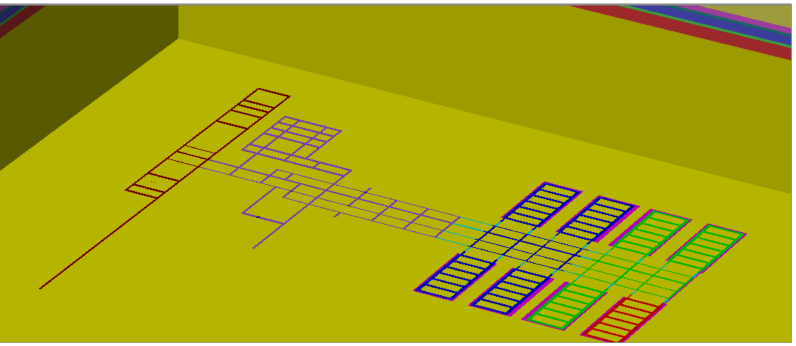
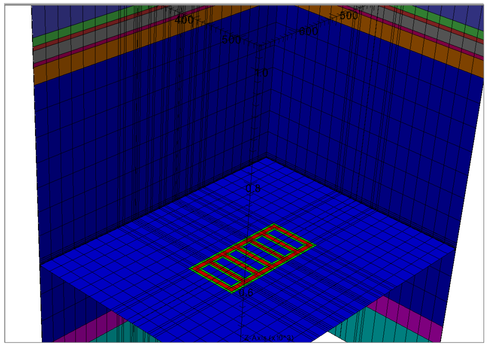
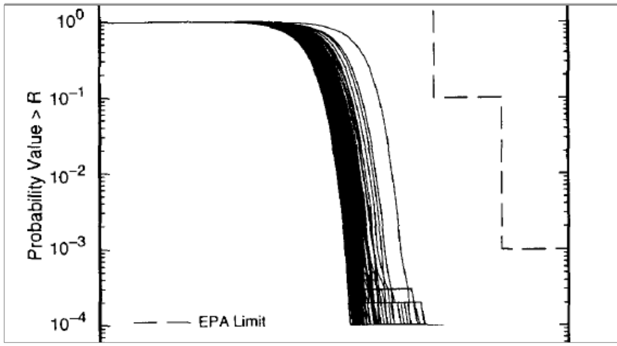
SAND2015-4298C

Exceptional service in the national interest

Sandia National Laboratories







Waste Isolation Pilot Plant Performance Assessment Specific Functionalities to PFLOTRAN

