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Modeling Reactive Transport in Deformable Porous Media Using the Theory of Interacting Continua

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Abstract

This report gives an overview of the work done as part of an Early Career LDRD aimed at modeling flow induced damage of materials involving chemical reactions, deformation of the porous matrix, and complex flow phenomena. The numerical formulation is motivated by a mixture theory or theory of interacting continua type approach to coupling the behavior of the fluid and the porous matrix. Results for the proposed method are presented for several engineering problems of interest including carbon dioxide sequestration, hydraulic fracturing, and energetic materials applications. This work is intended to create a general framework for flow induced damage that can be further developed in each of the particular areas addressed below. The results show both convincing proof of the methodologies potential and the need for further validation of the models developed.

Acknowledgment

This work was conducted in collaboration with Mario J. Martinez, Patrick K. Notz, Joe Bishop and John N. Shadid. Their helpful discussions are gratefully acknowledged. This work also emanates from close interactions with Kalyana B. Nakshatrala and his students. Lastly, I would like to thank William W. Erikson, Michael L. Hobbs and Michael J. Kaneshige for giving me an introduction to, and continued guidance regarding energetic materials.

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Chapter 1

Introduction

This report focusses on modeling flow-induced damage of porous materials including effects from chemical reactions and deformation or fracture in the solid matrix. Although not composed entirely in the context of classical mixture theory, the numerical formulation used for this research has its origins in the Theory of Interacting Continua and can be derived with only marginal deviation. The ultimate goal of this research is to address a number of engineering problems of national interest that depend critically on the ability to model flow-induced damage of porous materials. The research reported herein has applications in geologic sequestration of anthropogenic carbon dioxide, ignition processes for energetic materials, and prediction of crack pervasiveness and hydrocarbon yields for hydraulic fracturing.

Problems of interest

As carbon dioxide is injected (as a supercritical fluid) into a geologic deposit for abatement, large pressures develop that could compromise the integrity of the reservoir rock. Several trapping mechanisms that prevent carbon dioxide from escaping back into the atmosphere are influenced both by deflections in the rock matrix and cracks that form as the load exceeds the strength of the rock. Large scale release of carbon dioxide can not only lead to detrimental environmental impact, but under certain circumstances can be lethal. Given that an enormous amount of carbon dioxide must be sequestered annually to keep up with production, tremendous emphasis has been placed on developing modeling technology able to address the coupled nature of engineering problems involved in sequestration. Another trapping mechanism is provided chemically by solid carbonates that form as the carbon dioxide reacts with the in-situ constituents like brine and other minerals. The dependence on chemical processes must be included to accurately judge the efficacy of geologic sequestration and is a critical component of this research. In addition to the work presented here, several numerical studies related to sequestration of carbon dioxide have been presented in [8, 14].

Rather than ensuring that carbon dioxide will stay trapped underground, the modeling needs in the field of hydraulic fracture are aimed at enabling hydrocarbons to escape from the reservoir materials. As a reservoir is hydraulically fractured, cracks allow gasses such as methane to escape so that the end yield for a drill site is much higher than it would be if the reservoir rock was not fractured. As a technology, hydraulic fracturing has been around for decades, but has seen a sharp rise in interest due to the economic challenges associated with energy needs. What once was considered a last resort for extracting hard to harvest resources has become standard practice because the economics of drilling in difficult locations has become attractive. Regardless of the economic advantages made available through hydraulic fracturing, most view the process as controversial due to the potential for damage to the environment. Most convincing objections are based on the potential for water sources to be polluted by chemical additives used to improve fracturing performance. There are several toxic ingredients in the additives that have been linked to numerous health problems. Once these additives have leached into an aquifer, it is permanently contaminated and no feasible recourse exists to deal with such an incident. Since the economic benefit shows so much potential for hydraulic fracturing there is considerable interest from the oil & gas industry and environmental protection agencies for a simulation technology able to predict the extent of damage that fracturing will do to a reservoir and model the flow of contaminants through the damaged material. The goal is to be able to predict, for a given site, the liability that water resources will be penetrated by the fracturing process.

Although on a much smaller scale, many of the coupled flow-damage-reaction processes associated with subsurface geological engineering problems have corollaries in the field of energetic materials. As energetic materials ignite, the outcome of the ignition (whether or not detonation occurs and the resulting violence of the detonation) is highly dependent on damage to the porous matrix. As cracks form, new surfaces emerge that accelerate chemical reactions. Conversely, pathways open up allowing reaction gasses to escape before pressure build-up occurs often leading to no detonation at all. Modeling these types of engineering problems is especially complex since the very safety features designed to ensure insensitive munitions in accident scenarios can actually cause more violent detonations due to their unintentional magnification of damage to the energetic material. For example energetic material can extrude through vents intended to allow reaction gasses to escape during cookoff. The result is a much more violent reaction than would have occurred if the material were properly confined.

Methodology

To remedy the shortcomings of standard partial differential equation based strategies for modeling these types of problems a hybrid approach is employed in which finite elements are used to model the flow and chemistry and non-local methods are used to model the damage and deformation in the porous media. To integrate both of these methods we use the Theory of Interacting Continua [6, 3] in which the behavior of the bulk material is assumed to act as a mixture of the individual material constituents. In this way we incorporate the influence of the flow on the deformation and damage and vise versa. Both the flow and damage models begin with very simple formulations, but are generalized such that more complex models can be implemented. For most of the examples presented, only ad-hoc models are used which are not rigorously validated. Formal validation will be the study of a forthcoming work. The models do however showcase the salient features of the framework that has been developed and give a demonstration to its potential.

Finite elements have been used extensively to model flow through heterogeneous porous media, but problems that involve discontinuities have presented a formidable challenge. Since finite elements are based on spatial derivatives, in regions of discontinuity it is troublesome to obtain a smooth solution. Often, for a pristine material the material coefficients are treated as time independent, but for the problems of interest mentioned above, as damage occurs several quantities of interest evolve in time. For example, as the pore pressure exceeds the maximum strength of the reservoir rock, cracks begin to form that allow fluid to flow much more easily. This can be conceptualized as a local increase in the permeability. Likewise, the presence of the fluid in the porous media can provide an additional internal force due to the pressure exerted on the surface of the pores. As the pore pressure increases, there is a resulting effect on the stress in the solid matrix. Although the constitutive behavior of the porous media doesn't change, one can treat the increase in stress as an effective stress that is added to the stress calculated from the constitutive law.

To accurately capture the localized changes in permeability, and displacement due to cracks, a non-local method is employed. The non-local method used in the formulation has an integral-based governing equation that easily incorporates discontinuities [9]. The term *non-local* is meant to convey that the solution at any point in the domain is influenced by points outside of the immediate vicinity of the point in question. This region of influence is referred to as the point's *horizon*. Using a state-based formulation, in a discrete sense the solution is obtained by summing the force-states of all points within the horizon to obtain a balance of linear momentum. As the points are pushed away from each other, by the pressure of the fluid in the porous media, the bonds between these representative particles are stretched. Cracks are incorporated as broken bonds between particles that form when the critical value of stretch is exceeded. In the formulation below, once the bonds for a particular particle begin to break, the percentage of broken bonds is treated as the damage for that point. This damage field is used to model changes in permeability. This method has been presented in the following references [12, 13, 11].

