Development of Three-Dimensional Models for WIPP Performance Assessment Using PFLOTRAN - 15073

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ABSTRACT

The Waste Isolation Pilot Plant (WIPP), located in southeastern New Mexico, has been developed by the U.S. Department of Energy (DOE) for the deep geologic disposal of transuranic (TRU) waste. WIPP performance assessment (PA) calculations estimate the probability and consequence of potential radionuclide releases from the repository to the accessible environment for a regulatory period of 10,000 years after facility closure. To date, WIPP PA calculations have employed multiple 2D numerical models requiring simplification of the mesh and processes. Introducing 3D numerical models within WIPP PA enables increasingly realistic representations of the WIPP subsurface domain and improved flexibility for incorporating relevant features. Furthermore, the increased computing capacity afforded by modern hardware architectures enables this 3D modeling. Modeling in 3D will be more flexible because less homogenization is required and better accuracy of the results can be obtained by making fewer assumptions and/or simplifications. The use of PFLOTRAN, a state-of-art massively parallel subsurface flow and reactive transport code, will enable this 3D modeling, and eliminate the need for multiple related, but decoupled 2D models. However, there are capabilities that PFLOTRAN must be demonstrated in order to fulfill requirements for WIPP PA.

INTRODUCTION

The Waste Isolation Pilot Plant (WIPP) is a mined underground facility operated by the U.S Department of Energy (DOE) to dispose transuranic (TRU) waste in a bedded salt formation in southeastern New Mexico. The U.S. Environmental Protection Agency (EPA) regulates the WIPP according to the environmental radiation protection standards for management (Subpart A) and disposal (Subparts B and C) of spent nuclear fuel and high-level and transuranic radioactive wastes set forth in Title 40 of the Code of Federal Regulations, Part 191 (40 CFR 191). The DOE demonstrates compliance with the containment requirements according to the certification and recertification criteria in Title 40 of the Code of Federal Regulations, Part 194 (40 CFR 194) by means of performance assessment (PA) calculations carried out by Sandia National Laboratories. WIPP PA calculations estimate the probability and consequences of potential radionuclide releases from the repository to the accessible environment for a regulatory period of 10,000 years after facility closure. Although computing technology has made significant advancement since the first PA calculations were concluded in the early 1990s, there has not been a substantial improvement in hardware and software used for WIPP PA calculations during the same years.

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The current WIPP PA uses a 2D immiscible multi-phase (air and brine) porous media flow simulation of the repository and surrounding rock formations using BRAGFLO. Introducing a 3D numerical model with increasingly realistic representations of the WIPP subsurface domain and improved flexibility for relevant features will ensure that the previous conservative approximations were valid and will provide more capacity for future development of WIPP PA simulations. We illustrate PFLOTRAN capabilities, discuss its ability to enhance PA, and address additional capabilities needed to ensure it meets PA requirements.

PFLOTRAN CAPABILITIES AND ADVANTAGES

Parallel Computing Capability

PFLOTRAN's ability to employ massively-parallel computing to solve scientific problems is one of the main reasons it was chosen for future WIPP PA. PFLOTRAN was developed with high-performance computing (HPC) in mind through DOE's SciDAC-II program. The code is founded upon the open-source Portable, Extensible Toolkit for Scientific Computation (PETSc) framework[1] and has been used to solve subsurface reactive multiphase flow and transport problems with up to 2 billion degrees of freedom on clusters with up to 265,000 processor cores on state of the art computing hardware.[2] PFLOTRAN's ability to efficiently utilize HPC will enable detailed 3D discretization of the WIPP domain. Parallel computing has been used in WIPP PA, where individual simulations (realizations) were run on separate processor cores. In the future, domain decomposition will be employed to distribute a single realization across multiple processor cores, enabling the solution of larger problems in less time.

Mesh in 3D

PFLOTRAN solves reactive transport and subsurface flow on either structured or unstructured grids via the finite volume method. A structured mesh can be generated internally by PFLOTRAN, while an unstructured mesh can be imported from an external mesh generation program such as Cubit developed by Sandia National Laboratories. PFLOTRAN can utilize hexahedron, tetrahedron, wedge, and pyramid mesh elements.