H. Park, G. Hammond

U.S. DEPARTMENT OF ENERGY

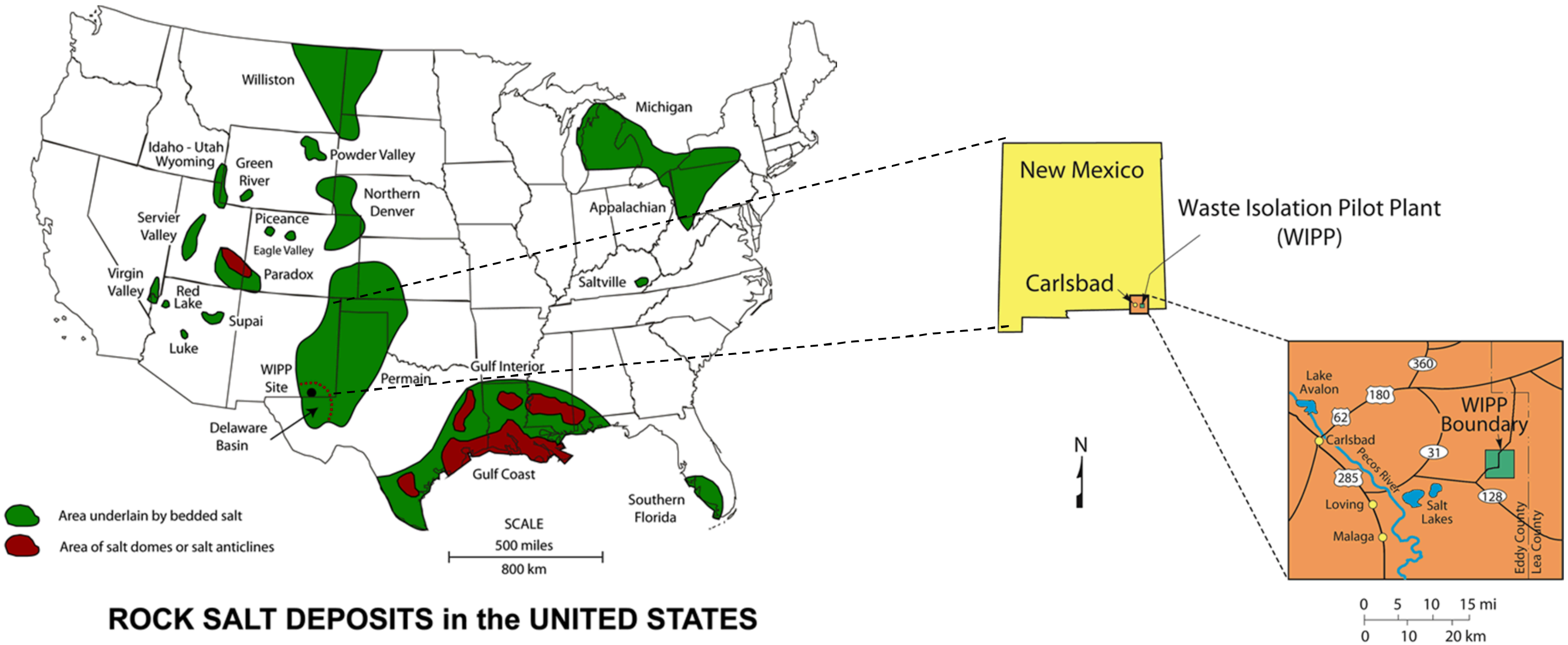
NNSA National Nuclear Security Administration

Sandia National Laboratories is a multi-program laboratory managed and operated by Sandia Corporation, a wholly owned subsidiary of Lockheed Martin Corporation, for the U.S. Department of Energy's National Nuclear Security Administration under contract DE-AC04-94AL85000. This research is funded by WIPP programs administered by the Office of Environmental Management (EM) of the U.S Department of Energy.

WHAT IS WASTE ISOLATION PILOT PLANT?

Waste Isolation Pilot Plant (WIPP)

- 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.

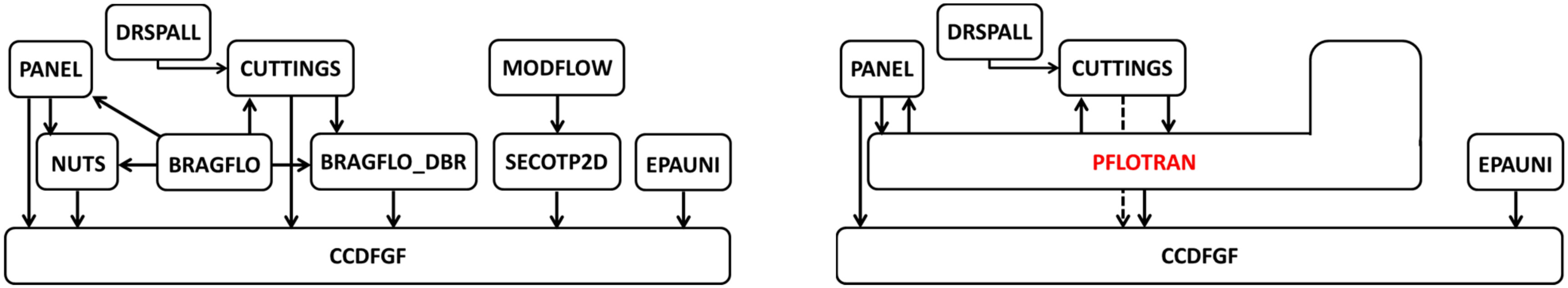


WIPP PA

- The DOE demonstrates compliance with containment requirements by means of performance assessment (PA) calculations conducted by Sandia National Laboratories (SNL) to Environmental Protection Agency (EPA)
  - Computer codes incorporating 24 peer-reviewed conceptual models
- WIPP 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.

