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Project title: Non-Darcian Flow, Imaging, and Coupled Constitutive Behavior of Heterogeneous Deforming Porous Media; Task 3: Testing paradigms of poro-elasto-plasticity

Summary:

This project employed a continuum approach to formulate an elastic constitutive model for Castlegate sandstone, based on the work of Zimmerman et al. (1986), Collins and Houlsby (1997), and Houlsby and Puzrin (2000). The resulting constitutive framework for high porosity sandstone is a) thermo-dynamically sound, (i.e., does not violate the 1st and 2nd law of thermodynamics), b) represents known material constitutive response, and c) able to be calibrated using available mechanical response data. To authenticate the accuracy of this model, a series of validation criteria were employed, using an existing mechanical response data set (Ingraham et al. 2013) for Castlegate sandstone. The resulting constitutive framework is applicable to high porosity sandstones in general, and is tractable for scientists and researchers endeavoring to solve problems of practical interest.

Motivation:

In developing constitutive models, researchers must balance the complexity of the mathematics required to represent all aspects of the material, with the ease of application. Although simplifying assumptions are necessary, some common assumptions, while convenient, often omit known mechanical behavior and/or lead to violation of fundamental laws of thermodynamics. Increasingly, computational modeling is used to better understand and predict rock behavior under loading conditions of interest to geologists, petrolemun engineers, etc. Use of a proper constitutive model is of the utmost importance, since the constitutive model is the mathematics that provides the relationship between stresses and deformations. An inaccurate constitutive model will provide incorrect deformation information under a given loading scenario.

The focus of this project was on development of an improved constitutitve model for the elastic response, which is essential because the elastic model: a) predicts the portion of the total strain that is recovered upon unloading, and b) is required to determine the irrecoverable plastic strain that remains upon unloading, knowing the total strain. Many experimental, theoretical and computational researchers have investigated methods for properly prediciting plastic strains; most use some form of classical plasticity in which plastic strains must be known at given stresses. These plastic strains are determined by backing the elastic strains out of the total strains; therefore, an inaccurate or superficial elastic model can result in significant error in the calculated plastic strain. A common experimental finding is that the plastic strain increment is not normal to the yield surface; however, the direction of the apparent actual plastic strain increment is greatly affected by the elastic constitutive model that is used to back the elastic strain out of the total strain. Thus, any successful effort to better model and predict plastic strain, and investigate apparent non-normality, requires use of an accurate elastic model.

Proposed Work and Revised Work Scope:

The original proposed work was to develop an integrated elasto-plastic constitutive framework, that is 1) thermodynamically sound, and 2) represents actual high porosity sandstone mechanical response (including stress and plastic strain dependence of elastic moduli). The common mathematical method for handling observed non-normality of the plastic strain increment (e.g., via a separate plastic potential), is known to violate the laws of thermodynamics under certain loading regimes, resulting in numerical instability during computer simulations. The proposed work starts from the laws of thermodynamics to develop the constitutive model (vs. commonly used phenomenological methods), thus insuring these laws are satisfied. An actual mechanical response data set, from Castlegate sandstone, was used to develop the general expressions for the constutive model (these general expressions are applicable to any high porosity sandstone), and to calibrate the model to the particular block of Castelgate sandstone.

