Using TOUGH2 to Model the Coupled Effects of Gas Generation, Repository Consolidation, and Multiphase Brine and Gas Flow at the Waste Isolation Pilot Plant

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Introduction
The Waste Isolation Pilot Plant (WIPP) is a U.S. Department of Energy facility designed to demonstrate the safe underground disposal of transuranic waste. The WIPP repository lies within the Salado Formation, a thick sequence of bedded pure and impure halite with thin, laterally continuous interbeds of anhydrite. The underground waste storage area is designed to have eight waste disposal panels, each of which will contain seven waste disposal rooms. Each disposal room, approximately 4 m high, 10 m wide, and 91 m long, is to be filled with steel drums containing contact-handled (CH) transuranic (TRU) waste. Following waste emplacement, each room will be backfilled with crushed salt. Due to deviatoric stress introduced by excavation, the walls of the waste disposal rooms in the repository will deform over time, consolidating waste containers and salt backfill, thereby decreasing the void volume of the repository.

Gas may be generated from the emplaced waste by anoxic corrosion reactions between steel and brine, and by microbial degradation. Gas generation could produce elevated pressures within the disposal rooms. If repository pressures approach lithostatic, backstress on the room walls will force room expansion and/or Salado fracturing, mitigating further pressure increases. Elevated pressures could drive gas release from the repository and enhance contaminant movement towards regulatory boundaries. Gas pressure in the disposal rooms is strongly influenced not only by the gas-generation rate, but also by changes in gas-storage volume caused by creep closure and/or expansion of the rooms, and by gas release from the rooms into the surrounding rock. Long-term repository assessment must consider the processes of gas generation, room closure and expansion due to salt creep, and multiphase (brine and gas) fluid flow, as well as the complex coupling between these three processes.

Stone (1992) used the mechanical creep closure code SANCHO (Stone et al., 1985) to simulate the closure of a single, perfectly sealed disposal room filled with waste and backfill. SANCHO uses constitutive models to describe salt creep, waste consolidation, and backfill consolidation. Five different gas-generation rate histories were simulated (Figure 1a), differentiated by a rate multiplier, f, which ranged from 0.0 (no gas generation) to 1.0 (expected gas generation under brine-dominated conditions). The results of the SANCHO f-series simulations provide a relationship between gas generation, room closure (Figure 1b), and room pressure (Figure 1c) for a perfectly sealed room. Several methods for coupling this relationship with multiphase fluid flow into and out of a room were examined by Freeze et al. (in press a). Two of the methods are described below.

Model Development
TOUGH2 was employed to couple the processes of gas generation, room closure/consolidation, and multiphase brine and gas flow. Two empirically-based methods for approximating salt creep and room consolidation were implemented in TOUGH2: the pressure-time-porosity line interpolation approach and the fluid-phase-salt approach. Both approaches utilized links to the SANCHO f-series simulation results to calculate room-void-volume changes with time during a simulation.

The Salado Formation was conceptualized as a homogeneous halite containing single anhydrite interbeds above and below the disposal room (Figure 2). A single, isolated, half-width disposal room (with symmetry across the centerline assumed) was simulated. Each of the four regions (disposal room, halite, upper interbed, and lower interbed) in the fluid-flow continuum was defined by a different set of physical properties. The interbeds provide the preferred path for gas release from the room because of a low threshold (gas-entry) pressure and a high intrinsic permeability relative to the halite. Direct connections between interbed elements and elements on the edge of the disposal room were specified (Figure 2). These connections had large transmissivities, representative of fracture-like connections. Gas generation was simulated by placing a number of gas sources within the modeled disposal room.

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Pressure-Time-Porosity Line Interpolation Approach

The room porosity vs. time and room pressure vs. time results from the five SANCHO f-series simulations (Figures 1b and 1c, respectively) were used to calculate a set of three-dimensional pressure-time-porosity lines (functions). One pressure-time-porosity line corresponds to each of the five SANCHO simulations. At each TOUGH2/EOS8 time step, a room porosity value is obtained by linear interpolation between the two pressure-time-porosity lines which bound the current simulated time and room gas pressure conditions. The simulated room porosity is then adjusted to the value determined from the interpolation. With this pressure-time-porosity line interpolation process (also referred to as the pressure lines method), the SANCHO-simulated relationship between room porosity (closure), pressure, and time, was transferred to TOUGH2/EOS8 where it was simulated in conjunction with multiphase fluid flow.