CURRENT PA VS PFLOTRAN

Current PA Description



Codes	Description
BRAGFLO	Simulates porous media flow in surrounding the repository over 10,000 years
NUTS	Calculates radionuclide transports in the Salado Formation including the repository
BRAGFLO-DBR	Predicts release from the repository to the environment via borehole intrusion
MODFLOW	Used to calculate flow field away from the repository in the Culebra member of the Rustler Formation
SECOTP2D	Computes radionuclide transport in fractured porous media (Culebra)

Current PA vs PFLOTRAN

Codes	Current PA	PFLOTRAN
BRAGFLO	- Immiscible - Isothermal - Two-phase flow	- **Miscible** - **Anisothermal** - Multiphase Flow - **Diffusion**
NUTS	- Multicomponent transport - Single porosity - Constant sorption - Single continuum model	- Chemical reactions - Dissolution/precipitation - **Multi-rate sorption** - **Multi-continuum model**
General Comparison	- **2D** - Structured grid - **Parallel with single core simulations** - Limitations on simulation size - Many I/O interface required - Network of coupled 2D simulations - **Simplified process models and coarse mesh** for quicker overall calculation time.	- **3D** - Unstructured/structured grid - **Massively parallel** - Simulation size only depends on hardware capability - Needs to develop WIPP required functionalities - **Detailed process models and high mesh resolution**, but overall PA calculation may be longer

Other Advantages of PFLOTRAN

- **Open source development**
  - A research community that leverages innovation in subsurface and computational sciences.
- In-house code development expertise
  - **Mulitiple Sandians are PFLOTRAN developers with authorization to commit changes to the code.**
- PFLOTRAN is managed under a modern support infrastructure.
  - **Distributed through source control management, Mercurial**
  - **Central source repository resides on Bitbucket**
  - Comprehensive regression and unit testing using Python
  - Automated build, test, release through Buildbot
- PFLOTRAN HDF5 file formats
  - **Compatible with open source visualization tools** (i.e. VisIt and Paraview)
- It will be managed under QA if PFLOTRAN is accepted to be used for PA

PFLOTRAN DEVELOPMENT

PFLOTRAN Enhancements testing

- Integration of empirically based WIPP specific functionalities
  - Well production at a specified bottom-hole pressure
  - Gas generation from iron corrosion and microbial degradation of cellulosics
  - Interpolating porosity of materials that undergo creep closure
  - Calculating porosity and permeability of materials that fractures
  - Klinkenberg effect on gas permeability
  - Applying Redlich-Kwong-Soave equation of state for gas density
  - Material map changes at human intrusion and creep closure
- Testing PFLOTRAN in 2D mode for direct comparison of the current verification and validation plan for BRAGFLO

Gas generation

- In WIPP PA, gas generation is assumed to be caused by anoxic corrosion of steel drums and microbial degradation of cellulosics, plastics and rubbers.
- The two gas generation reaction used in BRAGFLO are described as

$$q_{rgc} = \left(R_{ci} S_{b,eff} + R_{ch} S_g^*\right) D_s \rho_{Fe} X_c \left(\mathrm{H_2}|\mathrm{Fe}\right) M_{H_2}$$

$$q_{rgm} = \left(R_{mi} S_{b,eff} + R_{mh} S_g^*\right) D_c y \left(\mathrm{H_2}|\mathrm{C}\right) M_{H_2}$$

- Both gas generation source terms only depend on saturation of brine and gas, and the rest are experimental constants.

Gas generation

- Waste drum generates gas from iron corrosion and microbial activity
- One cell in the middle is characterized as waste drums
- Other cells represent soil with permeability of 1.0E-17 (Dewey Lake Red Beds)

