SubTER Grand Challenge Roundtable: Imaging Geophysical and Geochemical Signals in the Subsurface

The Grand Challenge SubTER Panel (Dr. Marcia McNutt, Chair)
DOE Leads: Margaret Coleman, Julio Friedmann, Doug Hollett, and Harriet Kung

Introduction

The future of the world's energy production and deployment is closely tied to our understanding of the subsurface, as well as our capabilities in subsurface or geologic engineering. Developments over the past ten years, including the growth of natural gas and petroleum extraction from shale or mudstones, the disposal of produced fluids from oil and natural gas wells, the desire to expand geothermal energy generation, the growing need and expectation for subsurface storage of CO_2, and the potential geological disposal of spent nuclear fuel have heightened the need for dramatic improvements in subsurface science, technology, and engineering. While commercially related improvements are continually being made primarily by industry, there remain large gaps between current and desired capabilities to understand, predict, and control subsurface processes underpinning technologies that dominate the U.S. energy supply.

To address these concerns, Secretary Moniz asked multiple offices within the Department of Energy to establish a crosscutting technology team to accelerate improvements in subsurface engineering. Named SubTER (Subsurface Technology and Engineering RD&D Crosscutting Team), the multi-disciplinary team from headquarters and the National Labs in 2014 identified a core objective of "adaptive control of subsurface fractures and fluid flow."

As part of this effort, and at the direction of the Secretary of Energy, the Offices of Fossil Energy, Energy Efficiency and Renewable Energy, and Science convened a one-day Roundtable on July 21, 2015. The offices asked leading experts and accomplished researchers in geophysics and geochemistry from universities, government, industry and national labs to provide their individual opinions based on their experiences that the Department would use to frame a new but related Grand Challenge: *imaging geophysical and geochemical signals in the subsurface.* This specific Grand Challenge was first identified by the Office of Science-Basic Energy Sciences at a Roundtable meeting on May 22, 2015 as part of the continued SubTER strategic planning.

At the July meeting, the Department asked the individual attendees for their opinions concerning the challenge of fracture networks with associated fluid flow and reaction, recognizing that this would require dramatic improvement in fidelity, resolution, and conceptual understanding. Progress around the Grand Challenge would likely require a 5-10 year sustained and coordinated multi-disciplinary effort among the members of the SubTER team.

Key Conclusion

History has shown that well-coordinated multidisciplinary initiatives can advance complex areas of basic geoscience in conjunction with advancing applied science and technology. The SubTER team realized that the key insight lay in broadening traditional efforts well beyond conventional disciplines of geophysics and geochemistry. In short***, progress on the grand challenge would likely require a set of multidisciplinary teams focused on discrete problems with some novel approaches and R&D platforms.***

An analogy the SubTER team proposed to the Grand Challenge space was the major advances in **earthquake science** over the past several decades. Traditionally the domain of earthquake seismologists, accelerated progress since the 1990's occurred by transforming the field into a more coordinated system level science incorporating multiple disciplines, including mineral physics, laboratory experimentation, advanced mathematics and high performance computing, paleoseismology, remote sensing and geodesy, and field geology. New facilities, shared by the community in question, were required, such as the San Andreas Fault Observatory at Depth, seismic and geodetic networks, and open data centers. Community governed Centers of Excellence such as the Southern California Earthquake Center were used to organize the community and synthesize the results of the research. The result was transformative; dramatic scientific and technical advancement in understanding the physics and risks of earthquakes.

Key research focal areas

The roundtable participants provided their individual thoughts on a number of key subtopics under the Grand Challenge that are considered essential to making fundamental progress on imaging the subsurface. These subtopics consist of five questions/issues in subsurface imaging and potential approaches to address these issues, as summarized in Table 1. It must be underscored that links and connections between these five subtopics are real and complex, and that concurrent progress on all these questions is essential to achieving Grand Challenge Goals. The potential approaches identified below represent the SubTER team's findings based on the individual feedback from the roundtable participants and are intended to set the initial framework for tackling the Grand Challenge for SubTER.