The current WIPP PA porous media flow simulation domain is a cross-section of the WIPP from north to south that stretches 46 km across and 1km tall. This mesh is only 68 by 33 elements, therefore elements range from 27.5cm to 12 km in size. Fig. 1. illustrates the discretization and zonation of parameters used in the WIPP PA BRAGFLO simulation. The current WIPP PA also employs a flaring grid, which simplifies calculation by representing 3D phenomena within a 2D grid. However, this is a further simplification. PFLOTRAN will employ HPC to accommodate the more accurate 3D mesh.

Flexibility of Database

PFLOTRAN leverages the open-source HDF5 (hierarchical data format) library to collectively and independently read and write data in parallel to a binary formatted file.[3] HDF5 is efficient and provides significant flexibility in the variety of data that can be stored. PFLOTRAN can extract realization-dependent information automatically from a database file stored in HDF5.

This information includes material properties, zonation of materials, specification of initial and boundary conditions, etc. PFLOTRAN output written in HDF5 is compatible with open-source visualization tools such as VisIt and Paraview for rendering 3D images and animations.

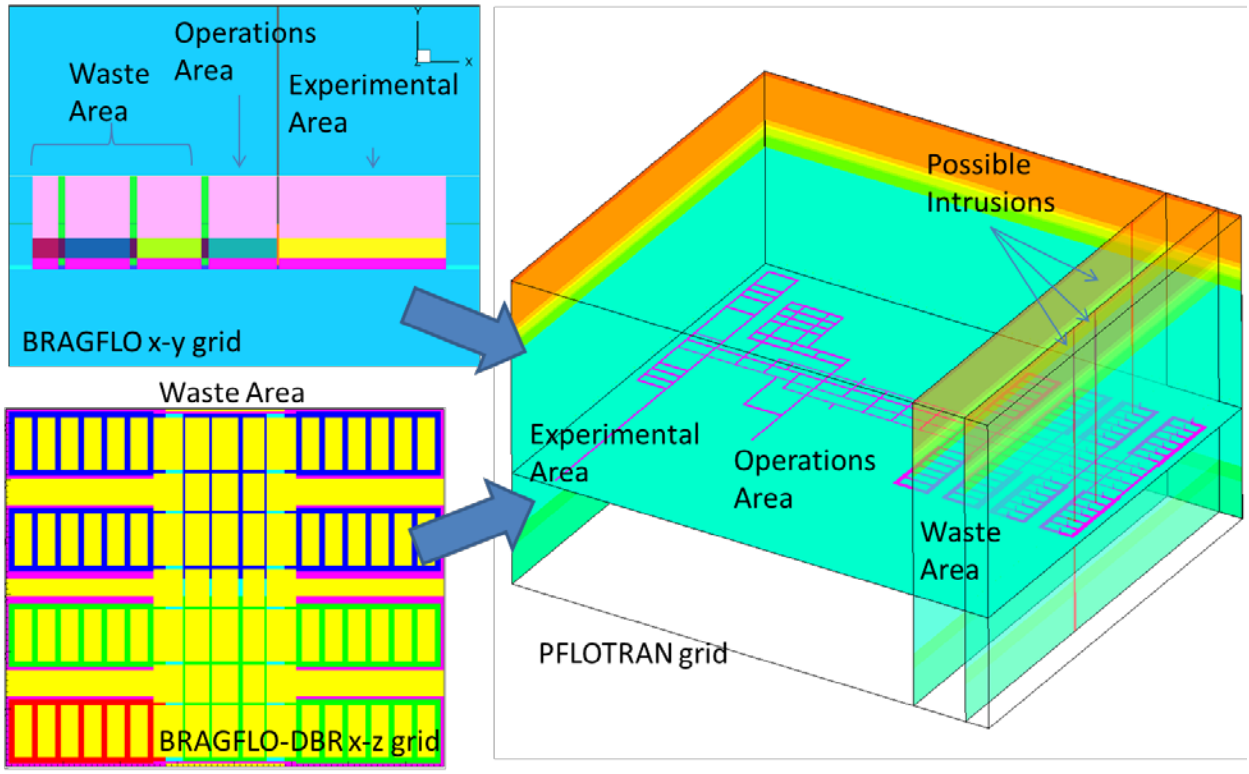

Fig. 1. This illustrates the current WIPP PA decoupled 2D grids (left) and more detailed 3D grid that can be simulated with PFLOTRAN (right).