Fluid-Phase-Salt Approach

The fluid-phase-salt approach uses the Darcy flow of a highly-viscous fluid phase to represent salt creep. To implement this approach, a three-phase, three-component equation-of-state module, EOS8 (brine, hydrogen, "dead" oil) was created by Karsten Pruess at Lawrence Berkeley Laboratories. The "dead" oil phase was used to represent "fluid" salt. In TOUGH2/EOS8, the flow properties of the fluid-salt phase are selected such that the flow of salt into the disposal room approximates room closure. The fluid-phase-salt approach requires a dual continuum conceptualization in which salt-phase flow is confined to a separate salt-flow continuum (Figure 3) to avoid interference with gas and brine flow. The salt-flow continuum contains only two regions: disposal room and halite matrix. Multiphase brine and gas flow is confined to the same fluid-flow continuum (Figure 2) used with the pressure lines method. The interbeds are not included in the salt-flow continuum because they are not considered to have a significant impact on the physical process of room closure due to salt creep. With this approach, only the disposal room is common to both continuums. As a result, any impact of salt flow on multiphase brine and gas flow occurs through the pressure relationships within the disposal room.

The theoretical relationship between fluid (salt) flow and salt deformation, which governs the fluid-phase-salt approach, assumes that a pressure-controlled backstress opposes creep. This relationship fails to account for the additional backstress opposing room closure that is caused by the consolidation of the room contents, and consequently, does not accurately predict room closure when there is significant room consolidation. To overcome this difficulty, a method to approximate the consolidation-induced backstress was implemented in TOUGH2/EOS8. Using an artificial boundary, the disposal room is divided into two regions (Figure 3). The salt-accessible room region, which is connected to the salt-flow continuum, initially contains all three phases (salt, gas, and brine). The salt-inaccessible room region, which is connected to the fluid-flow continuum, contains only gas and brine. Salt flow into the disposal room, which comes only from the salt-flow continuum, is restricted by the artificial boundary to the salt-accessible region. Brine inflow, which comes only from the fluid-flow continuum, flows into the salt-inaccessible region of the room. Brine and gas can flow across the artificial boundary, making the entire room void volume available to brine and gas. However, brine and gas release from the room goes only to the fluid-flow continuum, brine and gas are not permitted to flow into the salt-flow continuum.

The model geometry and gas generation scheme are designed so that a pressure gradient from the salt-accessible region to the salt-inaccessible region is maintained during room closure. The resulting flow of gas from the salt-accessible region to the salt-inaccessible region is limited by a flow restriction (low transmissivity) specified across the artificial boundary. This flow restriction results in increased pressurization of the salt-accessible region as salt flows in, which in turn produces increased resistance to salt inflow. The additional resistance to salt inflow is analogous to the additional backstress caused by consolidation of the waste and backfill.

A calibration process was undertaken with TOUGH2/EOS8 to determine the combination of parameters controlling (1) salt-phase flow (i.e., salt viscosity) and (2) gas flow across the artificial boundary (i.e., transmissivity), that produced the best match with room closure and room pressure history results from the SANCHO f-series simulations. With the calibrated parameters, the fluid-phase-salt method slightly underestimated room pressure at high gas-generation rates ($f \geq 0.6$) and slightly overestimated room pressure at low rates ($f \leq 0.2$). However, the method captured a wide range of room closure and pressure behavior ($f=0.0$ to 1.0) with a single set of calibrated parameters. Qualitatively, the additional resistance to closure is similar to the resistance to closure provided by the compression of the waste and backfill in that it is more significant when there is greater room closure.

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Simulation Results

Two sets of TOUGH2/EOS8 simulations are discussed here: (1) sealed-room closure (no fluid flow into/out of room); and (2) fully coupled flow and closure. Results from numerous other simulations are described in Freeze et al. (in press b).

Sealed-Room Closure

A sealed room simulation, similar to the SANCHO conceptualization in that there was no fluid flow in or out of the room, was performed with gas-generation rate history (Figure 3a) that was quite different from the SANCHO f-series rate histories (Figure 1a). This non-f-series rate history was selected because actual gas generation in the repository could be quite different from the f-series rate history. The non-f-series rate history had gas-generation rates that did not always decrease with time and the specified times for rate switches were different from the f-series simulations. The total mass of gas generated was the same as for the f=1.0 case.

