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**Sandia National Laboratories  
Waste Isolation Pilot Plant**

**Analysis Plan for a Preliminary Comparison of BRAGFLO and  
PorSalsa Using a Simplified WIPP Test Problem**

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## 1. INTRODUCTION AND OBJECTIVES

This analysis plan directs a preliminary comparison of output of the numerical codes BRAGFLO and PorSalsa for WIPP-related simulations. In this study a simplified WIPP problem will be run with both codes and results compared.

BRAGFLO is the main numerical reservoir flow code used for performance assessment (PA) of the Waste Isolation Pilot Plant (WIPP) repository. It is a finite difference, cell centered, two-phase flow code used specifically to study flow behavior in the vicinity of the repository (Near Field). The code includes WIPP-specific sub-models including: closure of the repository due to salt creep; gas generation and brine consumption resulting from corrosion and biodegradation of waste; brine consumption due to hydration of MgO backfill; pressure-induced fracturing. The code also has the capability of time dependent material properties. BRAGFLO has a choice of solvers but primarily an LU direct solver has been used for WIPP compliance and programmatic calculations. A Conjugate Gradient Solver (CGS) has been used for undisturbed (no borehole intrusion) 3-D calculations. The combined two-phase flow and the WIPP-related processes is a complex subsurface flow problem. To date limitations with the LU solver and lack of availability of dynamic memory allocation have resulted in the use of a 2-D grid with a limited number of grid blocks for WIPP PA calculations.

PorSalsa is a finite element, thermal, two-phase flow and transport code written for massively parallel implementation (Martinez et al., 1997). The finite element discretization allows the use of unstructured grid. These and other features of the code are ideal for large-scale 3-D complex simulations and for problems that require a high resolution (refined grid).

The purpose of this study is to evaluate output of BRAGFLO WIPP-related calculations by comparing results with that of PorSalsa. To do a full-scale comparison of output, the above stated WIPP-specific sub-models would have to be coded in PorSalsa. However, such a comparison and associated code modifications is outside the scope of this study. This study will use a WIPP-type test problem with a simplified representation of the sub-models as described in Section 2, and only apply minor code modifications in PorSalsa.

Specifically, the objectives are:

- to evaluate output of BRAGFLO relative to PorSalsa using a simplified WIPP-type test problem,
- to investigate the possibility of using PorSalsa in WIPP PA programmatic calculations that require large-scale or high resolution modeling, and
- to investigate other areas where PorSalsa can supplement BRAGFLO in WIPP PA.

## 2. APPROACH

### 2.1 Description of test problem

A vector from the 1999 MgO hydration sensitivity study (WIPP PA, 1999), which is a subset of the undisturbed Scenario S1, has been selected for the test problem. The vector uses a three-dimensional grid representing the WIPP repository and near field. Because the WIPP vertical 2-D grid accounts for three-dimensional effects (radial flaring) that may not be reproducible in PorSalsa, use of a full 3-D grid was considered more appropriate. The choice of the 3-D grid will also assist in evaluating the efficiency of PorSalsa in solving larger WIPP-type problems in comparison with BRAGFLO.

Vector Information:

Replicate = 1  
Scenario = 1 (undisturbed 3-D)  
Vector = 97

Total run time = 10,000 years

Geometry, formation and fluid properties, treatment of sub-models, well treatment and material reset information together with the code modifications that will be made in PorSalsa are given in Table 1. Fig. 1 shows a horizontal cross-section representing repository location in Layer 4 (reproduced from the M99 study, WIPP PA, 1999). The 3-D grid, which was used for undisturbed performance calculations, assumes symmetry about a north-south line through the middle of the repository, so only the east half of the repository is modeled. Thus, only half of the Northern Equivalent Panel (NEP) and Southern Equivalent Panel (SEP) were included in the 3-D mesh.