Simplified PA Code System

The use of PFLOTRAN as a multiphase flow and reactive transport model to replace a series of connected PA models will centralize the simulation processes, minimize computation time used on intermediate inputs and outputs, and create a uniform PA model. The use of PFLOTRAN will centralize all subsurface process modeling (i.e. multiphase flow and reactive transport) within a single simulation framework, eliminating compute time used on intermediate steps (e.g., writing, mapping, and reading model inputs/outputs) and reducing potential data handling errors. The current expectation is that PFLOTRAN will complete calculations currently performed by five codes in WIPP PA:

- BRAGFLO simulates porous media flow in and surrounding the repository over 10,000 years
- NUTS calculates solute transport inside the repository
- BRAGFLO-DBR that predicts release from the repository to the environment via a borehole intrusion

- MODFLOW is used to simulate groundwater flow away from the repository in the Culebra member of the Rustler Formation
- SECOTP2D that computes radionuclide transport in Culebra.

Advanced Porous Media Calculation

PFLOTRAN considers additional physical processes that are not included in BRAGFLO. BRAGFLO cannot consider the effects of pressure or temperature on fluid properties because it does not utilize equation of state, nor consider an energy balance. PFLOTRAN has the capability to simulate simultaneous energy and mass flow, with fluid properties being general functions of pressure and temperature through equations of state. PFLOTRAN also calculates miscible multiphase flow that accounts for dissolution of gas in liquid phase and water vapor in gas phase. BRAGFLO considers only immiscible multiphase flow, where gases such as H_2 cannot dissolve into the aqueous phase [$H_2(aq)$].

ENHANCEMENTS FOR PFLOTRAN

Integration of Empirically Based WIPP Specific Functionalities within a Mechanistic Code [4]

The current approach to WIPP PA includes process models such as considering pressure-induced hydrofracture, creep closure, gas generation by corrosion and microbial activity, and a material property change in a grid for borehole intrusion. These process models are simplified representations of complex phenomenon and are not typically found in mainstream subsurface flow and transport codes. However, for WIPP these process models are required, as they represent processes expected to occur within the salt repository over time.

PFLOTRAN's WIPP gas generation model was implemented and successfully tested against the equivalent BRAGFLO model. The calculated pressure and saturation did not match exactly due to the effects from the assumption of immiscibility used by BRAGFLO, but they were within 10 % error. The accepted gas generation model described by WIPP PA has the form

$$q_r = M_{w,H_2}\left(s_{H_2,Fe}q_{rc} + s_{H_2,CH_2O}q_{rm}\right) \qquad \text{(Eq. 1)}$$

where q_{rc} is the rate of production of gas resulting from the corrosion of iron ($\text{mol Fe m}^{-3}s^{-1}$). q_{rm} is the rate of production of gas resulting from the microbial degradation of cellulosics ($\text{mol Fe m}^{-3}s^{-1}$). $s_{H_2,Fe}$ and s_{H_2,CH_2O} represent the stoichiometric coefficients, and M_{w,H_2} is the molecular weight of hydrogen gas. The end product of this equation is the gas production rate.

Creep closure of the mined disposal rooms at WIPP changes the effective porosity of the repository materials over time, and is crucial to calculating the repository fluid pressure. The WIPP PA requires PFLOTRAN to look-up pre-computed tables generated by a mechanical simulation using a finite element code, and interpolate effective porosity using pressure and time for waste material elements.