Imaging subsurface fractures and flow

Uncertainty remains about the detection of preexisting heterogeneity in fractures and fracture systems and about the changes that occur in a system after rock fracturing takes place. Current direct seismic imaging with a resolution of meters does not adequately resolve individual cracks and fractures that often control flow in the subsurface. Moreover, oil companies have substantial experience in imaging at depths of 1km or deeper, but they have limited abilities to image shallower fracture networks. The water table and the presence of groundwater in the first 500m often cause imaging to be more challenging.

*Potential Approaches***:**

- Directed field observation: Dedicated horizontal wells could obtain data about fracture networks through direct measurement, geophysical observation and interpretation, and geochemical tracers. Comparison of the fracture networks before and after hydraulic stimulation at a site could prove particularly useful, possibly using new approaches such as time-lapse mapping and direct acoustic signal creation using microencapsulated energetic materials. Nanotechnology presents another possibility – certain nanomaterials, nano-contrast agents, and microfabricated sensors can measure and record temperature, pressure, chemical environment, and other key properties at depth, and carbon nanotubes can align with electromagnetic fields to record changes in fracture networks (note: these approaches may prove very expensive, and energy companies have to date been reluctant to independently fund large-scale studies when brute-force approaches remain commercially attractive).
- Laboratory experimental set: cores, block samples, and possibly even architected geomaterials would undergo batteries of experiments that probed the effects of rock type, strain rate, prior deformation history, and confining pressure on fracture geometry and surface area. These would provide physical results to help understand the field observations and validate simulations.
- Novel Simulators: Traditional Darcy Flow models, such as conventional reservoir flow simulators, do not adequately represent the physics of fracture or flow in fracture networks well. Building "beyond Darcy" models was identified as a potentially very valuable step to appropriately representing the key physics and hydrology of such system. Such computational models would necessarily underlie more complex future models, such as coupled wave-propagation models.

The SubTER team agreed that field observatories of some sort were likely very important to this effort, and that substantial industrial participation was essential to ensure access to relevant field sites. The need to engage the current subsurface industry was a through-going theme of the rountable, for technical reasons, in the interest of economic access to the subsurface, and perhaps most importantly because the subsurface industry is the only way to deploy things at the scale required to have an actual impact, making the transition from theory to practice--so often missing in government-funded energy research and policy--a greater possibility.

Resolving and Interpreting Changes in Fluid Composition

Changes in fluid element and isotopic composition occur before and after injection. This problem requires research on multiple scales (atomic through reservoir). This is especially relevant for fluids used in hydraulic fracturing, but also relevant to questions of groundwater contamination, CO_2 and nuclear waste storage, and the performance of enhanced geothermal sites. Traditional sampling and laboratory work does not provide sufficient insight to help constrain a framework capable of predicting key hazards or long-term well and site performance.

Potential Approaches:

- Directed field observation: Some facilities and locations have extraordinary access to subsurface data. For example, Lawrence Livermore drilled 1000 wells on their campus, which could provide a very dense geochemical and hydrological data set for interrogation. Involving the EPA could provide access to thousands of more modern wells. Some universities have extensive land holdings, like the University of Texas System with some 2,000,000 acres in west Texas, which could potentially be involved in facilitating field observations and experiments. In addition, the government could partner with or compensate/incentivize oil and gas companies to study their dense networks of abandoned and producing wells.

Table1. Grand Challenge Summary

Unknowns	Solutions
Imaging subsurface fractures and flow (natural and induced)	A) Field observatory approach with horizontal wells with data collection pre-and post-hydraulic fracturing B) Use of contrast agents in stimulation fluids that enhance sonic or electromagnetic signals C) Remote sensing with seismic waves, electromagnetic fields, NMR, LIBS, LIDAR, etc. D) Laboratory analysis of core samples (before and after stimulation) E) Develop lab conditions that simulate subsurface conditions F) Use of nanoparticles that undergo phase changes as they transit the system G) Develop modeling approaches that cross scales and make predictions (recurring theme that runs through all solutions to unknowns)
Resolving and interpreting changes in fluid composition (understanding chemical changes before and during flow)	A) Field observatory approach that includes monitoring changes in porosity and permeability with different fluid injections B) Laboratory approach including experimental, modeling and analysis of fluids before, during and after development C) Use of nanoparticles that undergo chemical changes as they transit the system
Characterization of Reservoirs (composition, permeability, fluids, phases, etc.)	A) Further development of architected geo-materials (advanced sensors and contrast materials) B) Design and use of natural experiments from deep brines