The 3-D grid incorporates the following features:

- Plane of symmetry north-south at midpoint of central panels;
- 4 full panels + 2 half panels (North and South Equivalent Panels);
- Room-scale discretization in repository;
- Stratigraphic dip;
- Extends laterally beyond the land withdrawal boundary;
- Extends vertically about 50 m above and below the repository horizon;
- Some operations region and north end detail, but no shaft.

Table 1: Description of computational requirements for a simplified WIPP-type test problem

<b>Item</b>	<b>Description and assumptions</b>
Grid	The grid includes 6300 gridblocks with $NX = 25$ , $NY = 36$ and $NZ$ (vertical) = 7. $NX$ , $NY$ and $NZ$ are number of grid blocks in the X, Y and Z (vertical) directions, respectively. The grid thicknesses $\Delta X$ , $\Delta Y$ and $\Delta Z$ as well as gridblock elevations with the $1^\circ$ dip, will be as in the M99 study.
Rock properties	The test problem will have 17 rock types (or regions). For each region rock properties permeability, porosity, compressibility and characteristic curve model will be assigned. Gridblocks will be associated with a specific region using material type grid maps. For this undisturbed scenario problem, there will be only two maps: the first at start time (-5 years) and the second at time 0 years. The second map is required to re-assign rock properties to the repository after it has been filled with waste.
Fluid properties	For WIPP PA analysis, the gas phase is represented by hydrogen gas. Density of $H_2$ is obtained using the Soave-Redlich-Kwong (SRK) real gas equation of state given in Section 2.4. For viscosity of $H_2$ gas a constant value of $8.93389 \times 10^{-6}$ [Pa s] is used. The liquid phase is represented by brine. Density of brine is equal to density of water multiplied by 1.22 (specific gravity of brine). Viscosity of brine is kept constant at $2.1 \times 10^{-3}$ [Pa s]. Code changes will be made in PorSalsa to include these properties.
Characteristic curves	Equations representing modified Brooks-Corey curves as given in Section 2.3 will be used. In this model the effective saturation is modified to include residual gas saturation. Capillary pressure and relative permeability of gas are then calculated using the modified effective saturation. For capillary pressure the modified Brooks-Corey model will be used with and without an upper limit.
Gas generation and brine consumption	Since the chemical reaction models that are used for WIPP calculations are not available in PorSalsa, a simplification that avoids code modification would be the use of sink/source terms. This was the case with TOUGH28W (Christian-Frear and Webb, 1995). Thus, a constant gas injection will be applied to the repository area to represent gas generation. The amount of gas injection is given in Section 2.2. As described in Section 2.2 brine consumption will not be included.

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Creep closure	To avoid code modifications for creep closure, use final waste porosity as a constant value. In most cases waste porosity drops from its initial value to its minimum value in a few hundred years. Thus, modeling creep closure may be avoided if the minimum porosity is used as a simplification.
Anhydrite fracturing	Since Porsalsa does not have the model for pressure-induced anhydrite fracturing, this functionality will not be used in BRAGFLO.
Well treatment	For disturbed scenarios an intrusion borehole is included in the grid. The selected test problem is for undisturbed scenario. Well treatment will be used for gas injection.
Reset properties	PorSalsa does not allow resetting of material properties at pre-determined times (as is done in BRAGFLO). This may be accomplished by restarting the code at times of material reset. PorSalsa does have restart capabilities. For this test problem there will be one resetting of material properties and initial conditions for pressure and saturation in the waste area at time 0 years.

