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# MODIFYING TOUGH2 TO SUPPORT MODELING OF GAS-TRANPORT THROUGH SATURATED COMPACTED BENTONITE AS PART OF THE LARGE-SCALE GAS INJECTION TEST (LASGIT) IN SWEDEN

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## ABSTRACT

The LASGIT (Large Scale Gas Injection Test) project is a full-scale test of gas transport in bentonite at the Aspö Hard Rock Laboratory in Sweden. Simulating conditions in a deep geologic repository for spent fuel, an empty copper container surrounded by compacted bentonite blocks is placed within a large-diameter borehole in the host rock of the Hard Rock Laboratory. Once the buffer is completely saturated with groundwater, He gas is injected from ports on the container and monitored as it migrates from the container through the bentonite buffer to the host rock. The intent of the LASGIT experiment is to improve the understanding of gas migration through the engineered barrier of a deep geologic repository for spent fuel and to validate different modeling approaches which may be used in future safety assessments.

A preliminary gas-transport model of the LASGIT experiment was developed with a modified version of TOUGH2. This paper will describe the modifications to the TOUGH2 code, present the implementation of the LASGIT experiment in a numerical model and discuss preliminary model results.

Development of the gas-transport model required modifications to TOUGH2 to simulate expected gas transport mechanisms. While the mechanism for gas transport within bentonite is not well known, three potential mechanisms have been proposed (Hoch et al., 2004):

- conventional two-phase flow through a porous medium
- stress- or pressure- induced microscopic fracturing of the bentonite to provide pathways for gas flow
- stress- or pressure- induced macroscopic fracturing of the bentonite to provide pathways for gas flow

Each of these mechanisms may work individually or simultaneously. TOUGH2 was modified to include a pressure-dependent permeability function to simulate micro- or macro- fracturing and a permeability-dependent capillary pressure function to simulate fracture dilation. Additional modifications to TOUGH2 were implemented to simulate He gas.

A 3-D radial mesh was generated representing the copper container and the surrounding bentonite. The mesh is refined surrounding injection ports in the copper container used to inject gas at localized breach points. The 3D mesh was generated and the pressure and saturation model results were visualized with mView, a numeric model pre- and post-processor.

At present, the LASGIT experiment has been installed and the water saturation phase has begun. The preliminary model will be used to evaluate gas-injection test design, and will be further developed for detailed test analysis.

## INTRODUCTION

The Swedish KBS3 concept for deep geologic nuclear waste disposal involves placing copper containers of used nuclear fuel, surrounded by compacted bentonite blocks, within boreholes drilled into the floor of repository tunnels. After closure of the repository tunnel, the bentonite blocks will saturate and swell with the groundwater, sealing any gaps and providing an effective diffusion barrier against potential radionuclide release due to container failure.

While the containers are designed to prevent container failures, the breaching of a spent fuel container requires consideration in a performance assessment of a repository. Once a failed container has been penetrated by groundwater, corrosion of the steel insert under anaerobic conditions will generate hydrogen gas. If gas accumulates in the void space of the canister and reaches high enough pressures, gas may migrate through the bentonite by one or more potential gas transport mechanisms (Hoch et al., 2004):

- conventional two-phase flow through a porous medium
- stress- or pressure- induced microscopic fracturing of the bentonite to provide pathways for gas flow
- stress- or pressure- induced macroscopic fracturing of the bentonite, differing from microscopic fracturing only in the magnitude of the fracture generated.

For the repository safety case, an important question is whether gas generation and the consequent gas migration through the bentonite will decrease the effectiveness of the bentonite barrier.

A number of laboratory research studies have examined the migration of gas through bentonite. While the mechanisms for gas transport have not been definitively established, these studies have determined that gas does migrate through saturated bentonite once gas pressures have reached an entry threshold. Laboratory-scale results from Harrington and Horseman (2003) are consistent with the development of fracture-like pathways through the bentonite. Experimental data also suggest that very little water is expelled from the bentonite by the migrating gas, and once resaturated, the bentonite seems to reseal (Hoch et al., 2004).

