers (SPE) Journal 27(9), 219-226, SPE paper 50939.