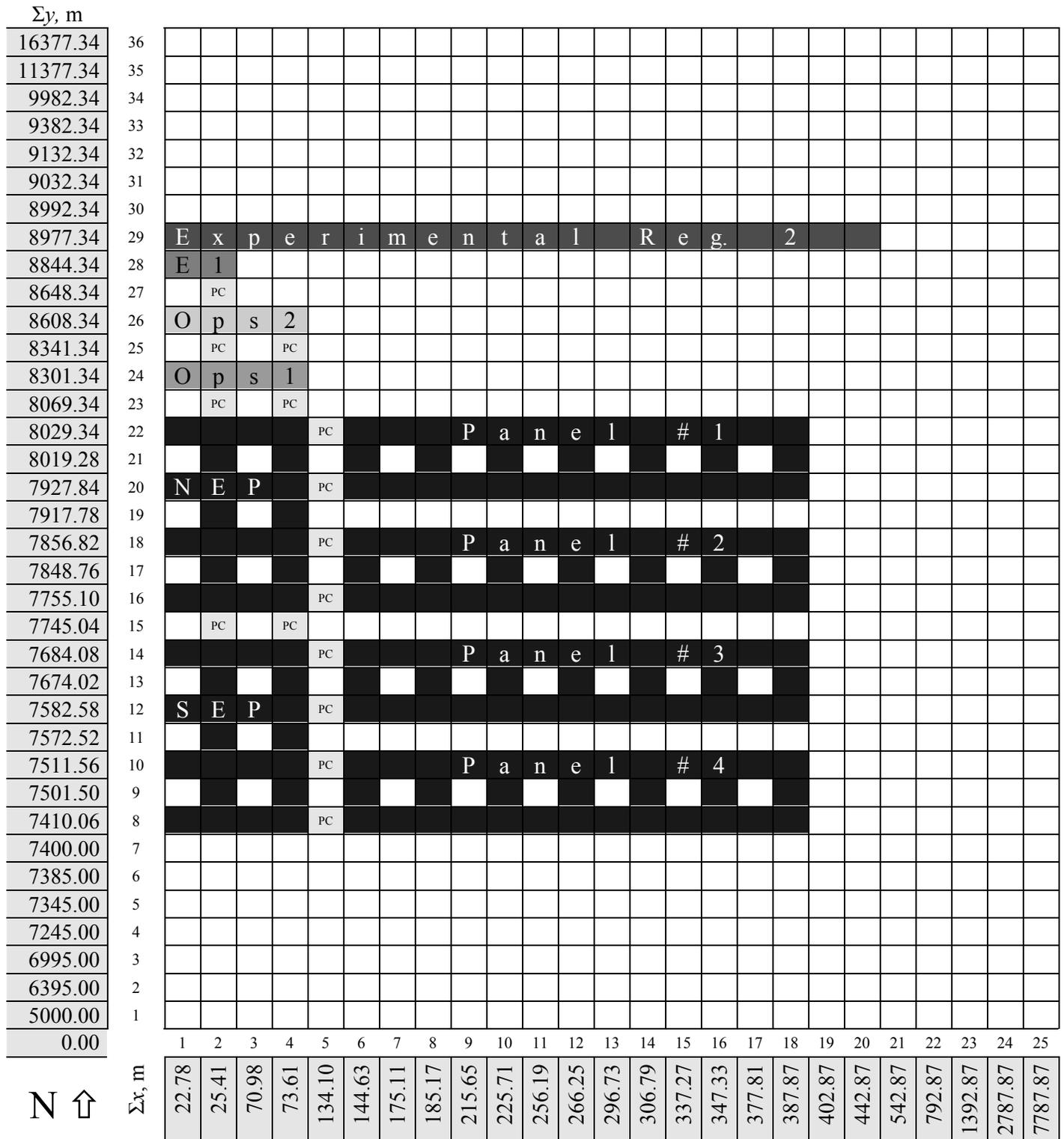


Fig.1: 3D BRAGFLO grid used in M99 Scenario S1, showing repository location in Layer 4. Axes indicate logical grid block numbers: (I,J,4) (from the M99 study, WIPP PA, 1999) (below). NEP and SEP represent Northern Equivalent Panel and Southern Equivalent Panel, respectively.

## 2.2 Sink/Source Terms

PorSalsa does not currently include the chemical reaction models (i.e. corrosion, biodegradation and MgO hydration models) that are part of WIPP performance assessment calculations. For this study the corrosion and biodegradation models will be simplified to avoid code modifications in PorSalsa. Gas generation due to corrosion and biodegradation will be modeled using constant gas injection. MgO hydration will be turned off.