Since the technology for non-local methods is still emerging, we elected in this first work to maintain a dichotomy between the flow solution and the deformation solution, maintaining separate meshes for both, managing the coupling in a weak fashion, and conducting information transfer between time steps. In future work we hope to integrate the formulation below into a single discretization that uses non-local methods for both the flow and deformation, but this is currently outside the scope of this work.

Overview

In the next sections we present the numerical formulation and some details regarding the implementation. Next, some numerical examples are presented that illustrate the proposed methods. Finally conclusions are drawn regarding the effectiveness of the methodology outlined in this report.

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Chapter 2

Numerical Formulation

As a general overview, the formulation below enables two simulations to run simultaneously, one finite element simulation to capture the flow and chemistry, and another non-local simulation to capture the deformation and cracking. As the simulations progress they mutually inform each other about the pressure of the fluid in the pores and the damage state of the matrix. In either simulation models are used to incorporate this data into the material coefficients. The models describe behavior such as how the permeability increases due to damage, or how the solid stress increases due to the pore pressure.

We start this section with the governing equations and the discretization for each physics and finish with an overview of the models used to engender the coupling.

Finite element flow and chemistry formulation

For the problems of interest presented in this work, the flow is modeled using Darcy's law [5] to compute the fluid velocity, along with a mass balance equation for pressure. In order to avoid numerical instabilities associated with mixed formulations [7, 2, 4], we use a single field approach whereby we solve for the pressure (denoted $p : \Omega \rightarrow \mathbb{R}$) using the mass balance equation and post-process the fluid velocity (denoted $\mathbf{v} : \Omega \rightarrow \mathbb{R}^{nd}$, where where "$nd$" is the number of spatial dimensions) once the pressure field has been determined. In the governing equations below we define Ω as a bounded open domain, and Γ its piecewise smooth boundary ($\Gamma := \bar{\Omega} - \Omega$, where $\bar{\Omega}$ is the set closure of Ω). We denote a spatial point by $\mathbf{x} \in \Omega$. The gradient and divergence operators with respect to $\mathbf{x}$ are, respectively, denoted by $\mathrm{grad}[\cdot]$ and $\mathrm{div}[\cdot]$.

Darcy flow

$$\mathbf{v} = \frac{k}{\mu}\left(-\mathrm{grad}[p] + \rho \mathbf{g}\right) \qquad \text{in } \Omega \tag{2.1}$$

Mass balance

$$\frac{\partial \rho}{\partial t} + \rho \,\mathrm{div}[\mathbf{v}] = \rho S \qquad \text{in } \Omega \tag{2.2}$$

In the equations above ρ is the fluid density, $k(\mathbf{x})$ is the permeability, μ is the coefficient of viscosity, $\mathbf{g}(\mathbf{x})$ is the specific body force, and $S(\mathbf{x})$ is the prescribed volumetric source term. To obtain a unique solution in the pressure field one typically enforces the following condition:

$$\int_{\Omega} p(\mathbf{x})\,\mathrm{d}\Omega = 0 \tag{2.3}$$

Another way to achieve uniqueness in the pressure field is to prescribe the pressure at a point to fix the datum, which is computationally the most convenient. In pressure-driven flows, there is no need to enforce additional conditions for uniqueness as the pressure is prescribed on a set of non-zero measure on the boundary.

Although this formulation may be extended to multiphase flows, to simplify the initial presentation we consider only isothermal single-phase flows composed of one fluid constituent. Under these assumptions we treat the fluid pressure as the pore pressure. For the remainder of this work we refer to the fluid pressure as the pore pressure.

The temperature in the system is modeled using an energy equation of the following form.

Energy

$$\rho C_p \frac{\partial T}{\partial t} - \mathrm{div}[\mathbf{q}] = \rho \dot{q} S \tag{2.4}$$

where C_p is the thermal coefficient, $\dot{q}$ is the chemical energy release rate and $\mathbf{q}$ is given for a diffusion constant κ as

$$\mathbf{q} = -\kappa \mathrm{grad}[T] \tag{2.5}$$

To track the evolution of chemical species in the domain, the following ordinary differential equation is used as the governing equation

Chemical species

$$\frac{\mathrm{d}X}{\mathrm{d}t} = -S \tag{2.6}$$

where X is the species concentration. For the examples presented in this work, we only consider simple reactions that can be modeled by tracking only one species such as A→B. The reaction rate is governed by a model of the form

Reaction rate

$$S = A \exp \frac{E}{RT} \left(\frac{p}{p_0} \right)^r X^n (1 - aX)^m \tag{2.7}$$

In the reaction rate above, there is an Arrhenius term with coefficient A that depends on the ideal gas constant, R, and coefficient E. There is also a pressure dependent term that depends on the fluid pressure. Finally, there is an autocatalytic term that depends on exponents n and m and coefficient a. The coefficients and exponents of the reaction rate are fit to data based on the problem of interest.

The above system involves three equations to be solved for fluid pressure, p, temperature, T, and species concentration X.

Weak formulation for the flow and chemistry problem

Let the weighting function corresponding to the pressure, temperature and species concentration be denoted by $q(\mathbf{x})$. The relevant function spaces are defined as

$$\mathscr{P} := \{p(\mathbf{x}) | p(\mathbf{x}) \in L_2(\Omega), \int_\Omega p(\mathbf{x})\,\mathrm{d}\Omega = 0\} \tag{2.8}$$

$$\mathscr{T} := \{T(\mathbf{x}) | T(\mathbf{x}) \in L_2(\Omega), \int_\Omega T(\mathbf{x})\,\mathrm{d}\Omega = 0\} \tag{2.9}$$

$$\mathscr{X} := \{X(\mathbf{x}) | X(\mathbf{x}) \in L_2(\Omega), \int_\Omega X(\mathbf{x})\,\mathrm{d}\Omega = 0\} \tag{2.10}$$

$$\mathscr{Q} := \{q(\mathbf{x}) | q(\mathbf{x}) \in L_2(\Omega), \int_\Omega q(\mathbf{x})\,\mathrm{d}\Omega = 0\} \tag{2.11}$$

where $L_2(\Omega)$ is the space of square integrable functions. Using the following notation for the standard L^2 inner product,

$$(\mathbf{a}; \mathbf{b}) = \int_\Omega \mathbf{a} \cdot \mathbf{b}\,\mathrm{d}\Omega \tag{2.12}$$

the classical Galerkin formulation can be written: Find $p(x) \in \mathscr{P}$, $T(x) \in \mathscr{T}$, and $X(x) \in \mathscr{X}$ such that

$$(q; \frac{\partial \rho}{\partial t}) + (q; \rho \mathrm{div}[\mathbf{v}]) - (q; \rho S) = 0 \tag{2.13}$$

$$(q; \rho C_p \frac{\partial T}{\partial t}) - (q; \mathrm{div}[\mathbf{q}]) - (q; \rho \dot{q} S) = 0 \tag{2.14}$$

$$(q; \frac{\mathrm{d}X}{\mathrm{d}T}) + (q; S) = 0 \tag{2.15}$$

$\forall q(x) \in \mathscr{Q}$.