Gas saturation initial condition

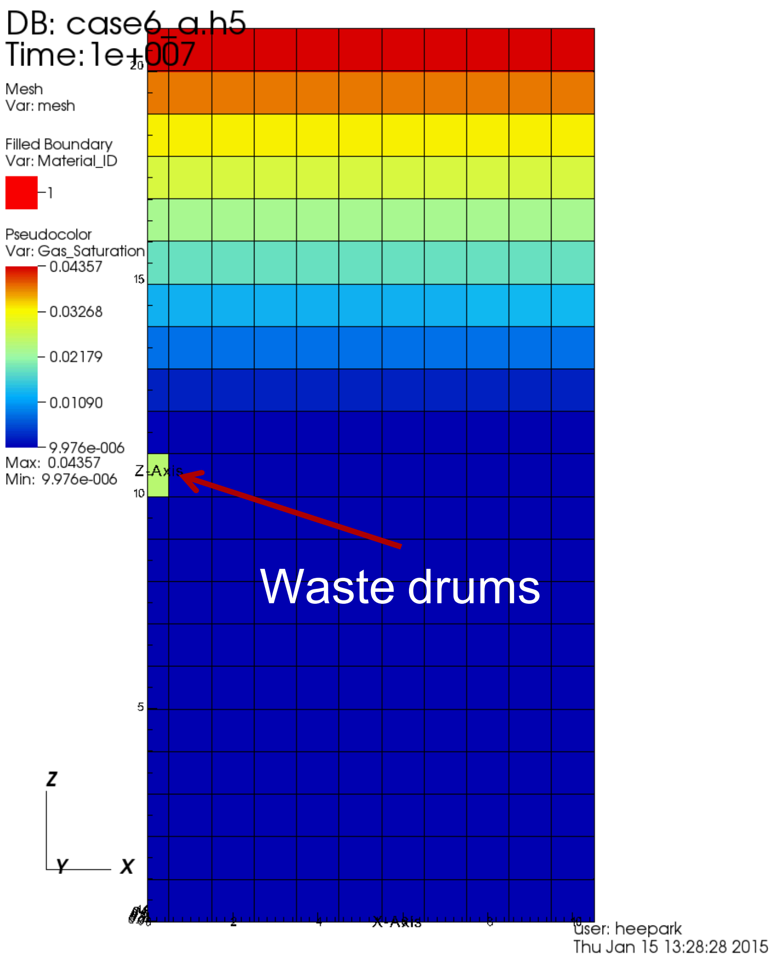
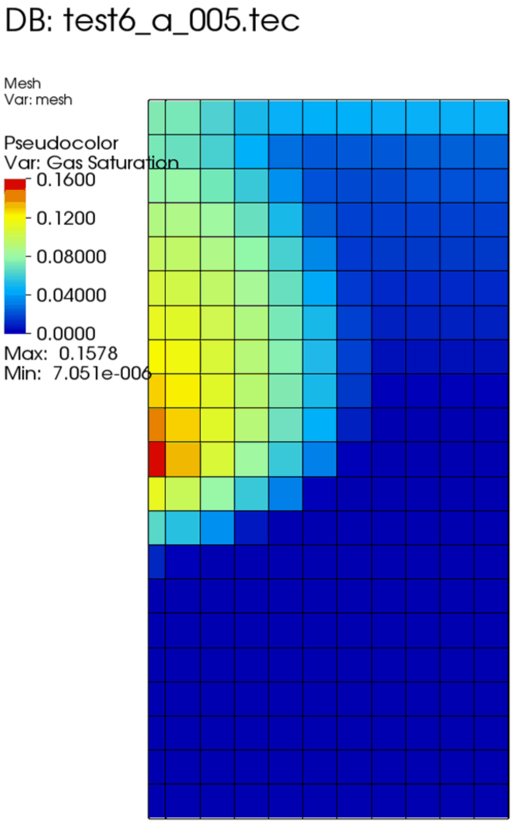