Non-f-series simulation results for both closure coupling methods are shown in Figure 4. The two methods produced significantly different responses. Differences in the respective responses were particularly evident at 750 years, 1,050 years, and 1,200 years. At 750 years, following a decrease to zero gas generation, the rate of room expansion slowed with the fluid-phase-salt method (Figure 4b) and gas pressure in the room decreased (Figure 4c) in response to the continued room expansion. With the pressure lines method, room expansion immediately reversed at 750 years (Figure 4b) and room pressure continued to increase (Figure 4c), albeit at a slower rate than during the first 750 years. It is reasonable to assume that effect of a decrease to zero gas generation in the room would gradually impact salt creep behavior as the salt approached a new equilibrium with the room pressure and the room void volume. This gradual response was correctly predicted by the fluid-phase-salt method. The pressure lines method response at 750 years was an artifact of the structure of the pressure-time-porosity lines. In the SANCHO simulations used to create the pressure-time-porosity lines, room pressure was relatively constant between 550 and 1,050 years (Figure 1c). This pressure trend is evident in the non f-series pressure lines method response between 750 and 1,050 years (Figure 4c).

At 1,050 years the pressure lines method predicted a change in room closure and room pressure response despite the fact that there was no change in gas-generation rate. The declining room pressure again appears to be an artifact of the SANCHO simulations, in which gas generation ended at 1,050 years. At 1,200 years, following an increase in gas-generation rate, the rate of room expansion increased with both methods. However, the room gas pressure increased for the fluid-phase-salt method and decreased for the pressure lines method. It is reasonable to assume that the resumption of gas-generation would increase room pressure which, in turn, would increase the rate of room expansion. However, the pressure lines method response again appears to be adversely influenced by the structure of the SANCHO-generated pressure lines.

These non f-series rate history simulations demonstrate that the use of the pressure-time-porosity line interpolation method skews results towards the SANCHO f-series results because time is used as one of the interpolation axes. The time axis indirectly contains information about the history of salt creep and backstress on the room walls. Thus, the backstress and room closure history described by each pressure-time-porosity line are specific to the SANCHO-simulated gas-generation rate history.

Coupled Flow and Closure

To examine the behavior of the fluid-phase-salt and pressure-time-porosity line interpolation methods under coupled flow and closure conditions, simulations were performed with the f=1.0 gas-generation rate history. Simulations were extended to 10,000 years to allow the comparison to encompass the complete period of gas release and migration. Simulation results for both coupling methods are shown in Figure 5. System behavior differs from the sealed room simulations in that after gas generation ends at 1,050 years, gas is being expelled from the room (Figure 5c) and the room void volume starts to decline again (re-closure of the room) (Figure 5a). As with the sealed room simulations, the two different coupling methods produced differences in simulation results. The differences are attributable to: (1) room closure calibration effects with the fluid-phase-salt method; and (2) different room conceptualizations for coupling of room closure with multiphase flow.

As noted previously, the fluid-phase-salt calibration process resulted in a slight underestimation of room pressure for high gas-generation rates and a slight overestimation of room pressure for low gas-generation rates. For the f=1.0 rate history, this calibration effect caused the fluid-phase-salt method to produce

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lower room pressures than the pressure lines method (Figure 5b). The lower room pressure translated to less gas expulsion (Figure 5c) and a larger room void volume (Figure 5a).

Differences between the coupling methods are also due to the different ways each method conceptualizes the disposal room. Multiphase flow is controlled by the gas- and brine-phase saturations within the room. These phase saturations impact both brine and gas expulsion through relative permeability relationships. For example, in simulations using the fluid-phase-salt method, brine inflow is typically confined to the small salt-inaccessible room region, producing high brine saturations and high relative permeability to brine. As a result, the fluid-phase-salt method produces more brine expulsion than does the pressure lines method. Additional simulations have shown that brine and gas expulsion under both the fluid-phase-salt and pressure lines methods is similar to brine expulsion from a fixed room, which is free of any closure coupling effects.

Conclusions
Two methods for coupling gas generation, disposal room closure/consolidation, and multiphase brine and gas flow at WIPP were examined using the TOUGH2/EOS8 code. Both methods incorporated links to the SANCHO f-series simulations (Stone, 1992), which coupled gas-generation rate with the mechanical creep closure of a room.