The LASGIT (Large Scale Gas Injection Test) project is a full-scale test of gas transport in bentonite at the Aspö Hard Rock Laboratory in Sweden. The intent of the LASGIT experiment is to improve the understanding of gas migration through the bentonite buffer under full-scale repository conditions and to validate different modeling approaches which may be used in future safety assessments.

The experiment set-up, illustrated in Figure 1, consists of a full size copper canister surrounded by bentonite buffer within an excavated deposition hole in the crystalline rock. The hole is sealed with a concrete lid, which represents the weight of the backfill. Once the buffer is completely saturated with natural and injected artificial groundwater, a series of gas-injection tests will be conducted, with helium gas injected from ports on the canister wall. Key parameters will be measured, including total pressure, pore water pressure, and temperature. The experiment is isothermal, since gas generation is expected to occur after heat output from the fuel is negligible.

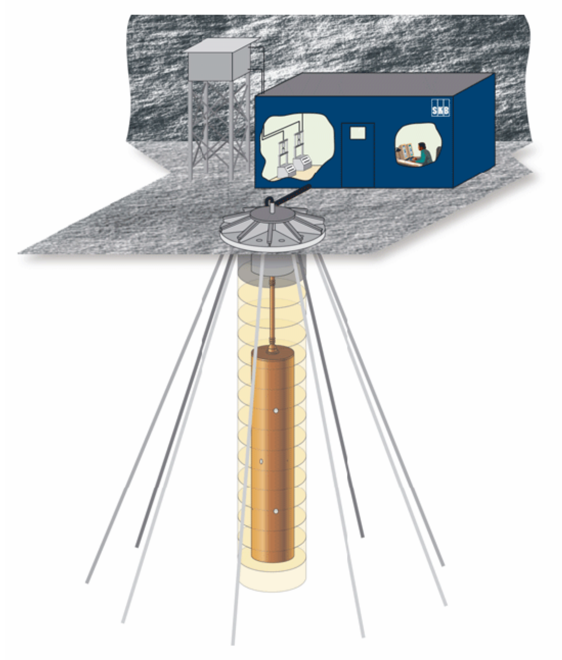

*Figure 1. LASGIT experimental set-up.*

Gas transport modeling of the LASGIT project will provide an evaluation of test design, as well as detailed test analysis. For the gas transport modeling of the LASGIT project, TOUGH2 will be modified to simulate potential gas transport mechanisms.

This paper will focus on modifications implemented in TOUGH2. Verification of these modifications using simple tests will also be presented, as well as the development of an initial model of the LASGIT system.

## TOUGH2 MODIFICATIONS

The following modifications to the TOUGH2 code were implemented:

1. Modification of permeability as a function of pressure. Increasing the permeability with increasing pressure effectively models micro/macro fracturing. Fracture directionality is also incorporated by only allowing modification of permeability for either horizontal or vertical connections. The choice of horizontal or vertical fracture directionality is intended to be based on the stress field inferred from measured total pressure.

2. Modification of capillary pressure according to permeability, which is dependent on pressure. Decreasing capillary pressure (note that capillary pressure is negative) as a function of permeability will simulate fracture dilation.

3. Compensation for the use of helium gas instead of air in the EOS3 module.

Additionally, two relative permeability functions and corresponding capillary pressure functions (Modified Brooks-Corey and Modified van Genuchten) included with iTOUGH2 (Finsterle, 1999) were incorporated into TOUGH2.

**Pressure Dependent Permeability Modifications**

TOUGH2 already implements basic pressure dependent gas permeability functions using the Klinkenberg approach. The Klinkenberg approach accounts for the effect of gas slippage in low-permeability porous media, i.e. the change in permeability of the gas phase due to the type of gas and the pressure differential across the media. For gases with small molecules or for low pressure differentials, gas permeability or gas slippage increases.

