

## Moving from 2D to 3D flow modeling for the Waste Isolation Pilot Plant Performance Assessment

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## INTRODUCTION

Performance Assessment (PA) for the Waste Isolation Pilot Plant (WIPP) is designed to evaluate the potential for consequential radionuclide release during a post-closure regulatory period of 10,000 years. Within the PA framework uncertainty is addressed through sampling of parameters and through a number of pre-determined scenarios for an undisturbed repository and a repository intruded by exploratory drilling. One of the primary calculations in the WIPP PA is a subsurface flow calculation in and around the WIPP repository for the 10,000-year post-closure period using a two-dimensional (2D) model.

The proposed replacement of waste panels in the WIPP challenges the assumption of east/west symmetry inherent in the 2D grid used in PA calculations of flow and transport near the repository. Therefore, a new three-dimensional (3D) model for use in PA is under development. While the 3D model is being developed, we will continue to use the 2D model for calculations. The purpose of the present task is to confirm that the 2D model domain is an adequate representation of the repository fluid flow within the updated disposal system geometry.

## METHODOLOGY

The current WIPP PA 2D flow simulations use a vertical grid based on assumptions that take advantage of the repository symmetry. The proposed replacement waste panels shown in the schematic of the repository in Figure 1 [1] introduce asymmetries into the repository design. The repository flow conceptual model has been updated to account for the new geometry and will be compared against simulations that are fully 3D.

### 2D and 3D simulation models

A WIPP-specific simulation module that is in the process of being added to existing software, PFLOTRAN [2], is used to verify and compare against the current 2D modeling results from purpose-built WIPP software BRAGFLO [3]. As shown in Figure 2, the 2D grid is ‘flared’ to be highly refined near the wellbore for an intrusion directly into a waste panel and has lower resolution in other areas away from the repository. The 2D grid ‘unbends’ the true L shape of the repository, in

that waste panels 11-19 are north of the rest of the repository in the model, whereas the true proposed replacement panels are west of the repository (See Figure 1). [4] describes the 2D model development in detail.

Previous work has established that PFLOTRAN can reproduce BRAGFLO simulation results similar to those used in compliance calculations to a high degree of precision [5]. Work since then has focused on running flow simulations on a fully 3D grid [6] [7]. The 3D grid shown in Figure 3 utilizes unstructured meshing, so it is highly refined near the intrusion wellbore in waste panel 5, has a moderate level of resolution for the rest of the repository structure and is very coarse far from the repository. [6] describes the 3D grid development. At the current stage of development of the 3D model 96.5% of the simulations complete in the time allotted, as shown in Table I [7]. All 2D simulations run to completion.

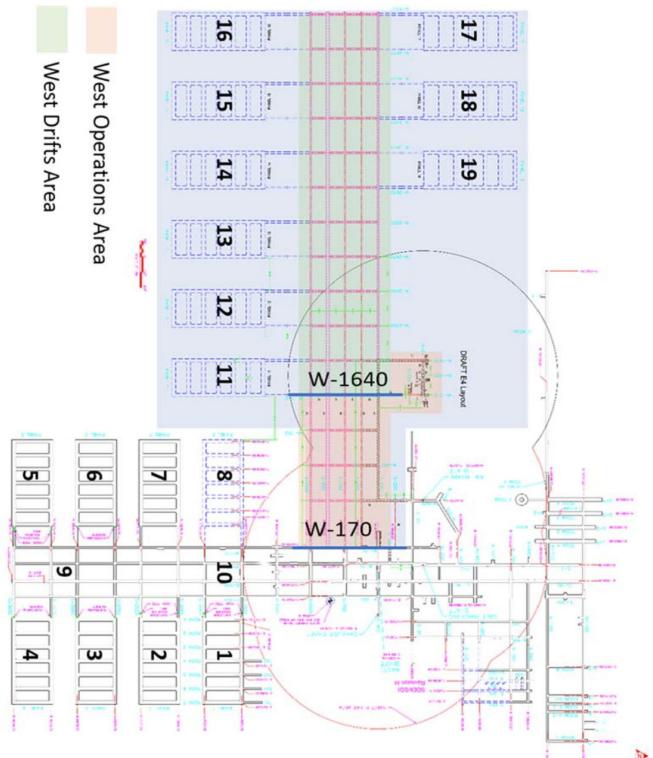


Fig. 1. Planview of the WIPP repository with proposed additional panels. North is to the right. Taken from [1].