Physical and Chemical Changes in Rock-Fluid Systems	A) Further development of architected geo-materials (advanced sensors and contrast materials) B) Design and use of natural experiments from deep brines C) Application of novel laboratory approaches to understand mineral-fluid interactions D) Geomicrobiology focused efforts E) Reactive Control of Subsurface Fluid Compositions and Pore Structures
Subsurface Stress Distribution and Dependent Seismicity	A) Remote sensing, in situ seismology, borehole geophysics B) 4D GPS navigation as order of magnitude increase in data density C) Lab experiments on constitutive relations D) Natural and potentially induced seismicity history E) Subsurface stress characterization F) Access to injection data G) Deployment of additional seismometers

- Comparison of changes in fluid compositions from field and laboratory measurements, and geochemical transport modeling: Reactive transport comprises a class of predictive models that can yield critical information on changes in fluid composition produced by the interaction of fracture fluids with the minerals and organic matter in subsurface formations. Such changes indirectly record the results of dissolution and precipitation reactions occurring at fluid-mineral and fluid-organic matter interfaces, which can substantially affect water quality, porosity and permeability. Comparison of measured compositions of produced waters from field observatories and laboratory studies with the predictions of reactive transport modeling was identified as an important means of monitoring the chemical changes resulting from hydraulic fracturing that are likely to impact the efficiency of oil and gas recovery from fractured shales. These types of models will also provide a basis for developing more complex models that predict the coupling of chemical and mechanical processes that are generally relevant to subsurface science such as fracturing, sequestration of energy by-products, geothermal systems, etc.. Currently, many geochemists produce datasets without reactive transport models to demonstrate how measurements in the lab or at one site can help to describe broader trends and changes in fluid composition in reservoirs. This area does not require much technology advancement (notable exceptions being in algorithm and theory development), but would benefit from targeted research directives to build a body of accomplishment and practice.
- Novel materials for subsurface interrogation: Many in the R&D community, including within industry, have considered or proposed “smart tracers”, “smart proppants”, and

similar reactive injectates that can provide time-lapse information on the geochemical and physical state of rocks and their associated fluids, or potentially, to affect water quality or manipulate fluid flow. The effort would leverage existing university and private sector efforts to design and develop a suite of these high-end scientific tools and consider the best opportunities to test, develop, and learn from their deployment.

Characterization of Reservoirs

The task of describing mineralogical/organic matter compositions, permeability, porosity, and saturating fluids within a subsurface reservoir remains a first-order technical challenge. Scaling remains a core challenge because eliminating the gap that exists between borehole data imaging (cm scale resolution) and regional-scale seismic imaging (m and km scale) requires bridging concepts and practices. This is particularly challenging as a "no-man's land" exists between these scales with very limited data and techniques. Inter-well measurements also present a challenge as it is difficult to detect reservoir heterogeneity in sites where drilling has not taken place. Understanding rock and reservoir heterogeneity is crucial to predicting the propagation, orientation, and connectivity of fractures.

Potential Approaches:

- Integrated field observation: In most industrial and research field sites, a small set of tools are applied and re-applied for characterization, and are static, one-time efforts. Again, orthogonal approaches applied over time have shown locally that immense progress is possible. These include remote sensing, electromagnetic surveys, microgravimetry and gravi-gradiometry, and combined passive and active acoustic geophysics in areas that are well resolved.
- Novel inversion approaches: The area of computational geophysics has grown tremendously in recent years. Conventional, deterministic inversion approaches have difficulty with the non-linear, highly uncertain initializations from flow in fractured media. Novel inversion approaches including stochastic, Bayesian, Boolean, and other mathematical frameworks show promise and may be much better suited to the fracture flow problem.
- Benchmarking and upgrading scaling approaches: One novel approach involved applying community methods for climate-modeling to solid-earth models. Climate scientists have devoted substantial energy to benchmarking to ensure that their models reflect the relevant components of the climate system. This involves running thousands of models (different initializations and differing physics), comparing them to observational data, identifying missing components and key areas of mismatch, and adding these into model sets. Dramatic improvements in standard models such as GENIE or LOSCAR reflect this approach, which could be useful for subsurface imaging.