For LASGIT modeling, micro/macro fracturing of the media rather than gas slippage is of interest. Consequently, an alternate relationship for modifying both gas and liquid permeability as a function of pressure was implemented to model micro/macro fracturing. For the LASGIT modeling, it is expected that gas slippage effects will be lumped into the pressure-dependent function defined to simulate micro/macro fracturing.

There are a number of possibilities for defining this function, and a simple linear function was selected for implementation, assuming a linear relationship between pressure and permeability. In this case, an initial pressure (P1) is defined representing the onset of pathway dilation, and an upper pressure (P2) is defined corresponding to the maximum increase in permeability. The intrinsic permeability (k) is calculated as defined below:

$$k = k_0 \qquad P < P_1 \qquad (1)$$

$$k = k_0\left(1 + (k\_factor - 1)\frac{P - P_1}{P - P_2}\right) \qquad P_1 < P < P_2 \qquad (2)$$

$$k = k_0 \times k\_factor \qquad P > P_2 \qquad (3)$$

where k is the modified absolute permeability, $k_o$ is the initial absolute permeability, k_factor is the maximum scaling factor and P is the current pressure.

The implementation of alternate pressure-dependent functions (e.g. parabolic, or asymptotic to P1 and P2) as required is straightforward.

Incorporating fracture directionality is less straightforward. Fractures are expected to propagate in the direction perpendicular to minimum stress. TOUGH2 is not a geomechanical code, so the stress state is not known nor calculated within the simulator. However, the actual stress state at the bentonite surfaces (canister, top lid, and rock wall) can be determined from the available LASGIT instrumentation. The total pressure (effective stress + pore pressure) and pore pressure transducers can be used to develop a stress map of the bentonite surface before the onset of testing. If we assume that the internal stress state of the bentonite can be interpolated from the surface stress, we can then determine the most likely orientation of fractures induced by the injection tests.

The fracture directionality determined from the measured stress state is incorporated by providing options to limit the connections to which pressure-dependent permeability modifications are made. Three options are provided for fracture directionality, which modify permeability for:

- all connections, simulating no fracture directionality
- horizontal connections, simulating horizontal fractures
- vertical connections, simulating vertical fractures

The determination of a horizontal or vertical connection is determined through the ISOT parameter in the CONNE record, which defines the directionality of each connection. In addition to limiting the connections with modified permeability, an additional scaling factor is provided to directly scale permeability for all, horizontal or vertical connections.

**Pressure Dependent Capillary Pressure Modifications**

Capillary pressure ($P_c$) describes the pressure differential between fluid and gas phases at the phase interface. It is usually parameterized as a function of liquid saturation, temperature, and air entry pressure ($P_e$). A high value for $P_e$ inhibits the movement of the gas phase by providing an additional threshold over which gas phase pressure must exceed liquid phase pressure to move the interface.

To simulate fracture dilation, pressure increases that would dilate a fracture result in a reduction in the air-entry pressure. Changes in permeability associated with fracture dilation are typically associated with changes in $P_e$. These associated changes are explicitly defined for a fracture, where both the permeability and the capillary pressure are a function of the fracture aperture. In low-permeability porous media, empirical relationships have been developed relating $P_e$ to the intrinsic permeability (Davies, 1991; Horseman, 2000). In the implemented TOUGH2 modifications, the air-entry pressure is effectively scaled by element permeability, which is, as described in the previous section, pressure-dependent (note that the modifications actually scale capillary pressure instead of air-entry pressure, as will be subsequently described).

In TOUGH2, capillary pressure is generally considered a property of a material type which is defined as a function of liquid saturation. TOUGH2 provides a number of different capillary pressure-saturation functions. The functions that will be used in the LASGIT modeling (van Genuchten, modified van Genuchten or modified Brooks-Corey) have five parameters, including air-entry pressure, which in the normal implementation is a constant value for each material type.