The pressure-time-porosity line interpolation method was useful for simulations with low gas-generation rates ($f \leq 0.2$) or with gas-generation rate histories similar to the SANCHO f-series. However, this method showed a tendency to introduce errors when the simulated gas-generation rate history involved high rates ($f > 0.4$) in a significantly different sequence than the f-series rate histories from which the pressure-time-porosity lines were derived. Under these conditions, the pressure lines method results tend to be skewed towards the SANCHO results.

The fluid-phase-salt method worked reasonably well under both f-series and non-f-series gas-generation rate histories. The dual room region conceptualization appeared not to adversely impact brine flow or gas release to the Salado Formation. The fluid-phase-salt method was calibrated in a manner such that it was accurate over the range of SANCHO f-series rate histories. It is uncertain whether the empirical calibration relationships can be extrapolated to gas-generation and room-closure conditions that are significantly outside the SANCHO f-series conditions.

The fluid-phase-salt method is thought to be a more reliable indicator of system behavior because it treats salt deformation as a viscous process and has a theoretical basis. However, it is a complex method that requires detailed calibration and may be difficult to implement in more complex repository geometries. The pressure lines method is thought to be less reliable due to the potential skewing of results towards SANCHO f-series results. However, due to its relative simplicity, the pressure lines method is easier to implement in multiphase flow codes, and pressure lines simulations run significantly faster (10 to 20 times) than fluid-phase-salt simulations.

References
Freeze, G.A., Larson, K.W., and P.B. Davies. in press a. *A Summary of Methods for Approximating Salt Creep and Disposal Room Closure in Numerical Models of Multiphase Flow*. SAND94-0251. Albuquerque, NM: Sandia National Laboratories.

Freeze, G.A., Larson, K.W., and P.B. Davies. in press b. *Coupled Multiphase Flow and Closure Analysis of Repository Response to Waste-Generated Gas at the Waste Isolation Pilot Plant (WIPP)*. SAND93-1986. Albuquerque, NM: Sandia National Laboratories.

Stone, C.M. 1992. "Creep Closure Behavior of Waste Disposal Rooms in Bedded Salt Due to Gas Generation Produced by Several Alternatives of the Engineered Alternatives Task Force," memorandum to B.M. Butcher (October 6). Albuquerque, NM: Sandia National Laboratories.