The WIPP PA hydrofracture model allows the porosity and permeability of certain materials to vary dynamically with the brine pressure when the pressure is within a specific range. For example, at pressures, p, below an initiation pressure, p_i, the porosity, ϕ, is computed from a constant rock compressibility, C_i:

$$\phi = \phi_0 \exp\left[C_i\left(p - p_0\right)\right], \quad p \le p_i \qquad \text{(Eq. 2)}$$

where ϕ_0 is the porosity at the reference pressure, p_0. The hydrofracture model changes the permeability of fracture materials, using the parallel plate analogy for flow in fractured rock:

$$k = k_i \left[\frac{\phi}{\phi_i}\right]^n \qquad \text{(Eq. 3)}$$

where k is the changed permeability, k_i is the permeability of intact material, ϕ is the porosity of altered material, ϕ_i is the porosity of intact material at $p = p_i$ using Eq. 2, n is an empirical parameter.

Lastly, it is crucial to have material property change capability on each element with time to simulate borehole intrusion. This capability will not only simulate the transport of radionuclide amid intrusion, but also re-initializes pressure and saturation of the domain for possible future intrusions. This function is applied for consolidation of shaft seal material.

Optimization of Runtime and Initial/Boundary Conditions

Applying physically realistic initial and boundary conditions is very important. The current WIPP PA runs a simulation from five years prior to closure of the WIPP to the time of closure in order to find the pressure field due to excavation and set as the initial condition. The same can be done with PFLOTRAN, the open volume and open shaft can be simulated up until the closure, save the simulation, change materials, and refine time steps to continue the problem.

The boundary condition is more complicated than the initial condition. It requires a balance between what is physically meaningful and what is numerically tractable. Currently BRAGFLO uses no-flow boundary conditions 20 km away from the repository. The extent of this model in three dimensions will be much more computationally expensive. Also, extreme element aspect ratios can cause inaccuracy in solution. Sensitivity studies regarding domain size and mesh resolution must be carried out to quantify their effects.

Similar to a challenge in boundary conditions, sensitivity studies regarding time step sizes, mesh resolution, convergence criteria, radionuclide transport intervals, and other parameters are required to optimize the runtime.

VERIFICATION AND VALIDATION PLAN FOR PFLOTRAN

PFLOTRAN will require its own verification and validation plan to ensure that all the functionalities are working as expected and producing the correct results. The document will be written following the requirements of the WIPP PA codes that PFLOTRAN will replace. It will include the fundamental equations and methods to calculate each process and model. A list of test cases will be designed to examine implemented functionalities much more closely and cover all the necessary requirements. Each functional test will have an objective, procedure, and acceptance criteria recorded in order to be replicated in the future. These tests will be a part of regression testing as well.

TEST CASE RESULTS

Calculating the 1D initial condition of the WIPP environment

This test demonstrates the saturation process over time in the disturbed rock zone (DRZ), which is fractured salt caused by distressing the salt bordering an excavation in the WIPP. Salado halite, a bedded salt formation, is initially fully saturated. When excavation occurs, porosity opens up in the fractured salt surrounding the excavation. This in turn causes desaturation in the DRZ and increases the permeability of the salt. The initial condition for this simulation is the following: excavated region or open air has moisture of 1% saturation (to define in hydrology terms), the DRZ is 40% saturated, and the intact Salado halite maintains its fully saturated status.[5]

The simulation illustrates how fully the saturated Salado region slowly wets the DRZ over time. The saturation of the DRZ is slow because the permeability of the intact halite is so low that water cannot quickly flow into it. Truly, the porosity, saturation, and permeability of the DRZ would not be as discontinuous as shown in this simulation, but it was assumed to be discrete. Also, this is only a demonstration of hydrologic aspect, completely disregarding creep closure of salt bedded formation, a natural recovery process.

Fig. 2. shows the wetting of the DRZ over 20,000 days or 54.8 years. The first subplot shows the defined material property of the regions, the second subplot shows liquid saturation of the regions, and the third subplot shows changes in pressure over time. PFLOTRAN and TOUGH2 results agree well. Such a test case could be used to satisfy WIPP PA requirements for two-phase flow and diffusion.