This thermodynamic approach requires that the elastic constitutive model must first be developed. This enables plastic strain to be determined from experimental total strain, by backing out the elastic strain predicted by the elastic constitutive model. Once the plastic strain is know at various stress states, a plastic constitutive model can be developed. The most noteworthy change to the work scope is as follows: the scope of work was reduced to include development of only the thermodynamically sound elastic constituve model. In the original proposal, we assumed that development of the elastic model would be a relatively straight-forward and simple task, allowing significant time to be spent on the plasticity model. However, two unforeseen items caused development of the elastic framework to be much more time-consuming and challenging than we expected. First, determining the proper mathematics to incorportating both a) stress dependence and b) plastic strain depenedence into the elastic moduli expressions was much more complex that we expected. Originally we planned to simply combine existing elastic models for stress dependence with those for plastic strain dependence; however, that approach is not thermodynamically sound, since it does not account properly for elastic-plastic coupling. Secondly, numerous inconsistencies and problems were uncovered with the experimental strain meaurements, once we started curve-fitting data to obtain actual expressions for the elastic strain and elastic moduli. This required intense re-examination of the strain data to separate test-artifacts from rock response, which further required an assessment of what the expected elastic response should be. This was an interative process, since the data must guide the model development, but we also needed to use the model to guide the process of scrubbing the artifacts out of the data. Therefore, for these two reasons, at the time of this report, only the elastic constitutive model has been developed. We are currently preparing a journal paper to publish the elastic model. Once this is complete, the original task of creating the plastic part of the model can be pursued. The remainder of this report will focus mostly on the process of creating the elastic constitutive framework, with some references to how this fits in the larger elasto-plastic constitutive frameowork.

Approach:

Systematic analyses of mechanical data for Castlegate (Ingraham et al. 2013), showed that the bulk modulus, K, evolves with mean stress and plastic volume strain during the hydrostatic portion of the loading. During the subsequent deviatoric loading, the shear modulus, G, evolves with von Mises equivalent shear stress and plastic shear strain. Using these dependencies, general expressions for the elastic moduli were formulated and assessed to insure thermodynamic consistency. Next, analytical and numerical techniques were applied to the Castlegate mechanical data set to obtain explicit expressions and material parameter values for the terms in the elastic moduli expressions. Gibbs function was derived using these specific elastic moduli expressions, thus completing the elastic modeling of the material.

Approach - Hyperplasticity:

The principle of hyperplasticity states that a complete constitutive relationship can be derived with 1) choice of an energy function (e.g., Gibbs function) and 2) a dissipation function or yield function. Using this principle, the elasticity approach (which we have completed) and plasticity approach (future work) of the constitutive framework are linked mathematically without the need for secondary assumptions. Although this principle has been outlined theoretically, the complete formulation has never been applied and validated against an actual mechanical data set for high porosity sandstone. However, results from hyperplasticity approaches for clays (e.g., Houlsby 1981a; Houlsby 1985) and soils (e.g., Houlsby 1981b; Collins 2003; Collins and Kelly 2002; Collins 2005) have been useful in developing our elastic framework for high porosity sandstone.

Assumptions:

The following assumptions were made in the development of a thermodynamically sound constitutive model for Castlegate sandstone.

1. Castlegate sandstone is assumed to be a continuum which is macroscopically homogeneous and isotropic. While velocity measurements, bedding plane, and the microscopic composition suggest use of a transversely isotropic (or even orthotropic) constitutive model, isotropy is a common first assumption in developing a new constitutive model, and will capture the most fundamental aspects of the sandstone behavior. Addititionally, an isotropic model is more easily calibrated for a specific sandstone, since experimental data is needed for evolution of only two independent elastic moduli (e.g., bulk modulus and shear modulus), whereas transverse isotropy, for example, requires experimental data to quantify the evolution of five independent moduli.

2. The constitutive response is independent of the third invariants of stress (J_3) and strain. While some researchers (including the data of Ingraham et al. 2013, used in this project) report a J_3 dependence for failure, there is currently insufficient data to accurately quantify J_3 dependence of elastic moduli. Ideally this would require tests conducted at constant mean stresss and constant shear stresss, with increasing Lode angle; to our knowledge, such tests have never been conducted on sandstone. Thus, future work could pursue a third invariant dependent constitutive relation.

3. Compressive forces/stresses are applied to the system quasi-statically; therefore, it is assumed that a) there are no inerial effects, b) rate –dependence can be neglected and c) any heat generated is dissipated so that the system can be considered macroscopically isothermal.