In examining the code, it was determined that modifying the capillary pressure directly, instead of modifying the air-entry pressure, would be a more straightforward approach. Modifying the capillary pressure directly allows the modifications to occur following the calculation of the pressure-dependent permeability, but before use of capillary pressure in assembling the matrix equations. This is the same location capillary pressure is scaled for block-by-block permeability modifications within TOUGH2. At this point in the code, before the capillary pressure modifications are implemented, capillary pressure has already been calculated from the capillary pressure function (e.g. van Genuchten). For the capillary pressure functions to be used in LASGIT modeling (van Genuchten, modified van Genuchten or modified Brooks-Corey), modifying the capillary pressure is equivalent to modifying the air-entry pressure.

Capillary pressure is modified according to one of three permeability-dependent functions:

Leverett function: $$P_c = P_{c0}\frac{1}{\sqrt{k}} \quad (4)$$

Direct function: $$P_c = P_{c0}\frac{k_0}{k} \quad (5)$$

Cubic law function: $$P_c = P_{c0}\frac{\sqrt[3]{k_0}}{\sqrt[3]{k}} \quad (6)$$

where $P_c$ is the modified capillary pressure, $P_{c0}$ is the initial capillary pressure calculated by the capillary pressure function, k is the modified absolute permeability and $k_0$ is the initial absolute permeability.

An additional check is added to the capillary pressure modifications to ensure that the resulting capillary pressure remains less than the maximum capillary pressure specified in the capillary pressure function input records.

## Helium Injection Gas

EOS3, the TOUGH2 EOS module to be used in the LASGIT work, assumes that air and water are the two components in the simulation. The actual injection gas to be used in the LASGIT test is helium, which has different properties than air. Compensation for this difference was accomplished as follows:

1. helium gas properties – Henry's coefficient (HC), molecular weight (AMA) and specific heat (CVAIR) were adjusted in the code for helium. Molecular weight and specific heat values, 4.003 g/mol and 5193.1 J/(kg K) respectively, were obtained from Reid et al. (1987). Henry's coefficient was calculated from a published value of the solubility of helium in water at 25°C and atmospheric pressure (Dack, 1975), at a value of $6.72 \times 10^{-11}$ mole fraction/Pa. This value is close to a Henry's coefficient calculated for helium gas tracer tests at the Grimsel Test Site in Switzerland of $6.53 \times 10^{-11}$ $Pa^{-1}$ (Senger et al., 1998).

Although Henry's coefficient is a function of temperature, EOS3 assumes a constant Henry's coefficient. Since the solubility of air in water is low, changes to the Henry's coefficient due to temperature are expected to have an insignificant impact on the calculated concentration of air in water. Helium has a lower solubility in water compared to air, and consequently this assumption of a temperature independent Henry's coefficient is still valid.

2. gas viscosity – In the new LASGIT modified version of TOUGH2, gas viscosity of helium can be calculated using the existing EOS3 approach for air (Hirschfelder et al. modified kinetic gas theory (Pruess et al., 1999)), or the Wilke method implemented in TMVOC (Pruess and Battistelli, 2002). Both of these viscosity functions are temperature and molar fraction dependent.

The Wilke viscosity calculation from TMVOC was added to EOS3 and modified to include helium. In the Wilke method, pure component phase viscosities are calculated from temperature-dependent polynomial functions published in Irvine and Liley (1984). The TMVOC version does not include helium specifically, although the Irvine and Liley (1984) reference contains values for helium.

## TOUGH2 VERIFICATION

The modifications to TOUGH2 were thoroughly verified with a series of simple verification tests that examined each modification separately and combined. Results of these verification tests were compared to spreadsheet calculations.

In addition, several gas-only simulations were compared to nSIGHTS, a well-test analysis model that simulates single-phase, one-dimensional, radial/non-radial flow with a borehole at the center of the modeled flow system and a user-defined pressure-dependent permeability function. Developed by INTERA Engineering for Sandia National

Laboratories, nSIGHTS has been qualified in support of the WIPP program (Intera Engineering, 2005). Figure 2 displays the differences between nSIGHTS and the modified TOUGH2 for a helium-only verification test with permeability modifications (k_factor = 10), no fracture directionality and no capillary pressure modifications. The small differences between the two models are attributed to the different discretization schemes of the two models.