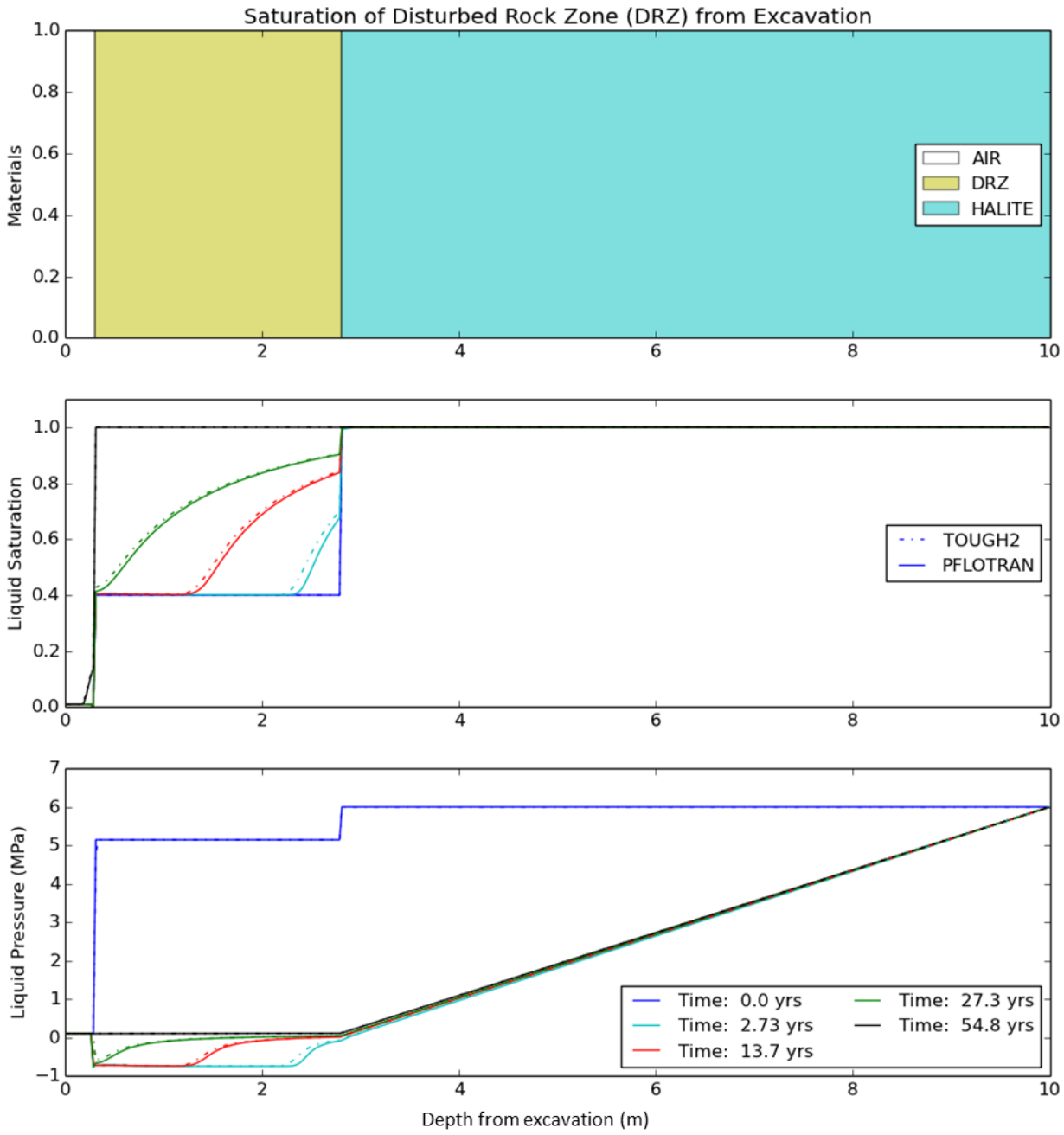

Fig. 2. This demonstrates agreement between TOUGH2 and PFLOTRAN over 20,000 days.

Well Production at a Specified Bottom-Hole Pressure

The purpose of this test is to verify that PFLOTRAN can simulate the performance of production wells in which the bottom-hole pressure is specified, in particular when two phases are present. This type of well model is often used to maintain a constant pressure at a specified location. This well model functions similar to a time-variable Dirichlet Boundary condition.