To determine the amount of gas injection rate that will be used BRAGFLO was rerun with the selected vector (Scenario 1, Vector 97), with gas generation rate as an output. For this run creep closure, anhydrite fracturing and MgO hydration were turned off. The selected vector does not include biodegradation, and thus the gas generation is due to corrosion only. The BRAGFLO output includes gas generation rate for each grid block in the waste area. The rates are summed over each grid block representing a panel. The resulting gas generation rate for each represented panel is shown in Fig. 2. The pressure and gas saturation in a selected grid block (Element 5970:  $i = 7$ ,  $j = 14$ ,  $k = 4$ ) are as shown in Figs. 3 and 4 respectively.

For this study the time varying gas generation rates will be replaced with constant injection rates. To capture the total cumulative gas generation for each panel with constant well injection rates, the gas generation rates in Fig. 2 were integrated over time. The calculated values are given in Table 2 together with the volume of each panel. The average panel gas generation rate will then be applied to each grid block in the panel in direct proportion to grid block volume. To simplify the test problem brine consumption will not be modeled.

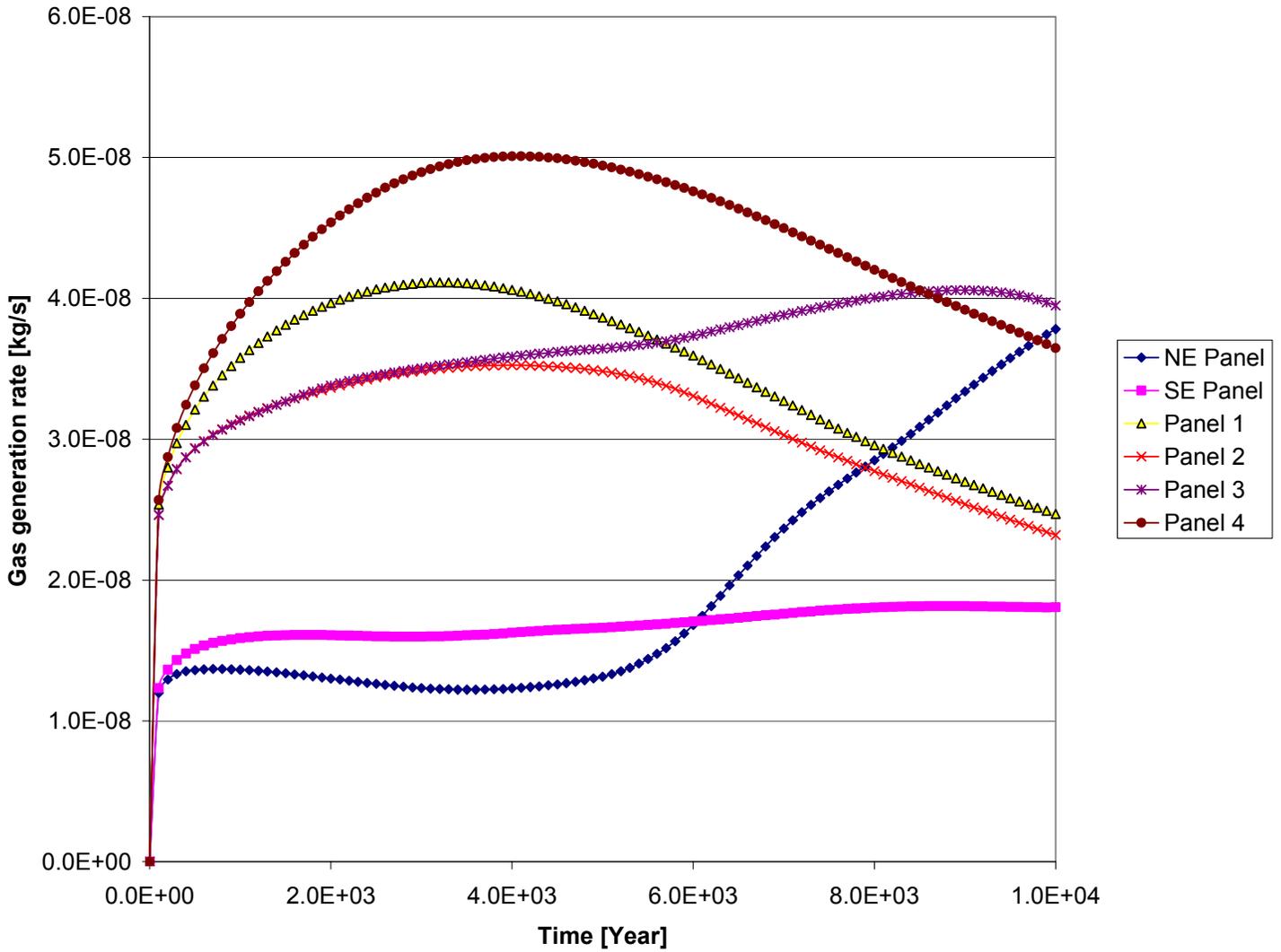


Fig.2: Average panel gas generation rate for selected vector (Scenario 1, Vector 97) from M99 study.