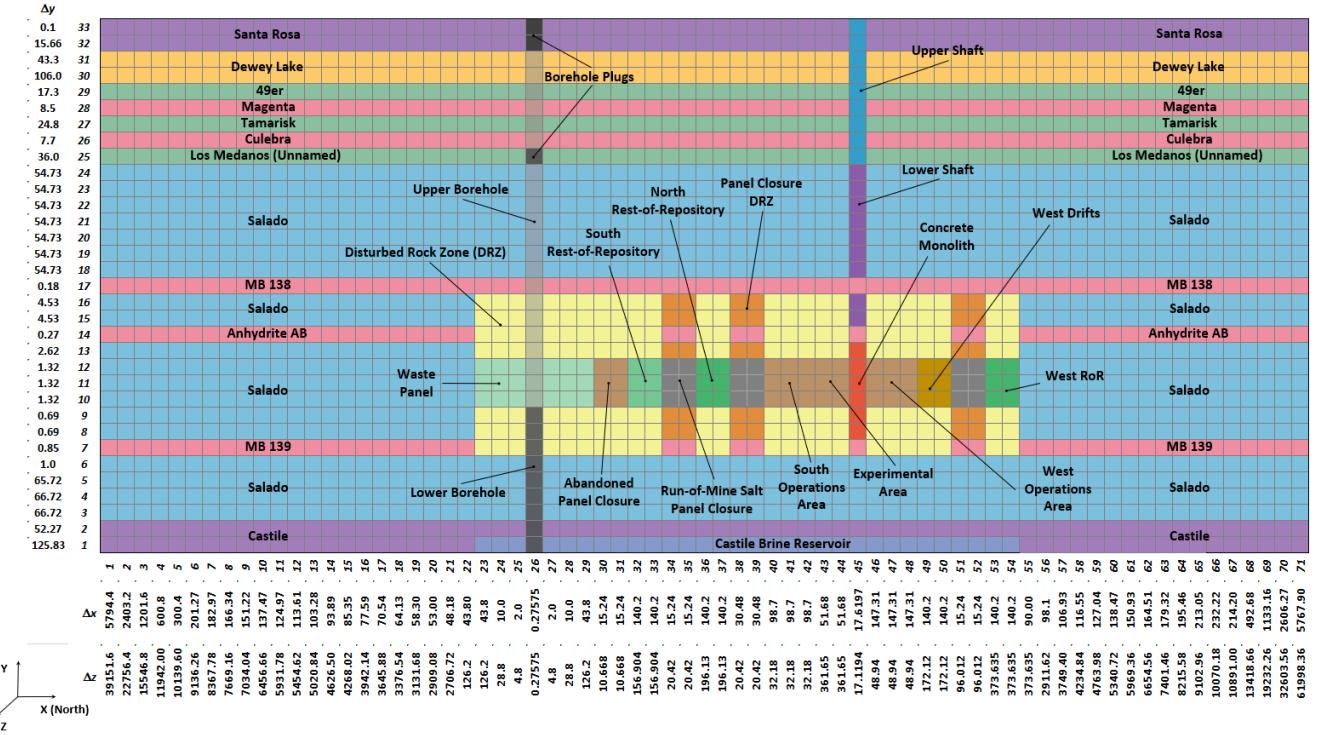


Fig. 2. Side view of the 2D ‘flared’ simulation grid. Grid cell size is not to scale. Vertical dimensions are given on the left and horizontal dimensions are below. North is to the right.