4. The elastic moduli evolve with both stress and plastic strain, such that the bulk modulus is a function of mean stress and plastic volume strain, $K(\sigma,\varepsilon^p)$ and the shear modulus is a function of shear stress and plastic shear strain, $G(\tau,\gamma^p)$. Additionally, we assumed that that there are

no cross dependencies (e.g., *K* depends on mean stress, σ, but not shear stress, τ, and *G* depends on shear stress, τ, but not mean stress, σ.) Since the bulk modulus analyses were performed using hydrostatic test data, there is no way to assess a possible shear stress dependence, since shear stress was always zero. The deviatoric data set includes tests at five different mean stresses (30, 60, 90, 120, 150 MPa); however, we found that the shear modulus did not evolve with mean stress.

5. Plastic strain is not accumulated during unload-reload cycles during experiments. Therefore, the unload response is purely elastic (the plastic strain is constant during a given unload curve), such that the unload curves (conducted during each test, and the final unload) can be used to determine the exact form of the moduli dependence on stress and plastic strain.

Methods:
The following are a few of the criteria developed for selection of an appropriate analytical form of constitutive framework for Castlegate sandstone.

A. When the rock is not loaded (i.e., $\sigma_{ij} = 0$ and $\varepsilon_{ij}^{p} = 0$) the static elastic moduli should be similar to that of the dynamic elastic moduli derived from the velocity measurement of an undeformed specimen. While this assumes homogeneous isotropy and linear elasticity, this is acceptable, since the criteria is used only to provide guidance on sensible bounding values for the moduli expressions.

B. The elastic moduli are decreasing functions of the plastic strains. Therefore, as plastic strain increases (e.g., plastic strain in loop 3 is greater than loop 2), the calculated moduli at a given stress value in each subsequent loop must decrease (e.g., at given stress, modulus for loop 3 is smaller than for loop 2).

C. The resulting constitutive model must be in good agreement with experimental constitutive response data (i.e., Ingraham et al. 2013a, Ingraham et al. 2013b).

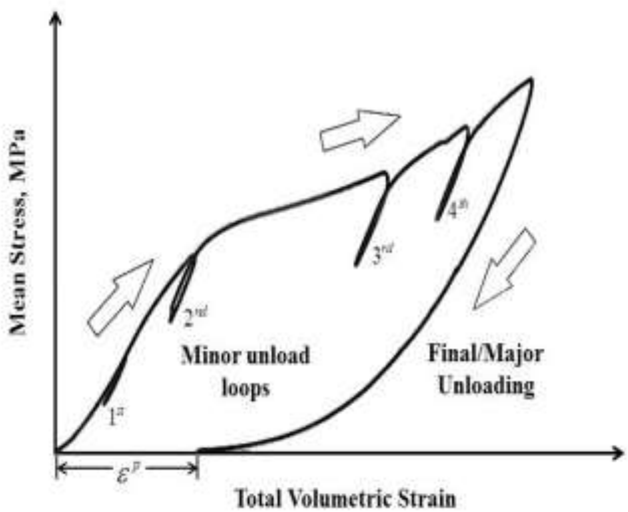
D. The resulting constitituve model must be thermodynamically consistent (Houlsby and Puzrin 2006, Dougill 1983).

Material:
Castlegate sandstone was chose for this project, because it is considered to be a reservoir analog rock, and because the project team has considerable experience in mechanical testing and modeling of this sandstone. Castlegate sandstone is a weakly-cemented fine to medium grained (~ 0.2mm grain size) rock, composed of 70-80% quartz, 5-10% clay with a small percentage of potassium feldspar, siderite, and lithics such as chert (DiGiovanni et al. 2000; DiGiovanni et al. 2001). The average porosity of the specimens used in this project was 26% (Ingraham et al. 2013), and specimens were cored parallel to bedding. Experimental investigation of the static and dynamic moduli of Castlegate sandstone found that the difference between the two moduli is negligible when the tangent modulus is obtained from the unloading loops during the test (i.e., not the final unload) (Plona and Cook 1995).