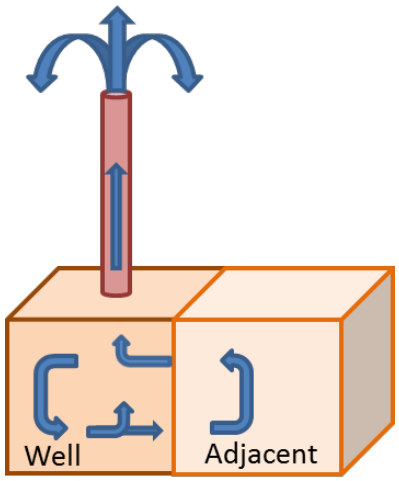

Fig. 3. A schematic description of the well production test case.

The test problem considers a horizontal one-dimensional reservoir with two grid blocks. Each grid block is a 10 m cube. Both grid blocks are initially at pressure 10 MPa and water saturation 0.5. Fluids consist of pure water and hydrogen gas. A single well with productivity index of 1.0 $\times 10^{-12}$ m^3 is completed in the first grid block at 0 s (an instant well) and is produced for 1000 s at a fixed flowing bottom-hole pressure of 1.0 MPa.

This model treats well deliverability by the inflow performance equation:

$$q_l = I\left(\frac{k_{rl}}{\mu_l}\right)\left(p_l - p_{wf}\right) \qquad \text{(Eq. 4)}$$

where

q = volumetric flow rate [m^3/s],
I = well productivity index [m^3],
k_r = relative permeability [-],
μ = viscosity [Pa·s],
p = pressure [Pa],

and subscripts

l = phase (brine or gas),
wf = flowing bottom hole.

Results from PFLTRAN, BRAGFLO, and TOUGH28W are shown in Fig. 4. Both water and gas are produced from the well grid block (grid block 1). As pressure is depleted from the well block, supporting flow from the adjacent grid block occurs. Both grid blocks become depleted, but the well block maintains a pressure below the adjacent grid block, as shown in Fig. 4. As the pressure declines, both the water and gas production rates decline.