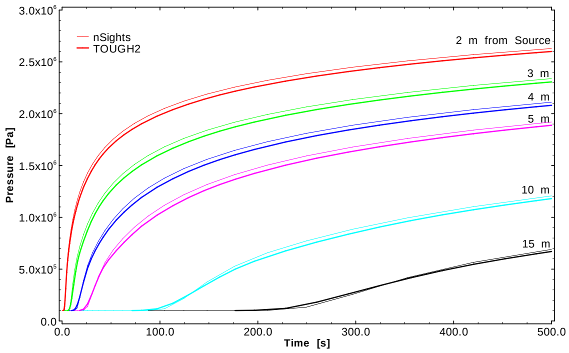


*Figure 2. Pressure time curve comparison between nSIGHTS and the modified TOUGH2. Pressure time curves taken at regular intervals along the model radius, half-way through the formation thickness.*

## INITIAL LASGIT MODELING

A preliminary gas-transport model of the LASGIT experiment was implemented with the modified TOUGH2 code, assuming water saturation is complete and gas injection testing has begun. Based on available data for the LASGIT project and assumed data where data was not available, this model is a starting point for future modeling, and ensures modifications to TOUGH2 are properly executed.

The initial model is a radial three-dimensional grid representing the bentonite buffer, with increased discretization around one injection port. The external boundaries of the simulated system are the physical limits of the bentonite, consisting of the rock walls of the emplacement hole, the top lid and the copper canister. Figure 3 shows a cut-away of the model, showing the model domain and prescribed pressure boundaries. Properties for the initial model, provided in Table 1, are based on known physical parameters of the LASGIT bentonite, as well as best estimate values for unknown parameters. These properties include parameters for the modified van Genuchten relative permeability and capillary pressure functions used in the initial model.

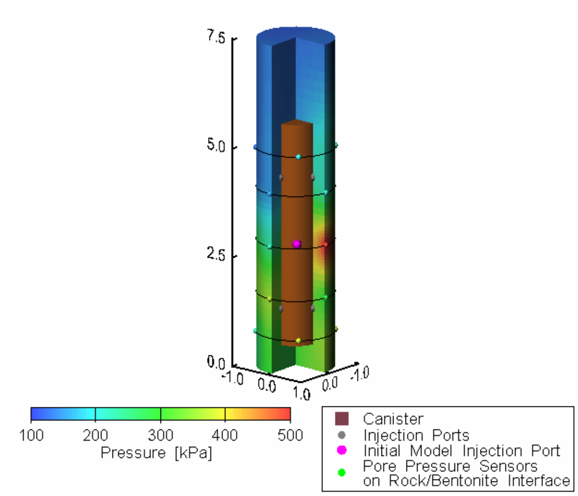


*Figure 3. Model domain showing initial pressures interpolated from measured pressures at the side rock/bentonite interface on October 31, 2005.*

*Table 1. Bentonite Properties for Initial Model.*

| Parameter | Best Estimate Value |
|---|---|
| Permeability | 1x10$^{-20}$ m$^2$ |
| Porosity | 0.4 |
| Rock Grain Density | 2780 kg/m$^3$ |
| Pore Compressibility | 3.58x10$^{-9}$ Pa$^{-1}$ |
| Gas Diffusion Coefficient | 1x10$^{-9}$ m$^2$/s |
| Residual Liquid Saturation | 0 |
| Residual Gas Saturation | 0 |
| Pore Size Distribution Index | 1.82 |
| Van Genuchten Gas Entry Pressure | 18 MPa |
| k_factor | 2 |
| $P_1$ | 1.5 MPa |
| $P_2$ | 20 MPa |

Dirichlet boundary conditions were established at the rock/bentonite interface on the external side and bottom boundaries of the model. Prescribed pressure values at these boundary conditions were interpolated from the latest pressure measurements at these boundaries (see Figure 3 and 4). Since the LASGIT experiment is still in the saturation phase, these boundary conditions will be updated in future iterations of the model, and will be made time dependent if required. The canister and top lid boundaries were assumed impermeable.