We use the mechanical data set (three principal stresses, strains in the three principal stress directions, and acoustic emissions) generated from a suite of true triaxial experiments previously conducted (Ingraham 2012, Ingraham et al., 2013 a,b) under an NSF-funded project. A suite of 25 tests were conducted at five different mean stresses (ranging from brittle failure through cataclastic flow), and under five different deviatoric stress states: axisymmetric compression (ASC, $\sigma_1 > \sigma_2 = \sigma_3$), pure shear (PS, $\sigma_2 = (\sigma_1 + \sigma_3)/2$), axisymmetric extension (ASE, $\sigma_3 < \sigma_2 = \sigma_1$), and two stress states in between: ASC/PS and PS/ASE. A hydrostatic test was also conducted. Acoustic emissions (AE) were used to identify the onset of strain localization (Ingraham et al., 2013b). After localization occurs, the rock cannot be considered as homogeoeous; therefore, our constitutive modeling work was restricted to pre-localization response.

Results:

The expression for the total volume strain equation was adapted from the form given by Zimmerman et al. (1986), who obtained a form for the total volume strain that was nonlinearly dependent on hydrostatic pressure, *P*, such that $\varepsilon = A\sigma - Be^{-(P/P*)} + D$, where *A*, *B*, *D* and *P** are fitting parameters obtained via least square regression. The values of the parameters, especially parameter *D*, were observed to vary within and across rock types (personal communication with R. Zimmerman, Decemember 2015). This nonlinear elastic response is seen in Castlegate sandstone, as shown in the figure below.



Next, we qualitatively confirmed the plastic strain dependence of the moduli, by simply assuming linear elastic unloading for the seven unload loops from the hydrostatic test: the total strain is partitioned into linear elastic plus plastic: $\varepsilon = p_1\sigma + \varepsilon^p$. The table below shows the results of the linear fit, and confirms that: 1) plastic strain increases during the hydrostatic loading, and 2) the modulus decreases with increasing plastic strain.

loop #	p_1 [1/MPa]	ε^p mm/mm]	R^2	$K = 1/p_1$ [MPa]
1	1.22E-04	1.03E-03	0.9992	8217
2	1.45E-04	1.19E-03	0.9996	6911
3	1.55E-04	1.27E-03	0.9996	6456
4	1.66E-04	1.25E-03	0.9999	6028
5	1.69E-04	1.29E-03	0.9998	5910
6	1.74E-04	1.31E-03	0.9995	5750
7	1.77E-04	1.35E-03	0.9998	5656

Next, we conducted a systematic analysis of each unload loop during hydrostatic loading, to obtain an general expression for the the elastic response, where the total volume strain is a function of mean stress and plastic volume strain, $\varepsilon = \varepsilon(\sigma, \varepsilon^p)$:

$$\varepsilon = a_1\sigma + a_2(1 - e^{-\frac{\sigma}{a3}}) + \varepsilon^p, \tag{1}$$

where $a_1 = a_{11} + a_{12}\varepsilon^p$, $a_2 = a_{21} + a_{22}\varepsilon^p$, and a_3 is a constant. Conducting a similar analysis using the unload loops during deviatoric loading, provided a similar expression for the total shear strain:

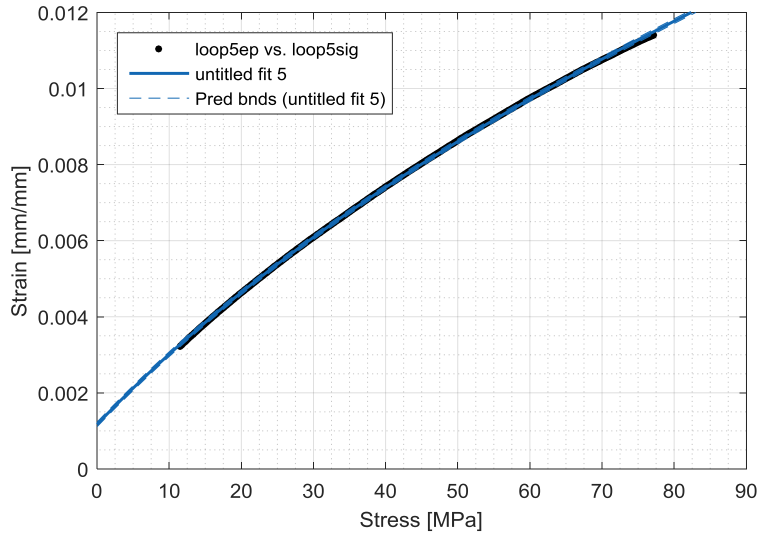
$$\gamma = b_1\sigma + b_2(1 - e^{-\frac{\tau}{b3}}) + \gamma^p, \tag{2}$$