Depending on the problem of interest or the boundary conditions required, terms in the above weak statements may be integrated by parts. In such cases appropriate terms on the boundary of the domain have been added.

Solid deformation and damage description

To model the deformation of the solid media we use a non-local method. The governing equations may be summarized as follows: The deformation of any point $\mathbf{x}$ is influenced by the action of a collection of particles, each denoted $\mathbf{x}'$, within a neighborhood defined by radius δ (referred to as the horizon). Interactions take place via bonds between the particles which we denote as $\langle \mathbf{x}' - \mathbf{x} \rangle$. The equation of motion for any particle at position $\mathbf{x}$ is written

$$\int_{\mathscr{B}_\mathbf{x}} \mathrm{T}(\mathbf{u}(\mathbf{x}') - \mathbf{u}(\mathbf{x}), \langle \mathbf{x}' - \mathbf{x} \rangle)\,\mathrm{dV}_{\mathbf{x}'} + \mathbf{b}(\mathbf{x}) = 0 \tag{2.16}$$

where $\mathscr{B}_\mathbf{x}$ is the neighborhood of the particle at $\mathbf{x}$, $\mathbf{u}$ is the displacement field, and $\mathbf{b}$ is the body force density, and T is a pairwise force function that gives the force vector per unit volume squared that defines the influence of the particle at $\mathbf{x}'$ on the particle at $\mathbf{x}$.

Discretized deformation formulation

If the body $\mathscr{B}_\mathbf{x}$ is discretized in the reference configuration into a finite number of cells, each with a single point at the centroid representing its position $\mathbf{x}$, the integral equation above may be replaced with the following discrete form

$$\sum_{i=0}^{N} \mathrm{T}(\mathbf{u}(\mathbf{x}') - \mathbf{u}(\mathbf{x}), \langle \mathbf{x}' - \mathbf{x} \rangle)\, \Delta \mathrm{V}_{\mathbf{x}'_i} + \mathbf{b}(\mathbf{x}) = 0 \tag{2.17}$$

where N is the number of cells, i, in the neighborhood of $\mathbf{x}$ with volume $\Delta \mathrm{V}_{\mathbf{x}'_i}$.

Constitutive model

The evaluation of the pairwise force function, T, requires a constitutive model to compute the force state in terms of the deformation state in the neighborhood of $\mathbf{x}$. In this work, we use the linear constitutive model presented in [10]. In the next section we show how this model is modified to account for the pore pressure of the fluid. The pairwise force acting on $\mathbf{x}$ can be expressed as a scalar force acting along the unit vector between the particles as follows

$$\mathrm{T}(\mathbf{u}(\mathbf{x}') - \mathbf{u}(\mathbf{x}), \langle \mathbf{x}' - \mathbf{x} \rangle) = \mathrm{T}\mathrm{M}(\mathbf{u}(\mathbf{x}') - \mathbf{u}(\mathbf{x}), \langle \mathbf{x}' - \mathbf{x} \rangle) \tag{2.18}$$

where T is the magnitude of the pairwise force and M is the unit vector pointing from the deformed position of $\mathbf{x}$ to the deformed position of $\mathbf{x}'$. The magnitude of the pairwise force is given as

$$\mathrm{T} = \frac{-3\psi}{m}\omega\chi + \frac{15\mu_s}{m}\omega\varepsilon \tag{2.19}$$

where m is the weighted volume at $\mathbf{x}$, χ is the length of the bond between $\mathbf{x}$ and $\mathbf{x}'$, ω is the value of the influence function, μ_s is a material parameter, and ε is the deviatoric extension of the bond. The dilatation scalar ψ is given as

$$\psi = K\Theta \tag{2.20}$$

where K is the bulk modulus of the material, and Θ is the peridynamic dilatation.

Coupling methodology based on damage modified permeability

To account for the influence of the fluid pore pressure in the peridynamic constitutive model, we introduce an effective dilatation scalar, $\bar{\psi}$, given as

$$\bar{\psi} = \psi - \alpha p \tag{2.21}$$

where p is the fluid pore pressure, and α is Biot's parameter. Equation (2.21) is motivated by a mixture theory approach to poroelasticity for which the interaction term is defined as a coefficient times the gradient of the fluid pressure, $\alpha\text{grad}[p]$. Typically, in the mixture theory approach, this additional term is added to the solid momentum equation by means of an effective stress, $\bar{\sigma} = \sigma + \sigma_p$, where σ is the elastic stress in the body and $\sigma_p = -\alpha p \mathbf{I}$ is the dilatation due to the fluid pressure. The previous approach takes advantage of the simple identiy $\text{div}[\sigma_p] = \alpha\text{grad}[p]$.

Figure 2.1 shows a diagram of both the effective stress principle and damage modified permeability. As shown in this figure, when cracks develop due to the pore pressure, interconnected flow pathways develop which significantly alter the flow field. Similarly, the presence of the fluid in the pores creates an additional stress contribution.

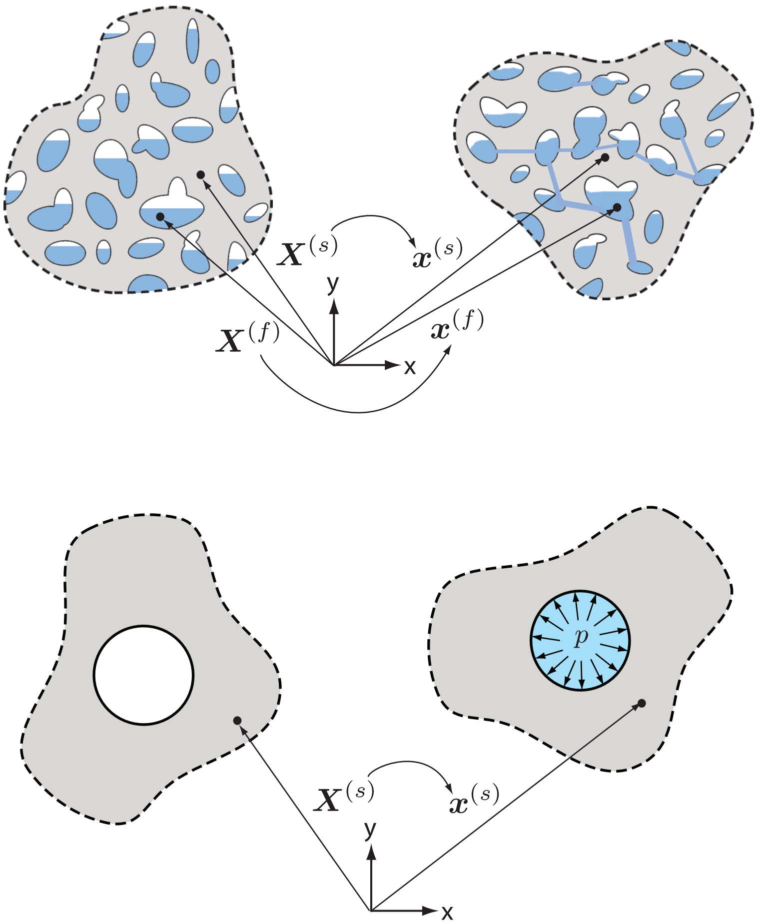

Figure 2.1. The undeformed (left) and deformed (right) configurations for the porous media, showing the damage modified permeability (top) and effective stress principle (bottom) of the proposed formulation.