Stone, C.M., R.D. Krieg, and Z.E. Beisinger. 1985. *SANCHO, A Finite Element Computer Program for the Quasistatic, Large Deformation, Inelastic Response of Two-Dimensional Solids*. SAND84-2618. Albuquerque, NM: Sandia National Laboratories.
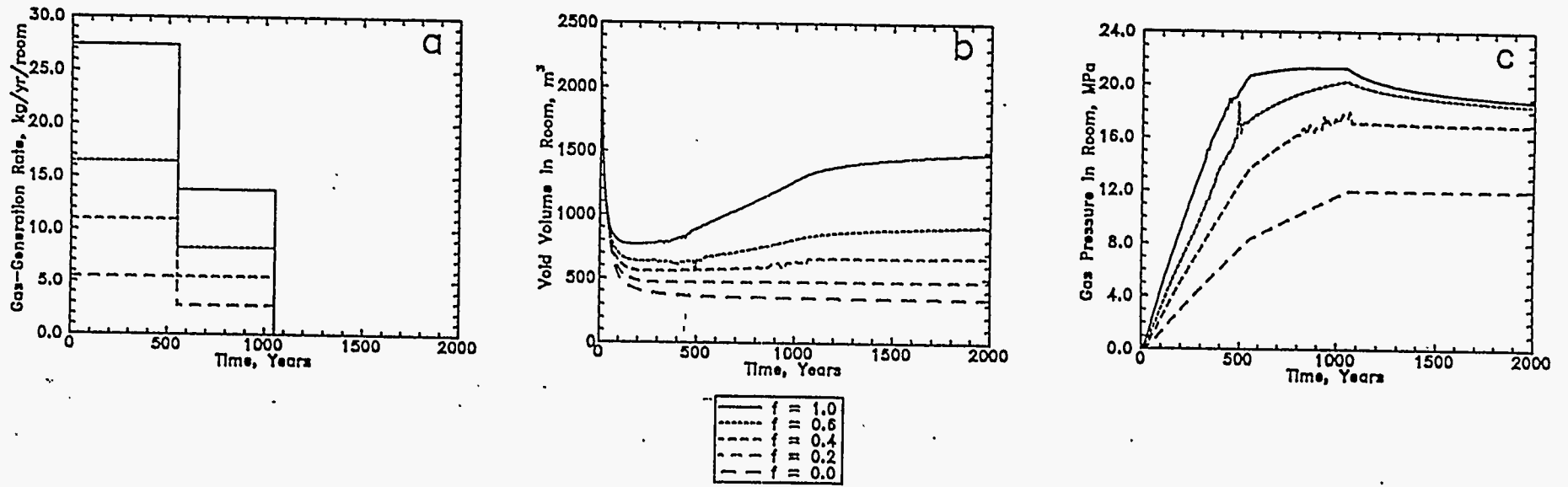
Figure 1. Gas-generation rate histories and SANCHO simulation results from Stone (1992).
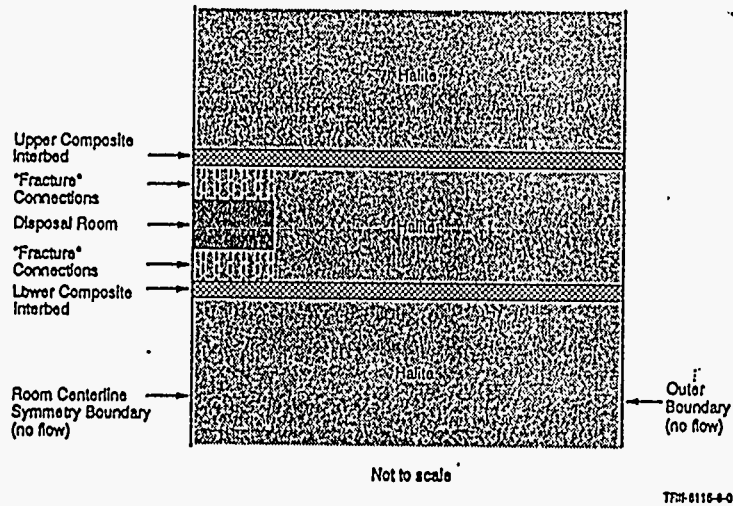

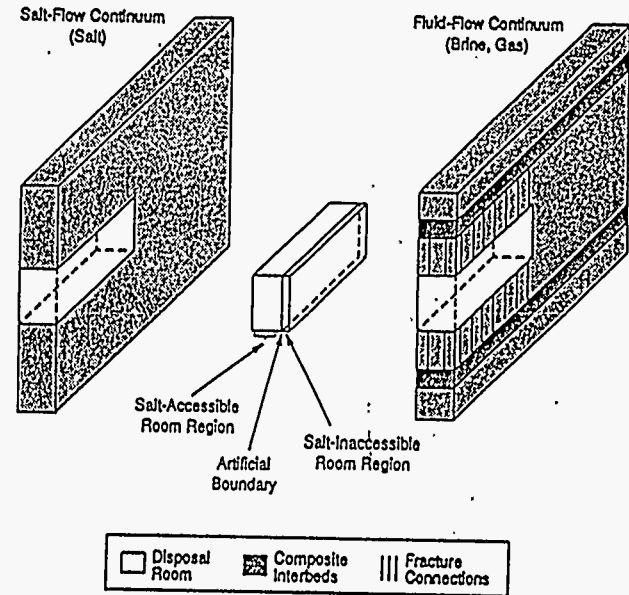Figure 2. Schematic representation of the fluid-flow continuum.