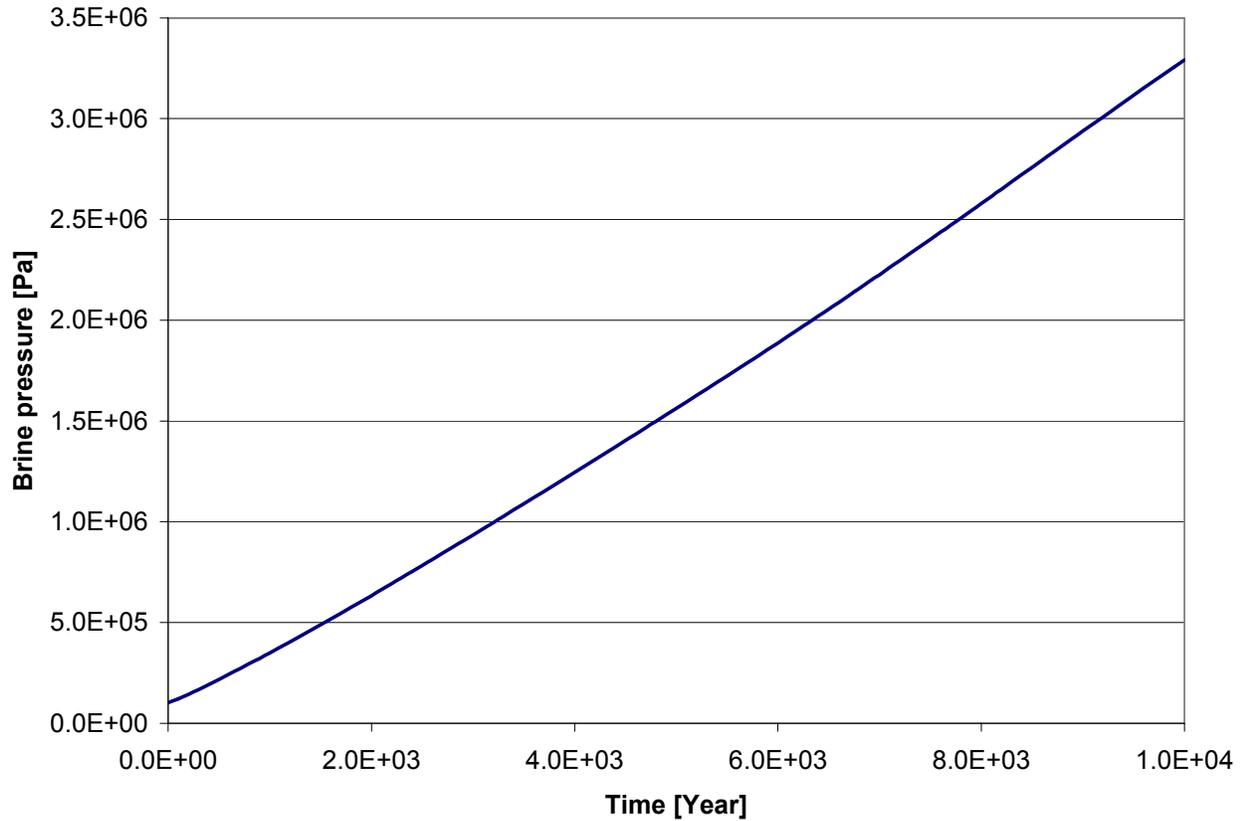


Fig.3: Brine pressure in a selected waste panel grid block (Element 5970,  $i = 7$ ,  $j = 14$ ,  $k = 4$ ) (Scenario 1, Vector 97 from M99 study with creep closure, MgO hydration and anhydrite fracturing turned off).