Likewise, we modify the permeability in the flow simulation based on the damage in the porous matrix. The permeability k is modified according to a linear relationship with the damage d:

$$k = (1-d)k_0 + d(k_f) \tag{2.22}$$

where the damage quantity varies from 0 (for no damage) to 1.0 (when all of a particles bonds are broken). The damage quantity, d is computed at the end of each time step and passed to the flow simulation as an element variable.

Chapter 3

Numerical Examples

In this section several numerical examples are presented that exhibit the features of the formulation presented above. It is intended that these examples give an overview of the capabilities developed as part of this research. Rigorous validation of the models used, convergence studies, etc. have not been performed. These will be the focus of forthcoming work.

Carbon dioxide sequestration

When it comes to addressing the environmental impact of the tremendous amount of carbon dioxide produced each year, storage in underground reservoirs has proven itself to be the most feasible option. In order to keep pace with carbon dioxide production, billions of tons must be sequestered each year. Because of these demands, the injection rate is high enough that unintended consequences can occur regarding the structural integrity of the reservoir. Studying the integrity of the reservoir is fundamental to successfully deploying this abatement strategy and can help reduce the chances of large-scale release of carbon dioxide back into the atmosphere if the reservoir fails to contain it.

The domain of a sequestration reservoir can be modeled using a system of layers. The bottom layer represents bedrock and is fixed in all directions and does not deform. On top of this, the next layer represents the aquifer in which the carbon dioxide will be injected. This layer is considered to be a porous media that deforms based on the pressure of the fluid in the pores. Resting on top of this layer is the caprock layer, which initially does not have any fluid in its pores, but is treated as a deformable material. The caprock deforms as a result of the deformation in the aquifer layer. Figure 3.1 shows the resulting deformation in the aquifer layer and the caprock due to carbon dioxide injection. As the fluid is injected, the pores expand causing the porous matrix to swell.

One quantity of interest related to the structural integrity of the reservoir is the amount of leakage given a particular injection rate. Figure 3.2 shows the results of a simplified simulation of a sequestration reservoir caprock under loading from injection. The domain is idealized in two dimensions as a specimen in tension. The domain of the simulation is representative of a small section of the caprock near the point of inflection, such that we ignore the bending moment created by the uplift and include only the tensile load. As the specimen is loaded beyond its material strength two cracks form in the center of the domain. Near these cracks, the permeability is greatly

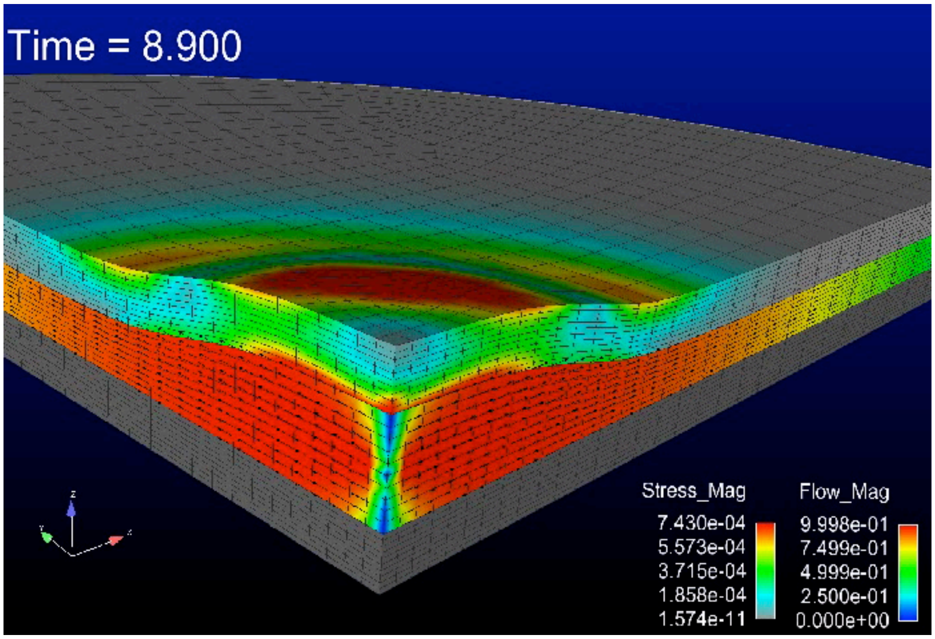

Figure 3.1. Simulation showing the deformation and stress generated in the caprock during injection.

increased allowing more flow to occur in these areas. To calculate the leak rate, the integral of the flux across the top surface can be computed.

Hydraulic fracturing

Hydraulic fracturing is used to release more hydrocarbons form a reservoir than otherwise would have been if the rock were left in a pristine state. There are several methods by which a reservoir is fractured, but the most common include pumping large quantities of water at extreme pressures into the reservoir and using propellants to generate pressure. Once the fracturing is completed, the water is removed and the gas is extracted. Among the various behaviors exhibited during hydraulic fracturing, there are two predominant observable characteristics related to the injection pressure and the crack growth rate.

For this simulations shown for this example, a 2D mesh was generated representing one quarter of a rock core cross section. Along the symmetry sides, symmetry boundary conditions are used for the flow, and rollers are used as the boundary condition for the deformation problem. On the inside surface, representing the borehole a constant injection rate is prescribed for the mass balance equation. The outer surface of the core is treated as an open boundary. Note that we have not included an chemistry in this simulation.

Figure 3.3 shows a snapshot of the results and provides a good illustration of the method used.