Figure by Heeho Park

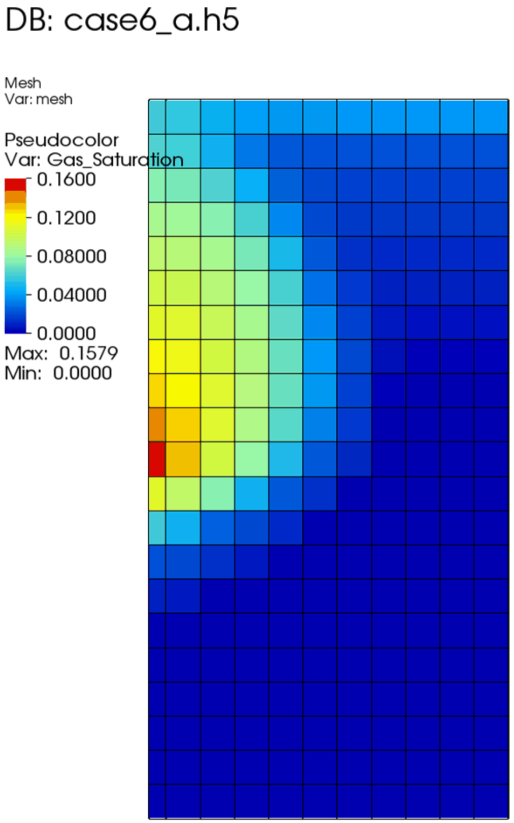
Gas generation

BRAGFLO



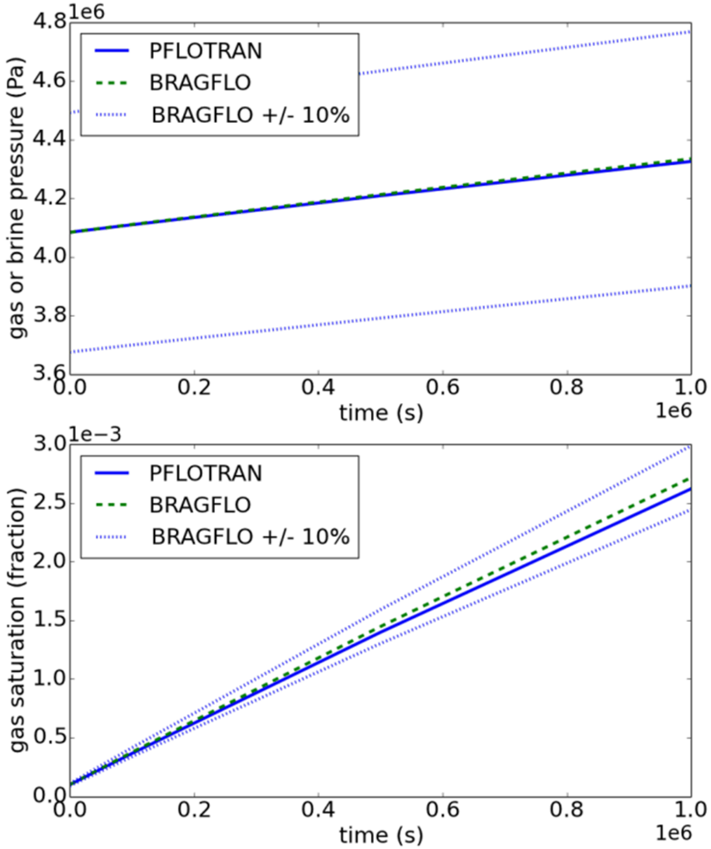
~160 years

PFLOTRAN



One cell gas generation

- A 10m cube with no-flow boundary condition waste material is simulated
- Difference due to miscibility vs immiscibility
- Capillary threshold pressure difference has been eliminated unlike the 2D case