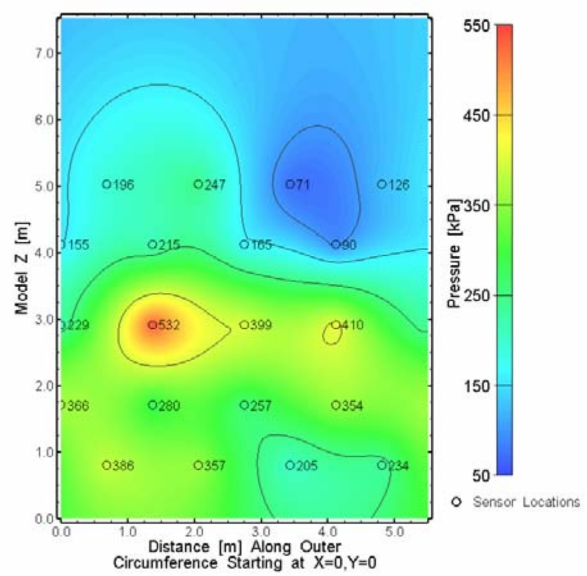


*Figure 4. Interpolated and measured pressures at side rock/bentonite interface on October 31, 2005. This figure shown the outer radius of the model domain, unrolled into a flat view.*

Initial pressures were set at a hydrostatic pressure profile and initial gas saturations at 0.03. After a steady-state partially-saturated pressure profile was reached, helium was injected into the system at one injection port at a constant rate of $2 \times 10^{-9}$ kg/s.

Figure 5 shows results from this model run after 2 years of continuous gas injection using the original TOUGH2 code and the modified TOUGH2 code. As expected, the pressure-dependent permeability and capillary pressure in the modified code results in the transport of gas over a larger area.

Further development of the model will include additional discretization around each injection port, and increased permeability near the canister wall.

Grid generation, model property, boundary and initial condition set-up and results processing was conducted using mView, software developed by INTERA with TOUGH2 model pre- and post-processing capabilities.

## SUMMARY AND FUTURE WORK

TOUGH2 was modified to model gas-transport through bentonite, incorporating potential coupled hydro-mechanical phenomena. Building on the initial application of the modified TOUGH2 code to the LASGIT experiment presented here, detailed models of the LASGIT experiment can be developed.

The next phase of modeling work is to evaluate hydraulic and gas test design with the TOUGH2 model. Test design evaluation will include a combination of deterministic modeling to iteratively obtain a sufficient response from each step of the test; probabilistic modeling which will assess the uncertainty of parameter values and the capability of the test of providing a suitable response over a range of parameter values; and inverse modeling to assess the non-uniqueness and possible low-confidence in parameter estimates. Probabilistic and inverse modeling with the modified TOUGH2 model will be accomplished within the paCalc framework. Developed by INTERA, paCalc is a performance assessment application with sampling and optimization utilities, with the capability of linking to any model executed through the command line.

Once LASGIT testing begins, the TOUGH2 model will be used to interpret test results and improve understanding of the gas migration through the bentonite buffer under repository conditions. As well, the modified TOUGH2 approach to gas-transport modeling will also be validated as a potential approach to be used in future safety assessments.