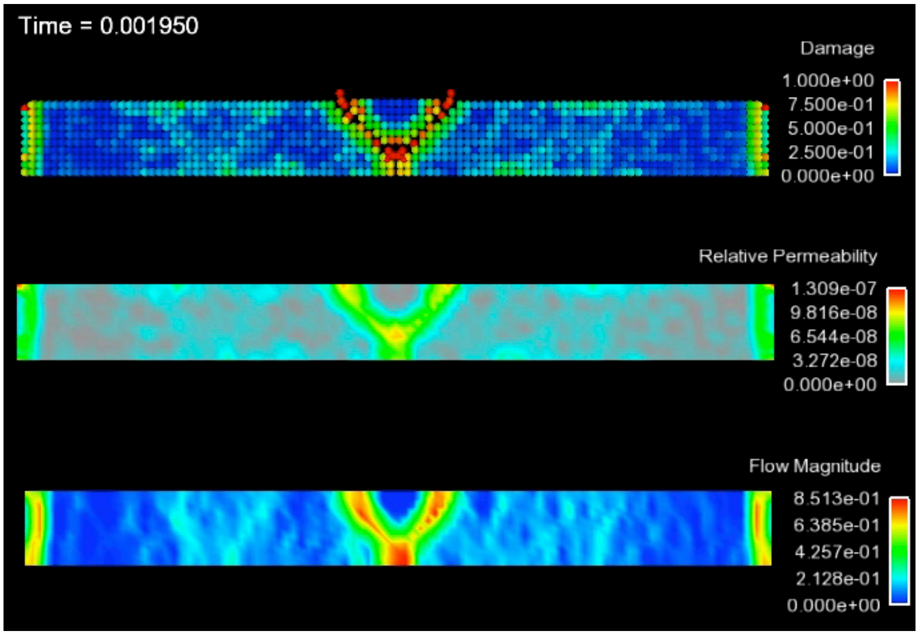

Figure 3.2. An instance in time near the end of a simulation of a carbon dioxide sequestration reservoir caprock failure showing a crack that has formed in the caprock, the permeability and the flow velocity.

On the left side of the figure is shown the finite element solutions for the pore pressure and velocity computed using the standard Galerkin formulation above. Since the porous media is treated as almost impermeable, the pressure is extremely high inside the crack, but drops quickly inside the material. Notice that the same holds for the fluid velocity since it is much easier for the fluid to flow inside the crack. The right side of the figure shows the results of the non-local simulation running in tandem. Note that the cracks correspond to locations of high pore pressure.

During the fracturing process, the fluid pressure in the borehole rises significantly until the crack forms. When the crack forms the pressure drops suddenly, depending on the material of the reservoir and the flow rate of the injection. The pressure at which the crack forms is known as the *breakdown pressure*. Under normal circumstances the pressure rises linearly until the breakdown pressure. Figure 3.4 shows the pressure in the borehole vs. time for the hydraulic fracture simulation. Notice that initially, the pressure is accurately captured, but a distinct breakdown pressure is not observed. This is most likely due to the material properties for the solid matrix not being properly selected. Another cause of this divergence from the expected solution may be due to damage that occurs in the immediate vicinity of the borehole which is non-physical. Damage near the borehole in the simulation acts to effectively increase the borehole volume leading to gradual pressure relief before the crack forms.

A much more challenging feature to capture than the breakdown pressure is the crack propagation rate since this is one of the fundamental characteristics of the fracturing process and deter-

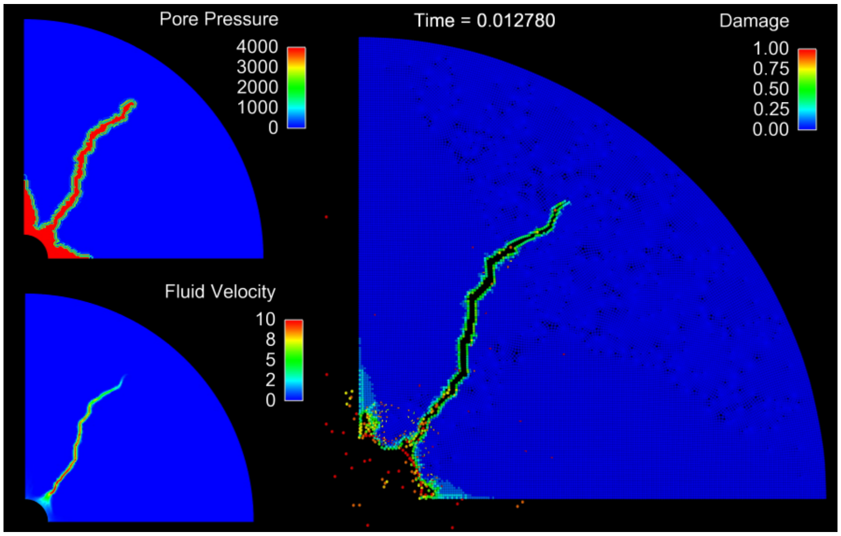

Figure 3.3. A snapshot in time taken of various quantities during the hydraulic fracture simulation. The upper left image shows the pore pressure both inside the crack and in the immediate vicinity of the porous media. The lower left image shows the fluid velocity. The damage is shown in the image on the right.

mines the extent of damage and in turn helps predict the extraction yield. It has been documented that if a constant pressure injection is used, once the crack forms it will propagate infinitely to the boundary of the domain. On the other hand if a constant injection rate is used, the rate at which the crack will grow depends on the injection rate. Experimental evidence suggests that for a constant injection rate, the crack will grow from the borehole according to the $2/3$ power law. Figure 3.5 shows the simulated crack length vs. time for various simulation constants. Although initially the simulated crack growth shows the expected behavior eventually the crack either propagates infinitely or ceases to propagate. Further investigation is required to determine if the $2/3$ power law can actually be captured using the proposed method. Initial consideration suggests that the bond strength and the elastic moduli of the porous media do not accurately reflect those used in the experiments.

Lastly Figure 3.6 shows that indeed the fluid races into the crack as expected when it opens up due to the pressure gradient that is created. Further work is required to adequately address

Energetic materials

Whereas in the previous examples, the damage was driven by injection pressure, for the energetic materials demonstrations, damage is a direct result of the chemical reactions that take place due to heating. A common technique for assessing the likelihood of detonation or the time to igni-