where $b_1 = b_{11} + b_{12}\gamma^p$, $b_2 = b_{21} + b_{22}\gamma^p$ and b_3 are constants. The table below displays the values for the material parameters obtained from curve fitting analysis. The expressions in Equations (1) and (2) are applicable to any high porosity sandstone, whereas the values of the material parameters in Table 3 are specific to this block of Castlegate sandstone.

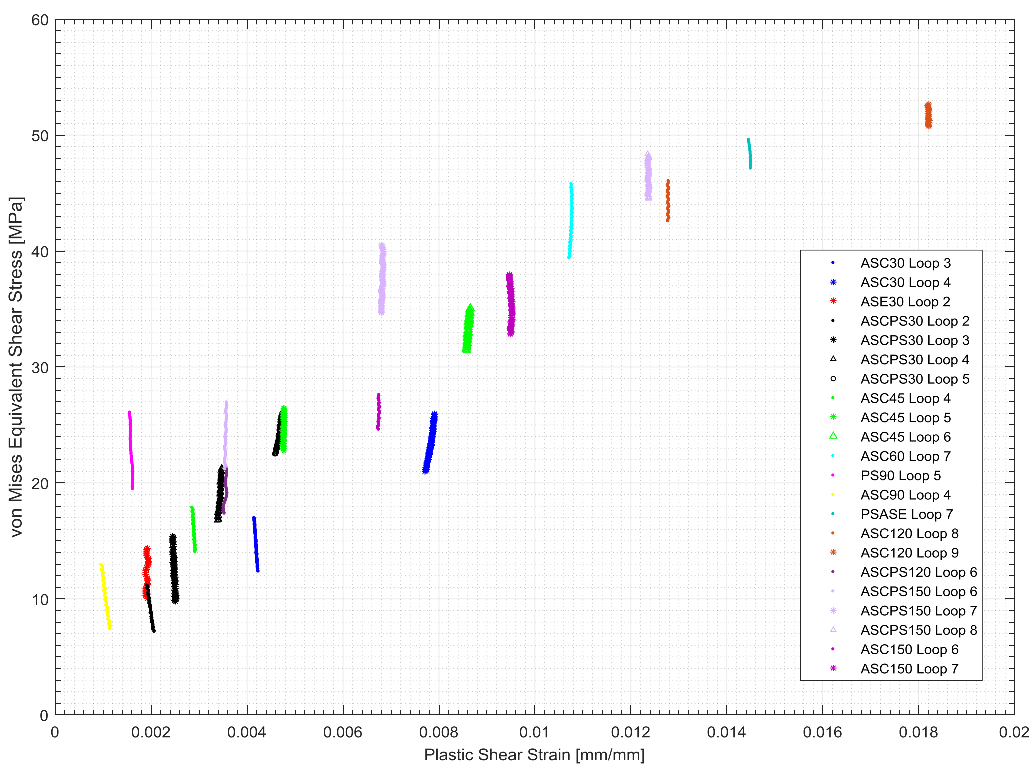
Values of material parameters obtained from curve fitting analysis

Volumetric	**Shear**	**Units**
$a_{11} = 8e-05$	$b_{11} = 6e-05$	$[\text{MPa}^{-1}]$
$a_{12} = 0$	$b_{12} = 0.0028$	$[\text{MPa}^{-1}]$
$a_{12} = 0.004$	$b_{21} = 0.0025$	$[\text{mm}/\text{mm}]$
$a_{22} = 0.8$	$b_{22} = 0$	$[-]$
$a_3 = 40$	$b_3 = 10$	$[\text{MPa}]$

The figure below shows the excellent fit between Equation (1) and the mechanical data from the unloading portion of loop five of the hydrostatic test.