## ACKNOWLEDGMENT

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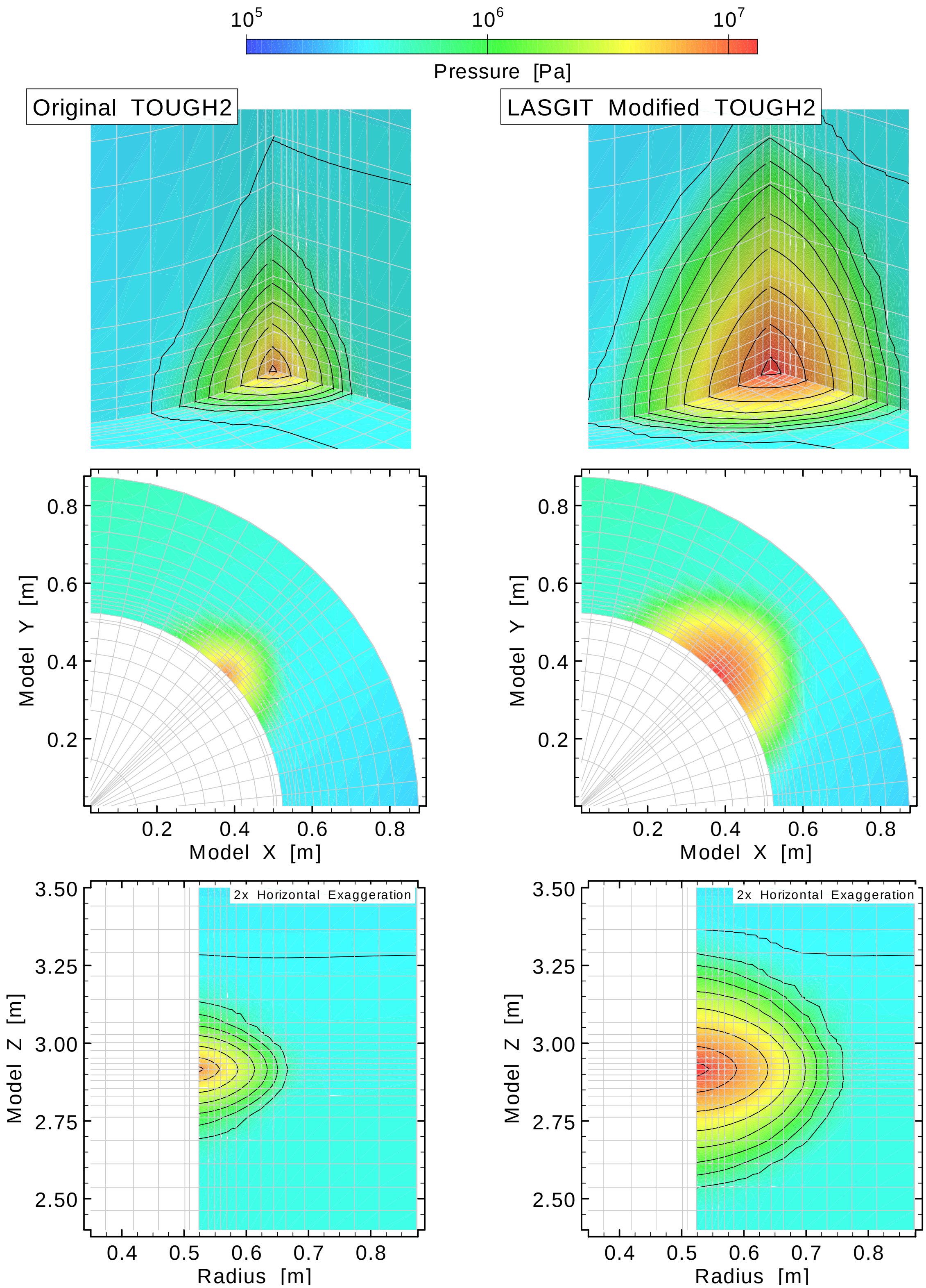


*Figure 5. Results of initial LASGIT model after 2 years of gas injection, shown (from top to bottom) in a 3D view, horizontal cross-section and vertical cross-section. The three plots on the left show results obtained using the original TOUGH2 code, and the three plots on the right show results obtained with the modified TOUGH2 code.*

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