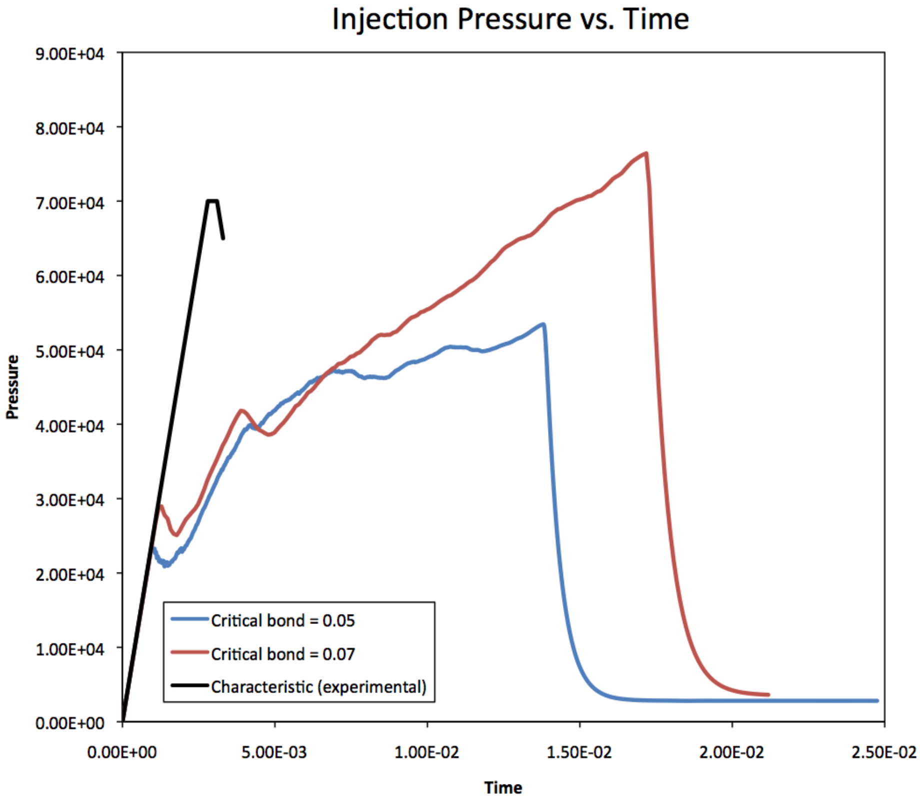

Figure 3.4. Fluid pressure vs. time. Once the crack begins to open up, the fluid pressure drops due to more volume being created for the fluid to fill.

tion for energetic materials in accident scenarios involves slow cookoff analysis. In slow cookoff, a small portion of explosives are confined in an aluminum anvil and heated to a certain temperature. Once the specified temperature is reached it is held constant until the explosive detonates or it becomes clear that ignition will not occur.

Recently, current research in the field of energetic materials has focused on the changes in permeability that result from the processes involved in ignition and the corresponding effects on the violence of the reaction. In some instances, damage to the energetic material enables reaction gases to escape before detonation leading to an insensitive munition. In other cases, damage to the energetic material leads to a more violent reaction since more surface area develops for the reaction to take place. To accurately asses safety metrics associated with accident scenarios requires technology able to incorporate both the chemical processes involved in ignition and the coupled feedback that occurs between the reaction gases and the porous material.

In [1], the authors present a diagram that illustrates the various damage causing mechanisms that occur during the ignition process. For a sample that is held at an elevated temperature, the leading cause of degradation in the energetic material (and resulting permeability change) is phase

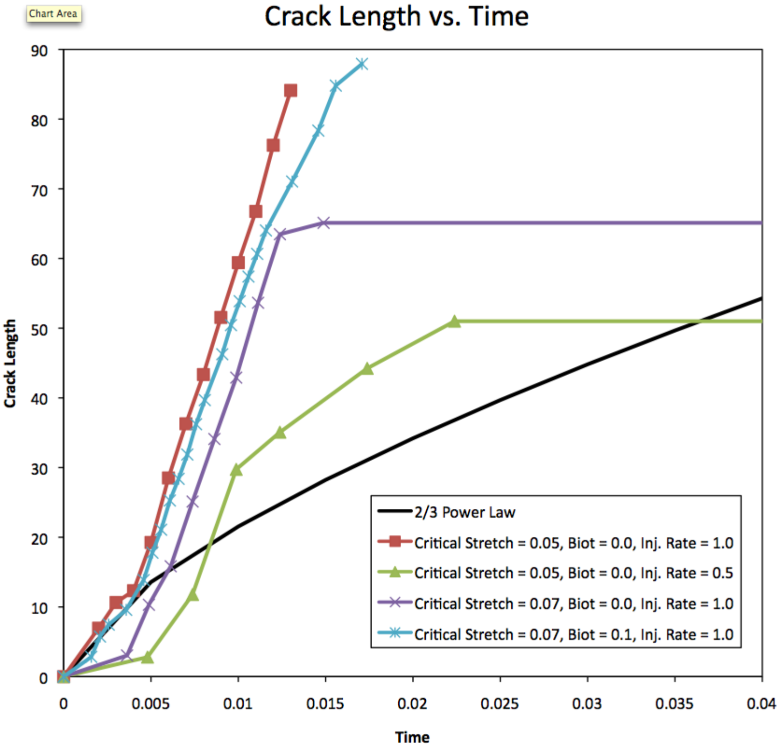

Figure 3.5. Crack length vs. time for the hydraulic fracture simulation. The representative curve in black is based on a $2/3$ power law, which is the expected crack growth rate.

change from condensed phase to gas phase. Next, the chemical reactions involved create additional permeability changes. Finally if the sample is cooled, the stress caused by contraction of the material leads to further permeability changes. To accurately predict the time to ignition one must consider these effects in the analysis.

Since no material is truly homogenous, we employ Karhunen-Loeve (KL) realizations to specify the bond strength throughout the domain for the following examples. In this way the damage propagation direction is randomized in such a way that cracks will follow the path of weakest bond strength. The helps prevent artificial tendencies for cracks to propagate in a particular direction. Figure 3.8 shows a plot of the bond strength for each element in a unit by unit domain. The bond strength is equivalent to a critical stretch or strain calculated in the material. Notice that the values range from 2% to 8% stretch.

Figure 3.9 shows the local permeability changes for an energetic material throughout the ignition process for points in time labeled A, B, and C. Until point A, the material remains essentially pristine since run-away has not occurred yet. Point A represents the start of the chemical reactions associated with ignition. At this point both the temperature and pressure rise significantly. The increase in pore pressure leads to the modified permeability. At point C the average permeability of the sample has changed by an order of magnitude. Figure 3.10 shows the results of the non-local

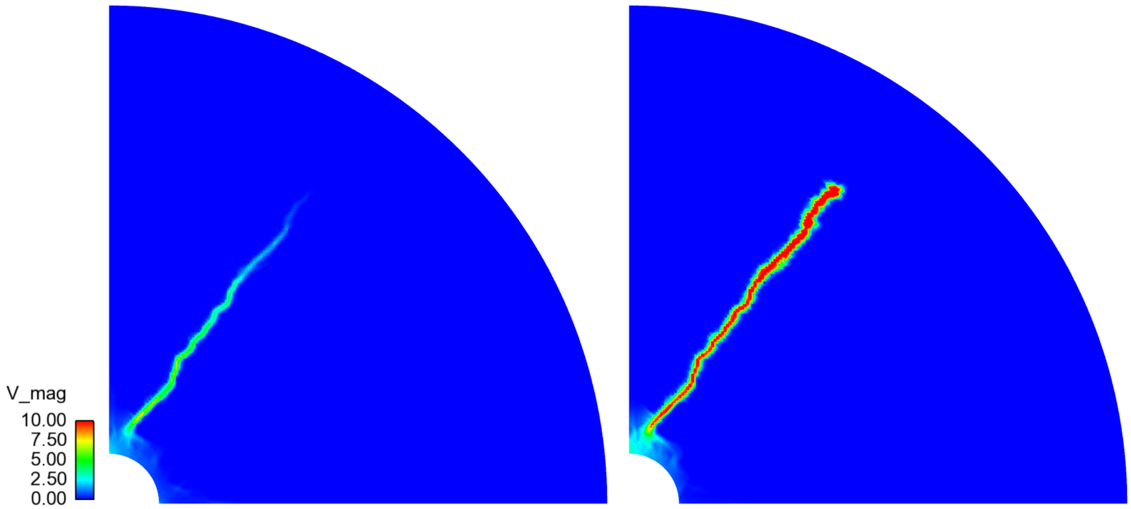

Figure 3.6. Fluid velocity in the crack before and after propagation. As the crack opens a pressure gradient develops from the high pressure in the borehole to the low pressure in the material. This causes a spike in the fluid velocity as it races into the crack from high pressure to low.