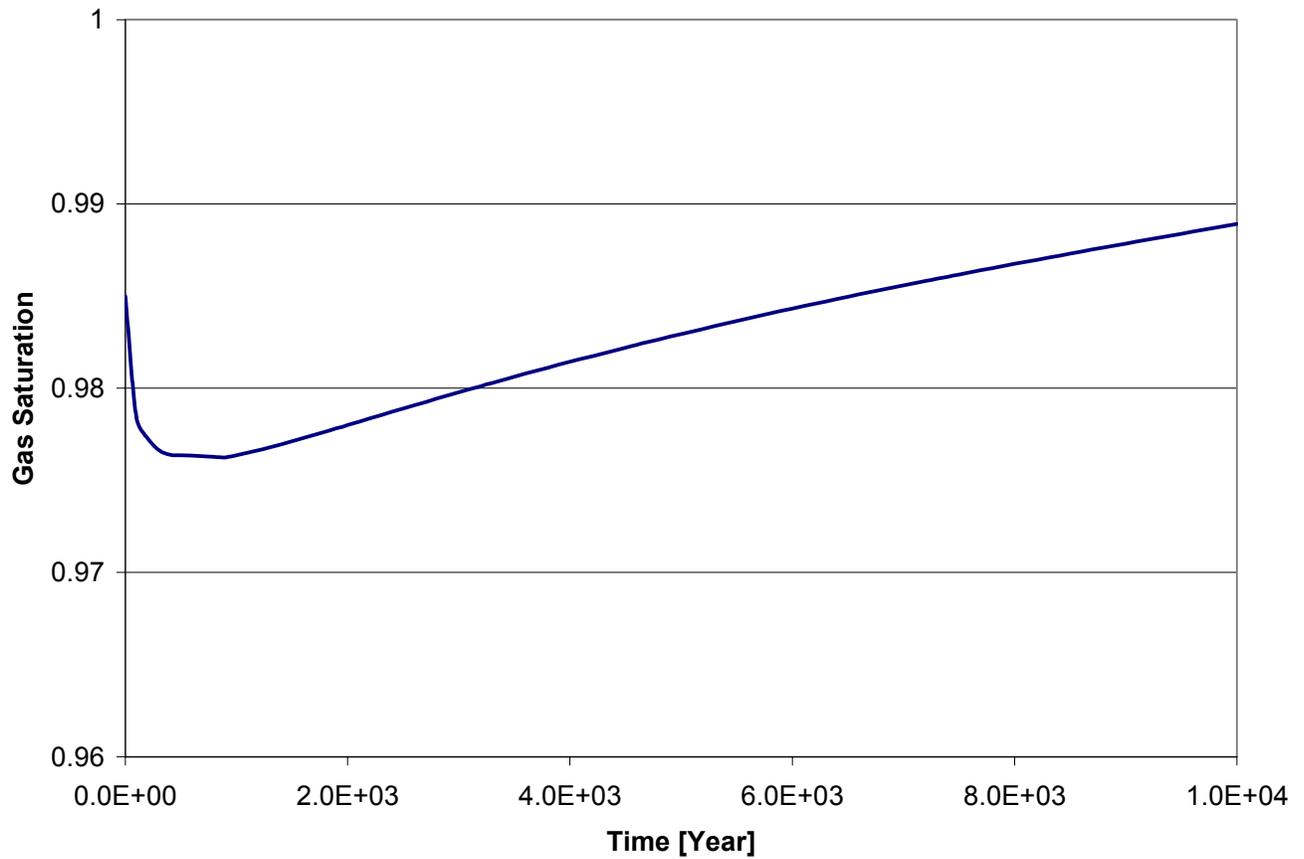


Fig.4: Gas saturation in a selected grid block (Element 5970,  $i = 7, j = 14, k = 4$ ) (Scenario 1, Vector 97 from M99 study with creep closure, MgO hydration and anhydrite fracturing turned off).

Table 2: Constant gas generation rate for each panel to be used as injection rate in the simplified WIPP-type test problem

Panel	Constant gas rate [kg/s]	Panel volume [m <sup>3</sup> ]
North Equivalent Panel	$1.912759 \times 10^{-8}$	$1.681906 \times 10^4$
South Equivalent Panel	$1.668324 \times 10^{-8}$	$1.681906 \times 10^4$
Panel # 1	$3.461631 \times 10^{-8}$	$4.570866 \times 10^4$
Panel # 2	$3.102832 \times 10^{-8}$	$4.570866 \times 10^4$
Panel # 3	$3.612200 \times 10^{-8}$	$4.570866 \times 10^4$
Panel # 4	$4.379232 \times 10^{-8}$	$4.570866 \times 10^4$

### 2.3 Characteristic curves

Relative permeability and capillary pressure will be computed using a modified version of the Brooks-Corey empirical relations (Brooks and Corey, 1964). The modified Brooks-Corey model includes the effects of residual gas saturation. The relevant equations are as shown below.

The modified Brooks-Corey model determines capillary pressure and relative permeabilities from:

Capillary Pressure:

$$P_c = P_t / S_{e_2}^{1/\lambda} \quad (1)$$

Relative Permeabilities:

$$k_{rw} = S_{e_1}^{(2+3\lambda)/\lambda} \quad (2)$$