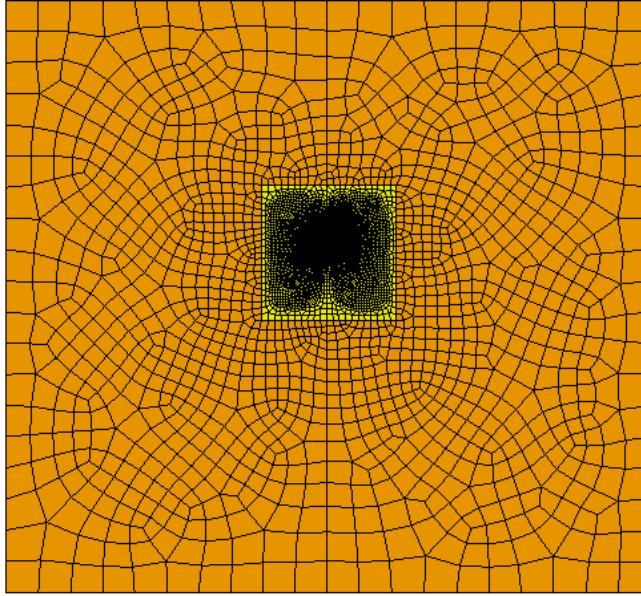


Fig. 3. Top view of the simulation grid generated for the 3D simulation domain. Left: Full model domain. The land-withdrawal boundary region is shown in yellow. Right: Detail of the repository mesh. North is to the right in both subfigures.

A Latin Hypercube sampling of size 100 is taken to create a replicate. In a full PA calculation 3 replicates are used. Here the results of a single replicate will be examined. Six scenarios are considered as shown in Table I, giving a total of 600 simulations used in this analysis.

### Comparison quantities

The aggregate results of the 600 simulations in replicate 1 are compared. This comparison between the 2D and 3D results focuses on brine pressures and saturations in the waste areas and brine flow up the borehole, as these values impact WIPP radionuclide releases. The 3D

simulations use the CRA-2019 WIPP parameters, while the 2D simulations use the updated APPA parameters [4]. The difference between the parameter values is minor and not impactful to this comparison.

In the 3D model each individual waste panel is modeled as a simulation volume, while in the 2D simulation all except the intrusion waste panel are lumped

TABLE I. Scenario descriptions and percentage that finished in the 3D simulation model [7]. E1 is wellbore intrusion through waste panel 5 and into a brine pocket in the Castille Reservoir below the repository. E2 is wellbore intrusion into the repository at waste panel 5.

| Scenario | Description                           | Percent of 3D Simulations completed |
|----------|---------------------------------------|-------------------------------------|
| S1-BF    | Undisturbed Repository                | 99%                                 |
| S2-BF    | E1 at 350 years                       | 96%                                 |
| S3-BF    | E1 at 1,000 years                     | 98%                                 |
| S4-BF    | E2 at 350 years                       | 97%                                 |
| S5-BF    | E2 at 1,000 years                     | 99%                                 |
| S6-BF    | E2 at 1,000 years; E1 at 2,000 years. | 99%                                 |