simulation of the deformation and damage in the energetic material. Notice that the regions surrounding the local permeability changes are fully damaged, meaning that for these representative particles, all of their bonds with neighboring particles have been broken.

Another issues of importance regarding the modeling of accident scenarios involving energetic materials is related to the integrity of the confinement. If the confinement is breached, gasses escape altering the outcome of the ignition. Anecdotal evidence suggests that in some cases the escape quenches the reaction such that no detonation occurs. In other cases, if material extrudes from the confinement the resulting detonation is extremely violent. Figure 3.11 shows both a comparison between two simulations where we either ignore or include the effects of confinement breach, and snapshots of the deformed state of the confinement for various points in the simulation that includes breach effects. Notice that including the damage to the confinement enables the pressure to be released once ignition occurs.

Finally, an additional quantity of interest for energetic materials analysis involves the fragmentation pattern of the confinement and the relative energy with which the fragments are projected at detonation. Figure 3.12 shows the results of a simulation of a short aluminum cylinder containing an energetic material that is slowly heated from below until ignition. For the sample on the left void space or *ullage* was left in the top of the container. This represents a common design practice. The sample on the right has no ullage. Figure 3.12 shows the difference in the size of the fragmentation pieces, and the number of projectiles between the two cases. The energy of the fragmented particles can be calculated using its mass and velocity.

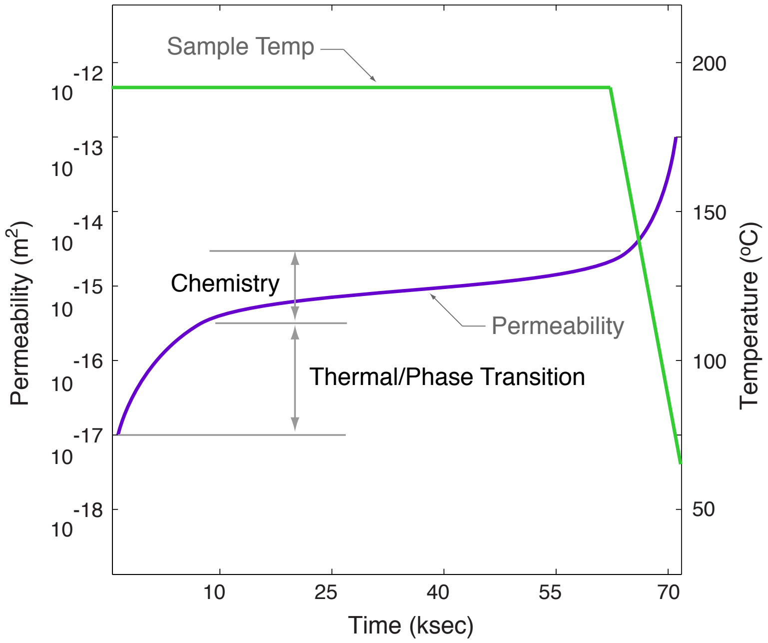

Figure 3.7. Factors leading to damage to the energetic material during various stages of ignition (recreated from [1]).

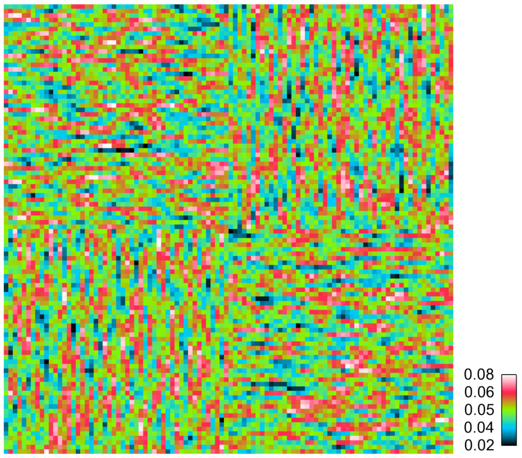

Figure 3.8. Elements colored by random bond strength. The bond strength field was created by doing a KL realization.