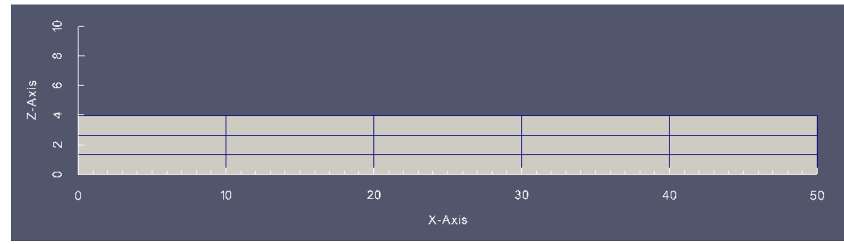


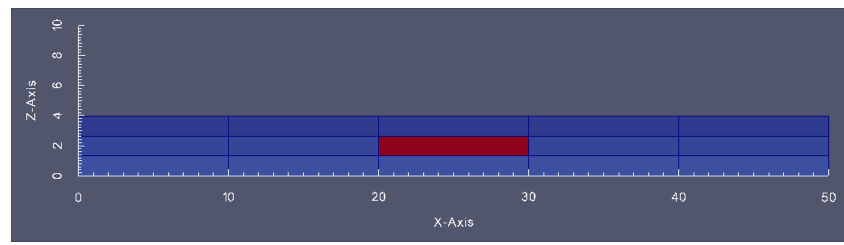
Creep Closure

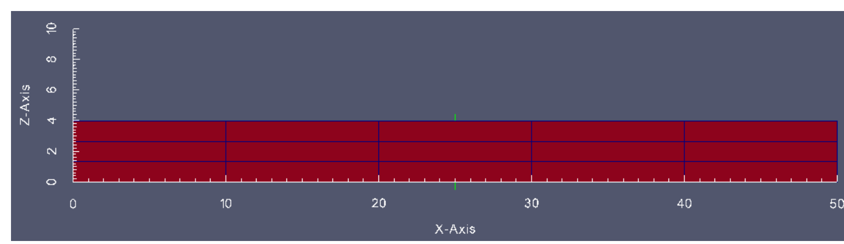
- The excavation of the WIPP will result in a plastic deformation of the salt material (creep) and resultant closure (creep closure) of excavated areas.
- The creep closure causes the reduction of void volume and increased repository pressure over time.
- Values of porosity are calculated as a function of time and brine pressure which were obtained by modeling deformation of a waste-filled room using a finite element structural mechanics code, SANTOS.
- The waste-filled room in PFLOTRAN is modeled as homogeneous high porosity porous media.

Creep Closure

- 50x4x1, 15 block cell that emulate 2D waste panel at WIPP
- The initial pressure is same as WIPP condition with no flow boundary condition
  - No gas generation
  - Gas generation in the center cell
  - Gas generation in all cells