In the field, advanced sensors and contrast agents (see Approaches under Imaging subsurface fractures and flow) could be useful. This may require identifying a small number of dedicated sites in which researchers can focus on studying heterogeneity. This effort will also likely require substantial computing resources (many thousands to millions of CPU-hours per calculation). A key outcome of this effort will be the ability to apply subsurface characterization techniques across a broad suite of conditions, as compared to current practices, that have far less transferability.

Physical and Chemical Changes in Rock-Fluid Systems

How minerals/mineral chemistry and the voids and fractures between minerals (i.e., pore spaces) change in terms of physical properties and chemical reactions (as opposed to fluids) is poorly understood. Physical changes (porosity, permeability, stress) and concurrent geochemical processes (redox state, dissolution, and precipitation) are both relevant and inherently coupled, particularly in fracture hydrology. There is an evolving field called "structural diagenesis" that attempts to understand these dynamic relationships. Additional emerging areas of uncertainty include the biological aspects of fracture fluids (role of both deep and shallow system microbes in chemical and physical reservoir changes) and whether they have long-term consequences on performance.

*Potential Approaches***:**

- Targeted field observation: Injecting and then recovering fluid may help researchers to understand changes in fracturing or mineralogical composition within a reservoir, though this technique may be of limited use to identify the locations of the changes. As discussed in previous sections, micro- or nanoparticle sensors could also be useful.
- Architected geomaterial experiments: Advances in synthesis and 3-D printing make it possible to create synthetic analogues of rocks that contain well-controlled compositions and distributions of pore spaces. This means that experimentalists can remove variability in the initial mineral structure and distribution to better isolate important processes (we currently have rapidly evolving national lab expertise in this area). Anticipated advances in the characterization of complex geomaterials at next generation national scientific user facilities are well-matched to that needed to build a scientific foundation for understanding physico-chemical reactions in the subsurface.
- Porosity and permeability evolution: New laboratory techniques, sample environments and methods of analysis are needed to transcend the empirical descriptions of the coupling between geochemistry and geophysical properties such as porosity, permeability and tortuosity.
- Novel interrogation techniques: The general principle consists of designing a sensor that changes its state when it interacts with some chemical or physical property. For example, seismic studies can identify the presence of gas, so a nanoparticle that releases gas when a geochemical reaction occurs could be detectible through standard seismic

mapping. This could help to identify and track reactions. The Advanced Energy Consortium (AEC), a group of companies and universities that conducts micro- and nanotechnology research for oil and gas recovery, has been conducting research in four primary thrust areas: mobility, nanomaterial sensors, contrast agents, and microfabricated sensors ("a lab on a chip") for the past 7 years working with 25 international universities. A government role in the AEC at this time could be well timed and differentiating.

- Laboratory studies of rock-fluid systems at borehole conditions, in which core is tomographically imaged before, during, and after fluid injection inform field studies of the same systems.

Subsurface Stress Distribution and Dependent Seismicity

Predictions of potentially induced seismicity can enable scientists to maximize yields and minimize negative potential impacts from technologies like enhanced geothermal systems, injection of produced water from oil and gas operations, and carbon and spent nuclear fuel storage. A better understanding of the dependencies that lead to induced seismicity requires dramatic improvements in characterizing the distribution of subsurface stress. Specific challenges include 3D stress measurement away from boreholes and monitoring changes in stress during perturbation. Another topic that requires additional research involves the conditions and thresholds for failure via induced seismicity, which may require new theoretical frameworks.

*Potential Approaches***:**

- Targeted field observation: Field-based approaches to understand subsurface stress distribution include borehole geophysics, induced seismicity monitoring, and airborne and other remote-sensing measurements. Close partnerships with NASA could open up the possibility of using radar or other remote-sensing techniques to detect stress distributions using new or existing observational platforms.
- Laboratory geomechanics: Lab experiments can continue to enhance our understanding of stress and strain. Both measuring and manipulating stress, in both natural and architected materials, in high- and low- strain rate settings are likely to provide important new observations and theoretical insights.
- Setting reliable and accurate natural seismic baselines is vital to understanding potentially induced seismicity. Working with states and regions that have, or are about to, increase the coverage of permanent and portable seismometers could help accelerate understanding.