$$k_{rg} = (1 - S_{e_2})^2 (1 - S_{e_2}^{(2+\lambda)/\lambda}) \quad (3)$$

The effective brine saturation  $S_{e_1}$  is defined as

$$S_{e_1} = \frac{S_w - S_{wr}}{1 - S_{wr}} \quad (4)$$

and the modified effective brine saturation  $S_{e_2}$  is defined as

$$S_{e_2} = \frac{S_w - S_{wr}}{1 - S_{gr} - S_{wr}}. \quad (5)$$

where  $P_t$  is threshold pressure and  $\lambda$  is pore size distribution parameter. Note that if this option is used with  $P_t = 0$ , then  $P_c$  is identically zero.

The modified Brooks-Corey model includes residual gas saturation in the calculation of the modified effective saturation ( $S_{e_2}$ ) for the gas phase relative permeability and the capillary pressure. Thus, the relative permeability of water is as in the original Brooks-Corey model.

## 2.4 Gas Density

The following describes the gas density function used in BRAGFLO. Other fluid properties are as described in Table 1. Although the gas density equations are for a mixture of gases, in the test problem the gas phase will be represented by hydrogen only (i.e. one component).

The density of gas is evaluated using the real gas equation of state:

$$\rho_g = \frac{(MW)_g P_g}{ZRT} \quad (6)$$

where  $Z$  = compressibility factor  
 $(MW)_g$  = gas phase molecular weight  
 $R$  = universal gas constant