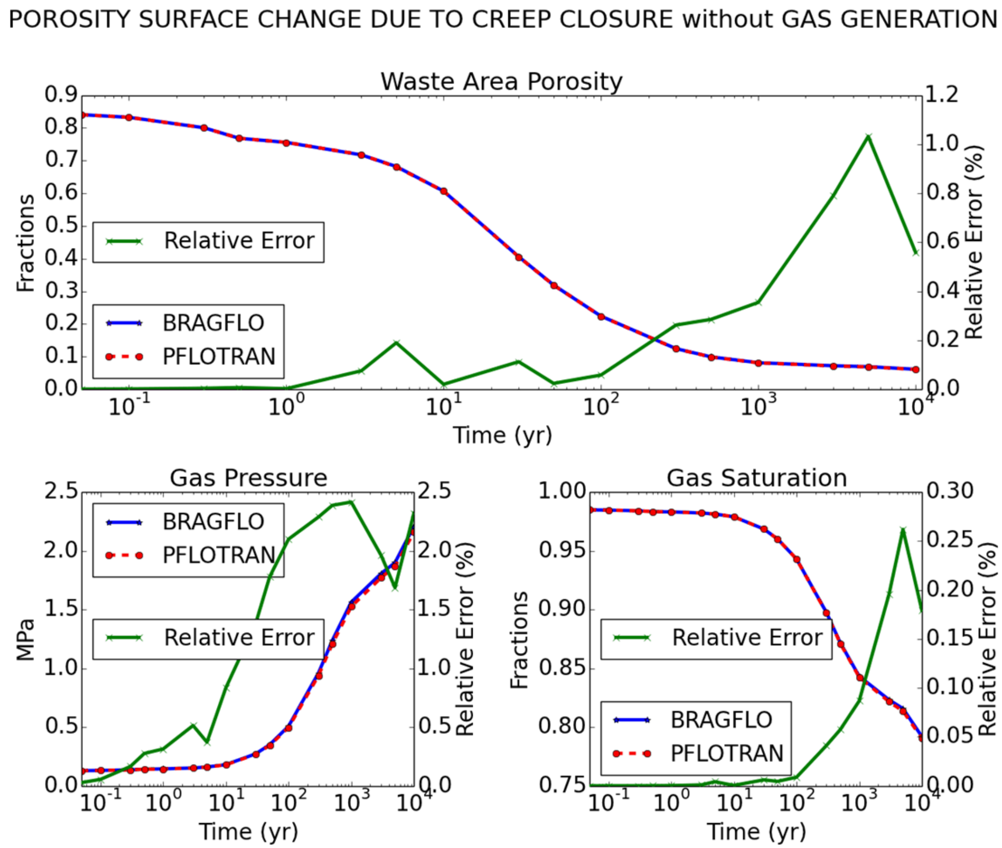






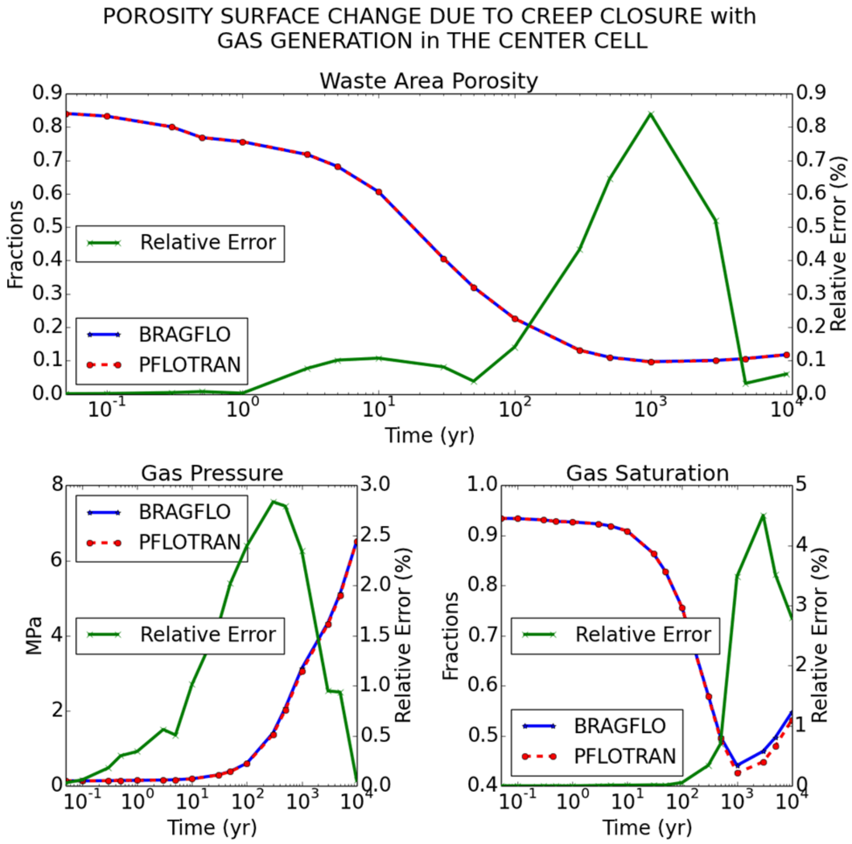
Creep Closure

- Phenomenon
  - Porosity of waste area decreases as salt creeps into and fills the open space
  - Gas pressure increases to 2.25MPa as void space decreases
  - Gas saturation decreases as void decreases
- Relative error is less than 2.5%