Other likely approaches

Both advanced computing and data manipulation techniques are crucial. In particular, techniques for big data analysis to process well, production, and microseismic data can also help to describe and predict patterns for induced seismicity. This effort will likely require access to proprietary data sets from industry, and may require specific efforts to gather, sanitize, federate, and share data for analysis.

Resource Considerations

Implementing these approaches will require a common set of additional resources, chiefly data and platforms. These include:

1. Increased access to sites and boreholes: these could be dedicated sites, active or pending industrial efforts, or sites under active regulation.
2. More advanced numerical and computational models: This will require access to high-performance computing (HPC) and other advanced computing resources, as well as some code development.
3. New types of laboratory experiments: This will require experimental design, some new facilities, and integration of existing facilities across DOE and with other agencies, industry and academia.
4. Targeted approaches – examples include airborne measurements and nanotechnology as well as other ground based and remote-sensing operations, including the use of natural tracers.
5. Large data set access and data-centric computing approaches – may involve combining existing datasets and promoting open access to public and private datasets.

The Roundtable participants estimate \$200-\$300 million of dedicated funds over a 5 to 10 year period to make substantial progress and achieve target goals. The level of funding is considered appropriate for a Grand Challenge initiative. It may also require new legal and contractual arrangements to execute the work, requiring partnerships and efforts between General Counsel at DOE, Labs, universities, companies, and possibly other agencies. This Grand Challenge initiative would involve students and early career scientists, thereby contributing to workforce development in geoscience and energy science.

Next Steps

The SubTER team identified a set of useful actions to pursue while a budget request is formulated, promulgated, and resolved. Such actions could be well undertaken in the context of SubTER's ongoing efforts.

Stakeholder outreach

At present, the initial ideas from the Roundtable participants require much more discussion within the research and industrial communities. The DOE could lead a series of meetings with key stakeholders around the country to add ideas and definition to the Grand Challenge undertaking, as well as to improve communication with researchers, practitioners, and the public.

Delineating and optimizing the collaborative approaches.

Effective use of these resources will require collaboration among government, industry, and academia. The Energy Frontier Research Centers (EFRCs) were highlighted as an effective research modality in promoting research partnerships, and they provide important lessons for future collaboration. The Advanced Energy Consortium (AEC) was also noted as a management structure successfully facilitating pre-competitive research across global universities with the potential to create a positive and disruptive change in the recovery of petroleum and gas from new and existing reservoirs. Both EFRCs and the AEC have demonstrated different levels of engagement with industry commensurate with the status of technology maturity.

While companies are much less likely to fund basic science when oil and natural gas prices drop (there are notable exceptions), joining industry-led research projects or “piggybacking” is a crucial strategy for efficient use of public resources. Individual companies and consortia are already researching many aspects of these five subtopics listed in Table 1. Therefore, DOE and other agencies can establish partnerships with the private sector to build upon industry research and use a single site/set of facilities for multiple studies. For example, if a company injects subsurface fluids into a reservoir, this presents an opportunity to add contrast agents to track chemical reactions and to accomplish multiple research objectives at once.

Furthermore, while interoffice and interagency collaboration can be beneficial, designating one office to own the project may lead to better control and streamlining of the project. Agencies like NSF, NASA and USGS can bring organizational ability and industry ties to the partnership, and all three organizations are very interested in open access to data. EPA involvement will also be useful, since this may help to address industry concerns that federal regulators will penalize companies for conducting field experiments with unknown effects upon the environment. New avenues of collaboration are possible through cooperative research projects organized by professional societies in the applied Earth sciences. An example is SEAM, a cooperative research model set up by the Society of Exploration Geophysicists to work with oil and service companies to build, and do simulations with, highly realistic Earth models.