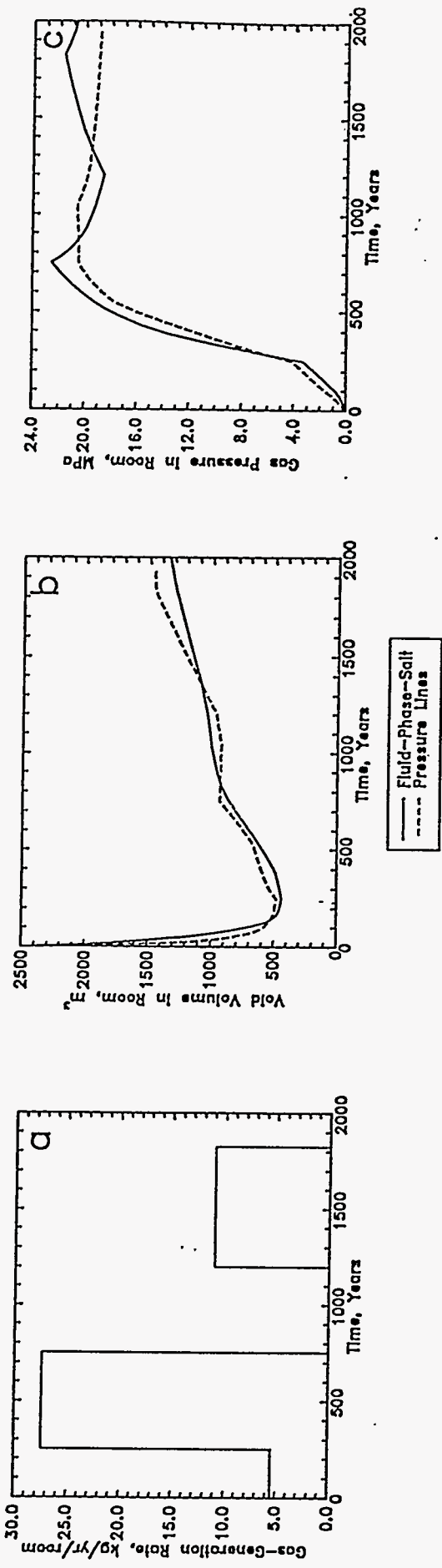Figure 3. System conceptualization with the fluid-phase-salt method.

Figure 4. Gas-generation rate history and simulation results from TOUGH2/EOS8 sealed room simulation.
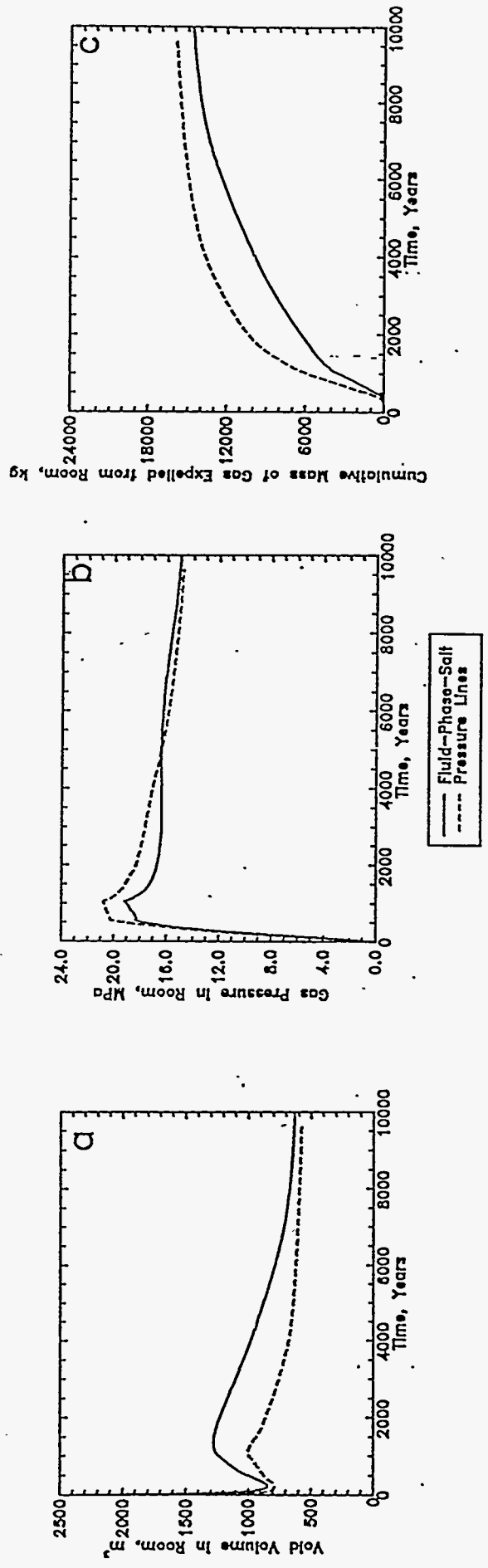

Figure 5. Simulation results from TOUGH2/EOS8 fully coupled flow and closure simulation with an f=1.0 gas-generation rate history.