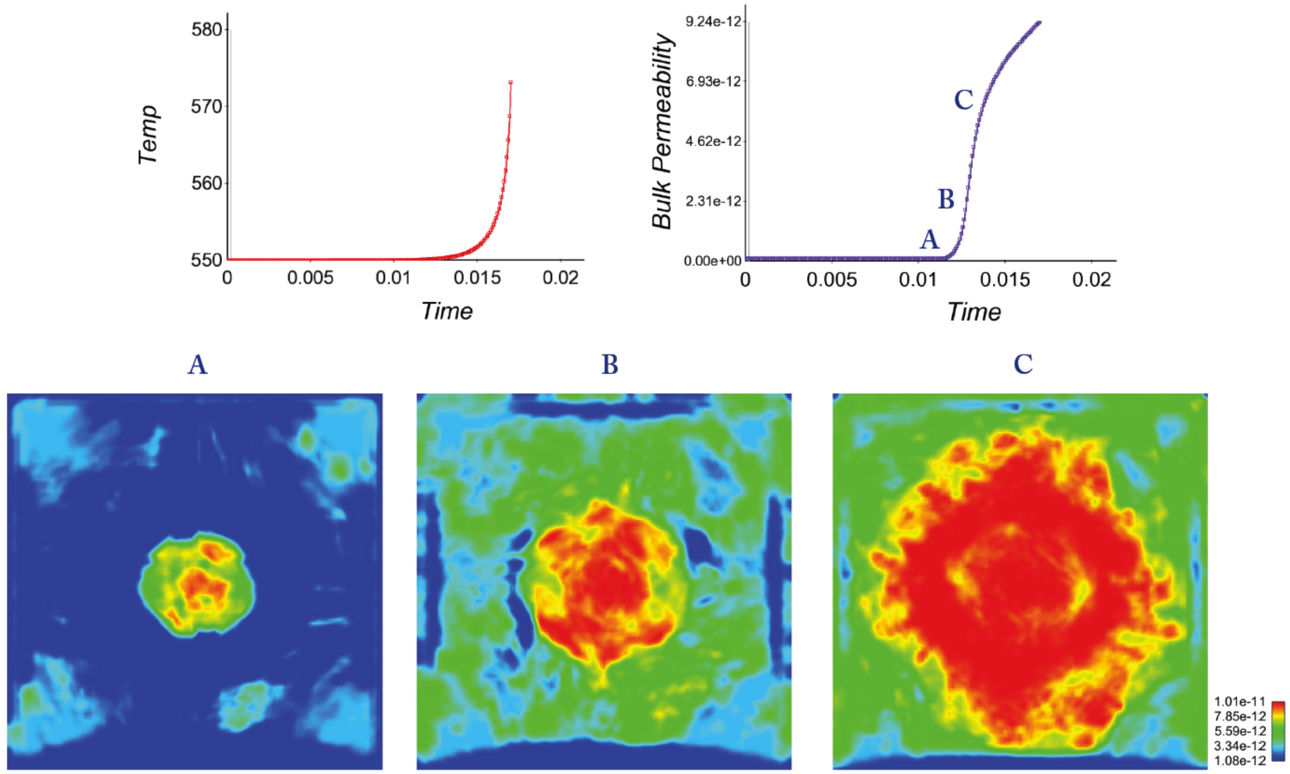

Figure 3.9. Evolution of permeability for various times during ignition.

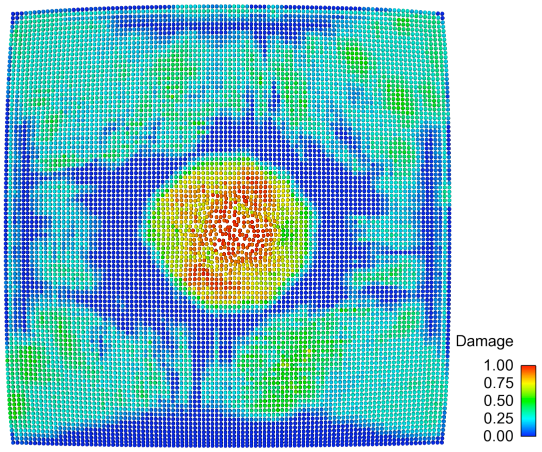

Figure 3.10. Results from the non-local method showing the regions of damage.

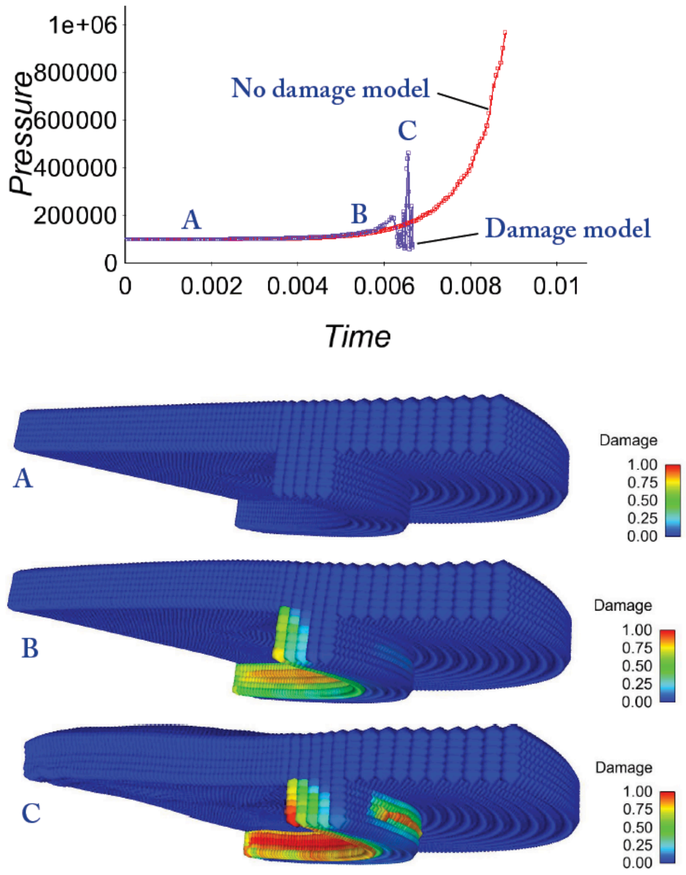

Figure 3.11. Damage conditions of the seal for various points in the ignition process. Once cracks propagate completely through the seal, ignition stalls as the pressure is released.

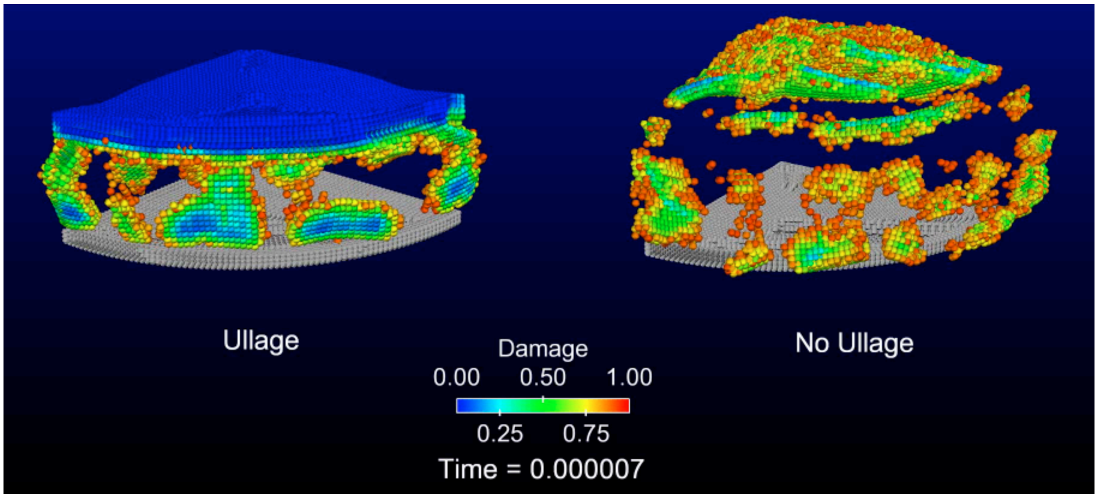

Figure 3.12. Fragmentation patterns dependent on the amount of ullage in the confinement.

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Chapter 4

Summary

In this report we have presented a computational methodology for analyzing engineering problems involving flow induced damage of porous materials using a mixture theory-like approach. The numerical formulation involves coupling two simultaneous simulations that track chemical reactions, flow characteristics, and damage evolution. The formulation presented was demonstrated for a wide variety of problems including carbon dioxide sequestration, hydraulic fracturing, and energetic materials. The results give an overview of the types of problems this methodology is appropriate for and demonstrates its features. It is intended that this report serve as a starting point for forthcoming works focusing on each problem individually, with more rigorous validation of the models involved and better representation of the material parameters. The result of these studies will be a powerful technology able to address many of the needs not currently met by existing methodologies.

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