Findings and Recommendations of the SubTER Team

The primary finding of the SubTER Team after receiving individual feedback from the roundtable participants is that ***now is a very good time to undertake a serious, concerted effort regarding this Grand Challenge topic***. Advances in materials science, manufacturing, scientific instrumentation, major DOE User Facilities, data processing, and computing power have reached a point where substantial progress is possible. This moment is matched by important growing needs to dramatically improve understanding and control of the subsurface, in particular regarding fracture generation, response, with associated fluid flow and reaction. Finally, global industrial efforts have created viable potential data sets, platforms, and partnerships that could serve to support a Grand Challenge initiative.

1. **We recommend the DOE add a Grand Challenge Effort to the ongoing SubTER cross-cutting effort**. This should be additive, and managed as a separate, coordinated, and complementary effort to the applied topics and tasks identified under SubTER.
2. **We recommend the DOE request the additional funds to support this undertaking**. We estimate the cost of an impactful Grand Challenge initiative to be on the order of $200-300M over a 10-year period.
3. **We recommend the DOE consider engaging existing assets in support of this effort**. This would potentially include increased access to HPC networks, major DOE User Facilities, other SubTER assets (such as FORGE), and General Counsel’s time and expertise in negotiating data access.
4. **We recommend additional outreach efforts to key stakeholders**. Such efforts are critically important to achieving the goals of the Grand Challenge in terms of additional resources, cost sharing, data access, and public and scientific acceptance.
5. **Early in the process set up a Center of Excellence** to organize the community and synthesize the results. The multiscale problem of the Grand Challenge involving multidisciplinary fields, will require a high level of coordination and integration for transformative progress to be achieved.

Appendix 1. Grand Challenge Participants

Gordon Brown, Stanford University

Florence Chen, Department of Energy

Margaret Coleman, Department of Energy

Don DePaolo, Lawrence Berkeley National Laboratory

Paul Fenter, Argonne National Laboratory

Julio Friedmann, Department of Energy

Carol Frost, National Science Foundation

Douglas Hollett, Department of Energy

Harriet Kung, Department of Energy

Marcia McNutt, American Association for the Advancement of Science

John Miller, Department of Energy

Michael Oristaglio, Yale University

Franklin Orr, Department of Energy

Tanja Pietrass, Department of Energy

Benjamin Phillips, NASA

Andrew Stack, Oak Ridge National Laboratory

Scott Tinker, Bureau of Economic Geology/University of Texas

Cecily Wolfe, U.S. Geological Survey

Appendix 2. Grand Challenge Roundtable Agenda

Agenda

Chair: Marcia McNutt (AAAS)
DOE Contact: Margaret Coleman (Office of Fossil Energy)

Morning Session

9:00 Opening Comments
Julio Friedmann, Harriet Kung, Doug Hollett
**Franklin Orr – Participating in a morning session*

9:15 – 10:15 What is possible in characterization and monitoring?
Focus: Resolution limits and fidelity for different geophysical and geochemical approaches.
SubTER Team Goal: Dramatic improvement in our ability to predict and manipulate subsurface flow and transport, particularly in faulted and fractured media
Michael Oristaglio (moderator)

10:15 Break

10:30 – 12:00 What is actionable? (such as disciplines, partners, and research platforms)
Focus: What actions could achieve progress on the grand challenge in 5-10 years. Discussion: Relevant disciplines, key partners and actors, key research platforms, etc.
Scott Tinker (moderator)

12:00 Lunch Open discussion

Afternoon Session

1:00 – 2:45 What is credible scope? (what can be done in what timeframe by whom?)
Focus: What are key programmatic elements and tasks to achieve progress on the grand challenge in 5-10 years.
SubTER Team Goal: Key planks and elements of a prospectus to propose to Sec. Moniz for budget consideration.
Don DePaolo (moderator)

2:45 Break

3:00 – 4:00 Prospectus for Secretary of Energy – recommendations in terms of budget, subjects/topics and scope that he can bring forward
Focus: What steps are necessary to bring the planks and elements into a prospectus.
SubTER Team Goal: Notional prospectus and setoff recommendations to propose to Sec. Moniz.
Marcia McNutt (moderator)

4:00 – 4:30 Conclusions and next steps