The figure below shows the shear stress vs. plastic strain for the unloading loops during deviatoric loading for several of the tests. Note that the line segments are mostly vertical, which means that the plastic strain dependence of the shear modulus has been correctly modeled and therefore the elastic strain has been properly backed out, such that the plastic shear strain is constant during elastic unloading. Note that if the elastic strain is not properly backed out, the plastic strain would inappropriately appear to increase or decrease during unloading.



Rearranging Equations (1) and (2) to collect the terms with plastic strain, we can see the role of each term more clearly. For hydrostatic loading, the expression for total volume strain given in equation (1) is

$$\varepsilon = \left[a_{11}\sigma + a_{21}(1 - e^{-\frac{\sigma}{a_3}}) \right] + \left[a_{12}\sigma + a_{22}(1 - e^{-\frac{\sigma}{a_3}}) + 1 \right] \varepsilon^p \quad , \tag{3}$$

where $a_{11}\sigma + a_{21}(1 - e^{-\frac{\sigma}{a3}})$ is the volume strain due to nonlinear elasticity, $\left[a_{12}\sigma + a_{22}(1 - e^{-\frac{\sigma}{a3}}) \right] \varepsilon^p$ is the volume strain due to nonlinear elastic-plastic coupling and ε^p is the plastic volume strain. Likewise, for deviatoric loading, the expression for total shear strain given in equation (2) is

$$\gamma = \left[b_{11}\tau + b_{21}(1 - e^{-\frac{\tau}{b_3}}) \right] + \left[b_{12}\tau + b_{22}(1 - e^{-\frac{\tau}{b_3}}) + 1 \right] \gamma^p \quad , \tag{4}$$

where $b_{11}\tau + b_{21}(1 - e^{-\frac{\tau}{b_3}})$ is the shear strain due to nonlinear elasticity, $\left[b_{12}\tau + b_{22}(1 - e^{-\frac{\tau}{b_3}}) \right] \gamma^p$ is the shear strain due to nonlinear elastic-plastic coupling and γ^p is the plastic shear strain.

Using our expressions for total strain during unloading, Equations (1)-(2), the bulk compliance, $1/K$, and the shear compliance, $1/G$, are found to be

$$\frac{\partial \varepsilon}{\partial \sigma} = \frac{1}{K(\sigma, \varepsilon^p)} = a_1 + \frac{a_2}{a_3} e^{-\frac{\sigma}{a_3}} \tag{5}$$

$$\frac{\partial \gamma}{\partial \tau} = \frac{1}{G(\tau, \gamma^p)} = b_1 + \frac{b_2}{b_3} e^{-\frac{\tau}{b_3}} \tag{6}$$

Next we determined the Gibbs function, which is assumed to be a function of both stress and plastic strain, such that $\Gamma = \Gamma(\sigma_{ij}, \varepsilon_{ij}^p) = \Gamma(\sigma, \tau, \varepsilon^p, \gamma^p)$. The total strain tensor is defined as $\varepsilon_{ij} = \frac{\partial \Gamma}{\partial \sigma_{ij}}$, where the total volume strain is $\varepsilon = \frac{\partial \Gamma}{\partial \sigma}$, and the total shear strain is $\gamma = \frac{\partial \Gamma}{\partial \tau}$.

Note that since work is focused on the elastic response, the plastic strain terms are considered to be independent variables. Therefore, from partial integration volume strain, $\varepsilon = \frac{\partial \Gamma}{\partial \sigma}$, and shear strain, $\gamma = \frac{\partial \Gamma}{\partial \tau}$, the elastic portion of the Gibbs functions is derived:

$$\begin{aligned}\Gamma(\sigma,\tau,\varepsilon^p,\gamma^p) = {} & \frac{1}{2}a_1\sigma^2 + \frac{1}{2}b_1\tau^2 \\ & + a_2\left(\sigma + a_3 e^{-\frac{\sigma}{a_3}}\right) + b_2\left(\tau + b_3 e^{-\frac{\tau}{b_3}}\right). \\ & + \sigma\varepsilon^p + \tau\gamma^p + \eta\left(\varepsilon^p,\gamma^p\right)\end{aligned} \qquad (7)$$