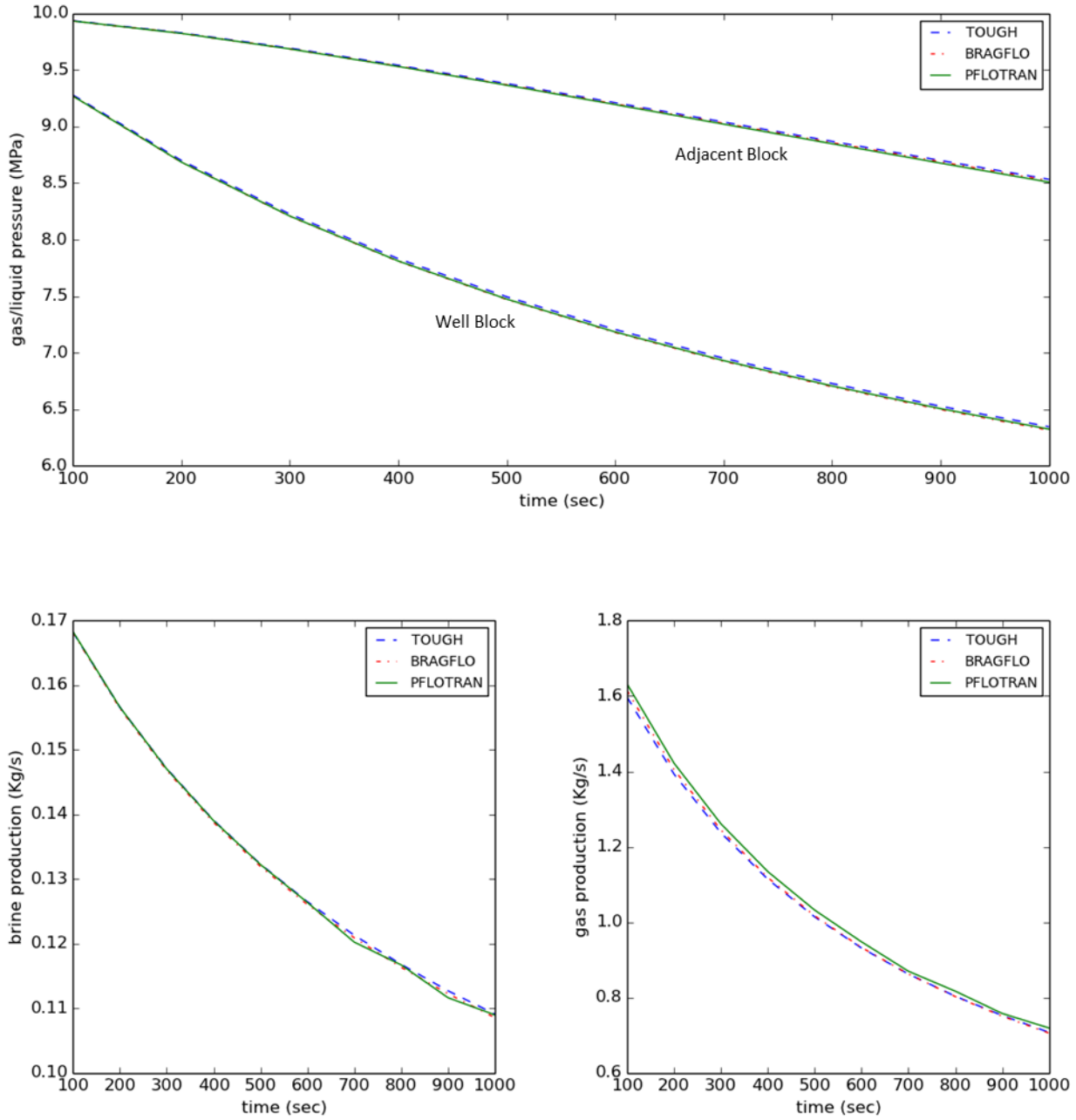

Fig. 4. Results from the well production test case simulation. Reservoir pressure response for well completed block (bottom line) and the adjacent block (top line) are shown in the upper plot. The lower plots show production rate of gas and brine of the well completed block. Data at time 0 s was unavailable from TOUGH.

CONCLUSIONS

The first WIPP PA was finished in the early 1990s with clever assumptions and painstaking simplifications because of the computing resources they had. The calculations were also performed with conservative parameters in order to have increased confidence in the results. The use of PFLOTRAN and 3D numerical model will utilize modern computing capabilities to

increase accuracy and provide more assurance than before, possibly enabling advancement of the WIPP in the future. PFLOTRAN will be employed to distribute a detailed 3D single realization problem across multiple processors; complete calculations for five different codes in WIPP PA; and apply realistic equations of state, energy balance, and miscibility. So far, test cases for WIPP-specific functionalities agreed agreeing with WIPP PA codes and TOUGH2, a multi-phase code released by Berkeley Lab Software Center. A research needs to be done in order to set proper boundary and initial condition to the 3D grid and optimize runtime to complete PA in a reasonable timeframe.

REFERENCES

1. S. BALAY, W. GROPP, L. C. MCINNES, and B. F. SMITH, *PETSc, the portable, extensible toolkit for scientific computation,* Argonne National Laboratory (1998).
2. G. E. HAMMOND, P. C. LICHTNER, and R. T. MILLS, *Evaluating the performance of parallel subsurface simulators: An illustrative example with PFLOTRAN*, no. 1, 208-228, Water Resources Research 50 (2014).
3. HDF Group. HDF5, *Hierarchical Data Format*, URL: http://www.hdfgroup.org/HDF5 (2013).
4. C. CAMPHOUSE, *Requirements Document & Validation and Verification Plan for BRAGFLO Version 6.02 ERMS# 558659,* Sandia National Laboratories, Albuquerque, NM (2012)
5. K. L. KUHLMAN, *Summary Results for Brine Migration Modeling Performed by LANL, LBNL, and SNL for the Used Fuel Disposition Program, FCRD-UFD-2014–000071, SAND2014–18217R.* Sandia National Laboratories, Albuquerque, NM (2014)