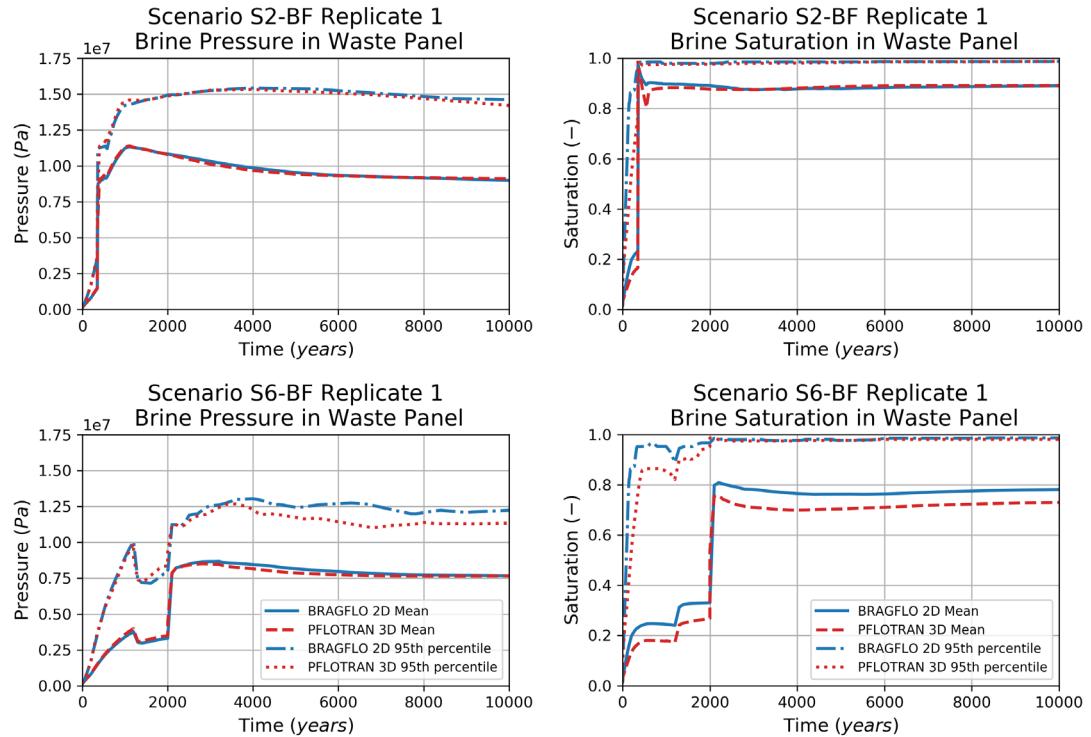


Fig. 4. Comparison of the 2D and 3D mean and 95<sup>th</sup> percentile simulation results in the intrusion waste panel for scenarios S2 (top) and S6 (bottom). Brine saturation (left) and pressure (right) are shown.

together into groups. For consistency between the models the 3D results in Panels 3, 4, 6, and 9 are lumped into the South Rest-of-Repository; Panels 1, 2, 7, 8, and 10 are in the North Rest-of-Repository; and Panels 11 through 19 are in the West Rest-of-Repository. The ‘Waste Panel’ in the 2D grid is waste panel 5 in the 3D grid. The comparison quantities are volume-averaged over their respective areas.

## RESULTS

Figure 4 shows the brine pressures and saturations for the mean and 95<sup>th</sup> percentile simulation for the intrusion waste panel in scenarios S2 and S6. In all waste areas and all scenarios, the brine pressure results in 2D follow the same trends as the 3D results over similar ranges throughout the 10,000 year simulation. 2D simulations show slightly lower mean brine pressures in the waste area in most scenarios at later times, and a larger range of brine pressures, including higher maximum pressures, in all waste areas compared to 3D.

Similarly, the brine saturation results from 2D follow the same trends as the 3D results (Figure 4-right). In some scenarios and areas, 2D shows a slightly higher mean brine saturation than 3D. In most cases the 2D results tend to show a larger range of brine saturations, which is consistent with the larger range of pressures.