Note that $\eta\left(\varepsilon^p,\gamma^p\right)$ must be either a scalar function of plastic strain, constant or zero. This completes the elasticity portion of the constitutive model. Knowing the Gibbs function, Γ, the strain increment can be predicted, as follows:

$$d\varepsilon_{ij} = \frac{\partial^2 \Gamma}{\partial \sigma_{ij}\partial \sigma_{kl}} d\sigma_{kl} + \frac{\partial^2 \Gamma}{\partial \sigma_{ij}\partial \varepsilon_{kl}^p} d\varepsilon_{kl}^p = M_{ijkl} d\sigma_{kl} \qquad (8)$$

The final step required to predict the strain increment is to predict plastic strain increment, $d\varepsilon_{kl}^p$. This can be done using some form of classical plasticity, e.g.:

$$d\varepsilon_{ij}^p = d\lambda \frac{\partial g}{\partial \sigma_{ij}} \qquad (9)$$

where the direction of the plastic strain increment is perpendicular to a plastic potential, *g*, and the magnitude of the plastic strain increment, $d\lambda$, is determined from the consistency condition, $df = 0$, where *f* is the yield function. The use of a plastic potential, *g*, is required because the plastic strain increment is typically not normal to the yield surface, *f*, for geomaterials.

Alternatively, Collins, Houlsby and colleagues (e.g., Puzrin and Houlsby 2001a; Collins and Hilder 2002; Collins 2002; Collins 2003; Collins and Muhunthan 2003) propose that normality can be achieved by using a yield surface in dissipative stress-space. In their formulation, the use of the plastic potential function is not required. Instead, they propose that a complete constitutive relationship can be derived with: 1) choice of an energy function (e.g., the Gibbs function we have already derived), and 2) a dissipation function or yield surface.

Future Work:
At the time of the completion of the grant, we have derived the Gibbs function and are currently preparing a paper to publish these results. In 2017, we will use our elastic constitutive model to back the elastic strains out of the total strains, in order to determine plastic strains and plastic strain increments in all the tests, covering various stress states. This will enable us to plot yield

surfaces, assess non-normality and predict band orientations for strain localization (and compare to experimentally observed band angles from Ingraham et al., 2013b). Addtionally, these resulting plastic strains can be used to investigate the efficacy of various plasticity approaches to predict plastic strain increments.

Presentations:

1. AGU Fall Meeting, December 2016, San Francisco, CA, "Constitutive Modelling for High Porosity Sandstone: Castlegate Sandstone," MC Richards, KA Issen, MD Ingraham.
2. AGU Fall Meeting, December 2016, San Francisco, CA, "Characterization of Dilatant Shear Bands in Castlegate Sandstone Using Micro-Computed Tomography," RE Rosenthal, KA Issen, MC Richards, MD Ingraham.
3. AGU Fall Meeting, December 2015, San Francisco, CA, "Evolution of Elastic Moduli for High Porosity Sandstone under True-Triaxial Stress Conditions," MC Richards, KA Issen, MD Ingraham.
4. AGU Fall Meeting, December 2014, San Francisco, CA, "Development of a thermodynamically consistent constitutive framework for Castlegate sandstone," MC Richards, MD Ingraham, KA Issen.
5. Engineering Mechanics Institute (EMI) Conference, Evanston IL, August 2013, "Examination of a Thermomechanics-based Constitutive Framework for Castlegate Sandstone," KA Issen.
6. Sandia National Laboratories, June 2013, Albuquerque NM, "Thermomechanics-based Constitutive Framework for Porous Geomaterials," KA Issen.

Student Awards:

1. Melissa C. Richards, AAUW Dissertation Year Fellowship ($20,000), 2017-18.
2. Rachel E. Rosenthal, Honorable Mention, NSF Graduate Research Fellowship Program, 2017.

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