For the compressibility factor (which defines the non-ideality of a gas) the Soave-Redlich-Kwong (SRK) (1949 and 1972) cubic equation of state was used:

$$Z^3 - Z^2 + (A^* - B^* - B^{*2})Z - A^*B^* = 0 \quad (7)$$

where

$$A^* = \frac{a_m P_g}{R^2 T^2} \quad (8)$$

$$B^* = \frac{b_m P_g}{RT} \quad (9)$$

$a_m$  and  $b_m$  are gas mixture parameters defined by the mixing rules for cubic equations:

$$a_m = \sum_i \sum_j y_i y_j (a_i a_j)^{1/2} (1 - k_{ij}) \quad (10)$$

$$b_m = \sum_i y_i b_i \quad (11)$$

where  $k_{ij}$  is the binary interaction coefficient. Tabulated values of  $k_{ij}$  for the SRK equations of state can be found in Reid et al. (1987, P. 83).  $a_i$  and  $b_i$  are pure component parameters given by:

$$a_i = \frac{0.42748 R^2 T_{crit}^2}{P_{crit}} [1 + 0.48(1 - T_r^{1/2})]^2 \quad (12)$$

$$b_i = \frac{0.08664 R T_{crit}}{P_{crit}} \quad (13)$$

where  $T_{crit}$  and  $P_{crit}$  are component critical temperature and pressure respectively.

### 3. SOFTWARE LIST

The numerical codes that will be used for the test are BRAGFLO version 4.40 and a modified PorSalsa that includes the necessary code changes as described in Table 1.

### 4. TASKS

Teklu Hadgu and Alex Treadway will coordinate analysis and documentation. Mehdi Eliassi will prepare input, run and prepare required output of PorSalsa. Mario Martinez will make necessary code changes in PorSalsa and assist Mehdi Eliassi in running PorSalsa. Mario Martinez will also provide technical support. Jim Bean will help in setting BRAGFLO input and output. Teklu Hadgu will make BRAGFLO runs and prepare output. The technical, QA and management reviewers will be Polly Hopkins, Mario Chavez and Kathryn Knowles, respectively. Estimated completion date of this study is September 1, 2001. Table 3 shows the work schedule.

Table 3: Estimate of work schedule

Task #	Task Description	Responsible Individual(s)	Deliverable(s)	Due Date
1	PorSalsa code modifications	Mario Martinez	Memo	5-31-01
2	Submit necessary information and data to run PorSalsa	Teklu Hadgu, Alex Treadway and Jim Bean	Data to Mehdi Eliassi	6-8-01
3	Set-up grid generation, material properties, initial conditions for PorSalsa	Mehdi Eliassi, Mario Martinez	PorSalsa input	6-15-01
4	Run test case on PorSalsa and BRAGFLO	Mehdi Eliassi, Mario Martinez, Teklu Hadgu	PorSalsa and BRAGFLO output	8-15-01
5	Plot results on Mustafa and other graphics packages	Mehdi Eliassi, Alex Treadway, Mario Martinez, Teklu Hadgu	Graphs to be used in report	8-24-01
6	Analyze and document results	Teklu Hadgu, Alex Treadway, Mehdi Eliassi	Analysis report	9-03-01

## 5. SPECIAL CONSIDERATIONS

No special considerations have been identified for this analysis.

## 6. APPLICABLE PROCEDURES

Analyses will be conducted in accordance with the quality assurance (QA) procedures listed below.

*Training:* Training will be performed in accordance with the requirements in NP 2-1, Qualification and Training.

*Parameter Development and Database Management:* Data used in this study was derived from the 1999 MgO hydration sensitivity study (WIPP PA, 1999), and not sampled directly from the parameter database.

*Computer Codes:* BRAGFLO 4.40 was qualified in accordance with NP 19-1 for single use. The platform on which BRAGFLO will be run is the Compaq Alpha, OpenVMS AXP, version 7.2. PorSalsa will be run on an Intel Pentium 2 Cluster with 100 Megabit switch Ethernet currently running in Red Hat 6.1 Linux. A user's manual for PorSalsa will be provided.

*Analysis and Documentation:* Documentation will meet the applicable requirements in NP 9-1.

*Reviews:* Reviews will be conducted and documented in accordance with NP 6-1 and NP 9-1, as appropriate.

## 7. REFERENCES

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