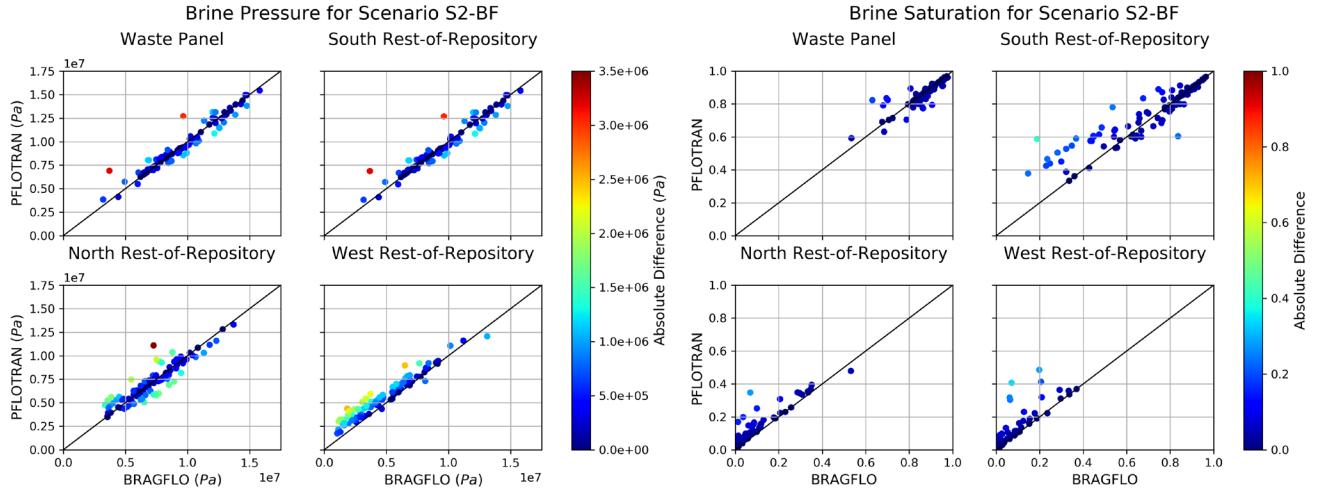


Fig. 5. Comparison of the 2D and 3D simulation results in all waste areas for scenario S2. Time-averaged brine saturation (left) and pressure (right) are shown for all replicate 1 simulations.

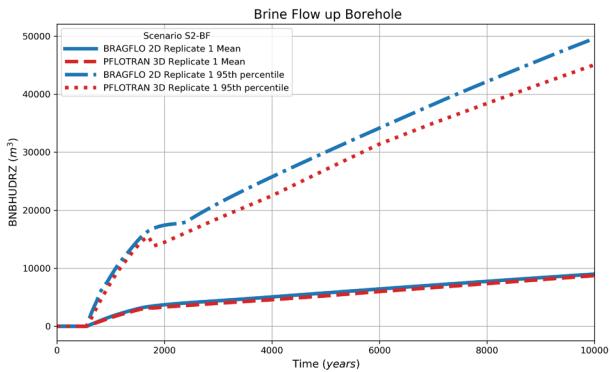


Fig. 6. Comparison of the 2D and 3D simulation results for flow up the borehole in scenario S2.

Figure 5 shows the time-averaged brine pressure (left) and saturation (right) for all the lumped waste areas. In some scenarios and areas, the 2D simulations show a slightly lower mean brine pressure, particularly in West Rest-of-Repository. However, in those cases the 2D results tend to show a larger range of brine pressures, including higher maximum pressures.

The 2D average brine saturation results also follow the same trends as the 3D results for all waste areas (Figure 5-right). The 2D geometry allows more brine flow down-dip, which results in higher brine saturations in the intrusion waste panel and lower brine saturations in up-dip West Rest-of-Repository. The latter is likely due to ‘unbending’ the L shape of the repository.

Figure 6 shows that brine flow up and down the wellbore shows similar trends in both 2D and 3D simulations. Cumulative flows in 2D are slightly greater than cumulative flows from 3D.

## CONCLUSIONS

A comparison was done between 2D BRAGFLO and 3D PFLOTRAN Salado flow models. Despite the difference in dimensionality, the models show similar trends in the quantities that drive WIPP PA releases (brine pressure, brine saturation, and brine flow up the borehole). The two models produce results that are similar in magnitude and range of uncertainty. Furthermore, the results for lumped waste regions are similar in 2D and 3D.

The agreement between the two models demonstrates that the unbending of the repository representation in the 2D model is an appropriate simplification of the 3D geometry and the 2D representation of the repository is adequate for estimating releases from the disposal system.

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