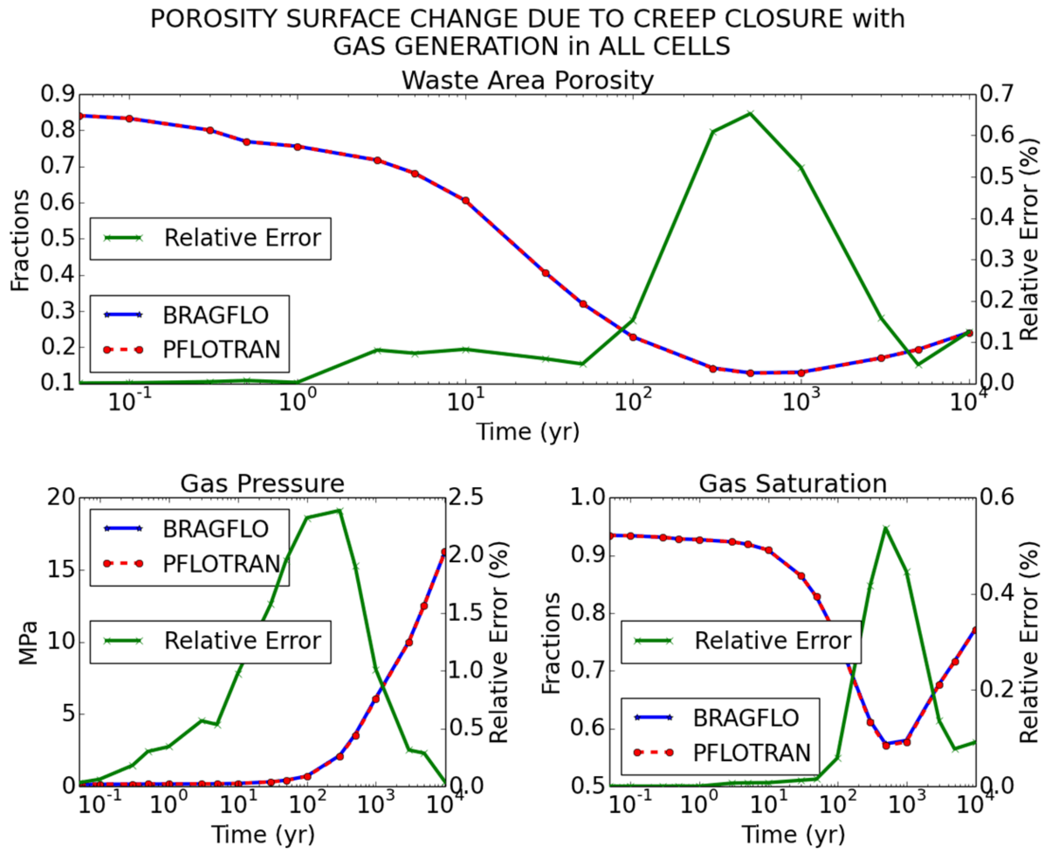
Creep Closure

- Phenomenon
  - Porosity opens up after 1000 years because of gas generation
  - Gas pressure increases higher than no gas generation case
  - Gas saturation increase after 1000 years
  - Gas pressure up to 6.5MPa
- Relative error is less than 5%



Creep Closure

- Phenomenon
  - Much more intensified gas generation is noticed when all cells are generating gas.
- Relative error is less than 2.5%



Well Production

- BRAGFLO can simulate a production well in which the bottom-hole pressure is specified with both brine and gas phases present.
- This model treats well deliverability by the inflow performance equation:

$$q_l = I\left(\frac{k_{rl}}{\mu_l}\right)\left(p_l - p_{wf}\right)$$

where

q = volumetric flow rate [m³/s],

I = well productivity index [m³],

k_{rl} = relative permeability [-],

↘ = viscosity [Pa•s],

p = pressure [Pa],

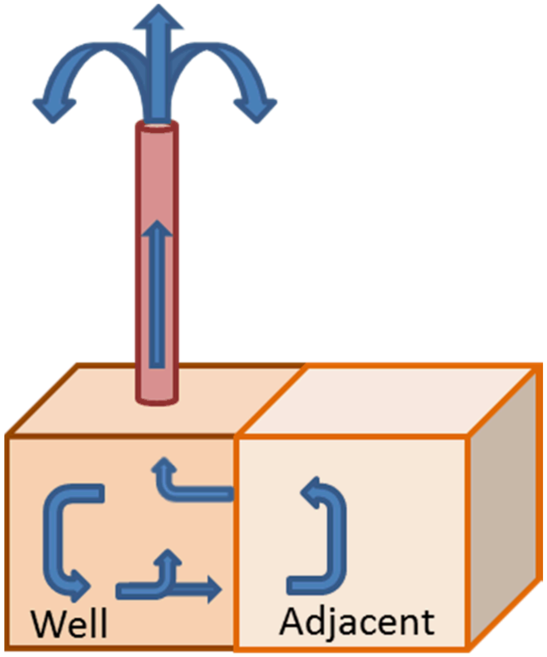
and subscripts

l = phase (brine or gas),

wf = flowing bottom hole.

Well Production

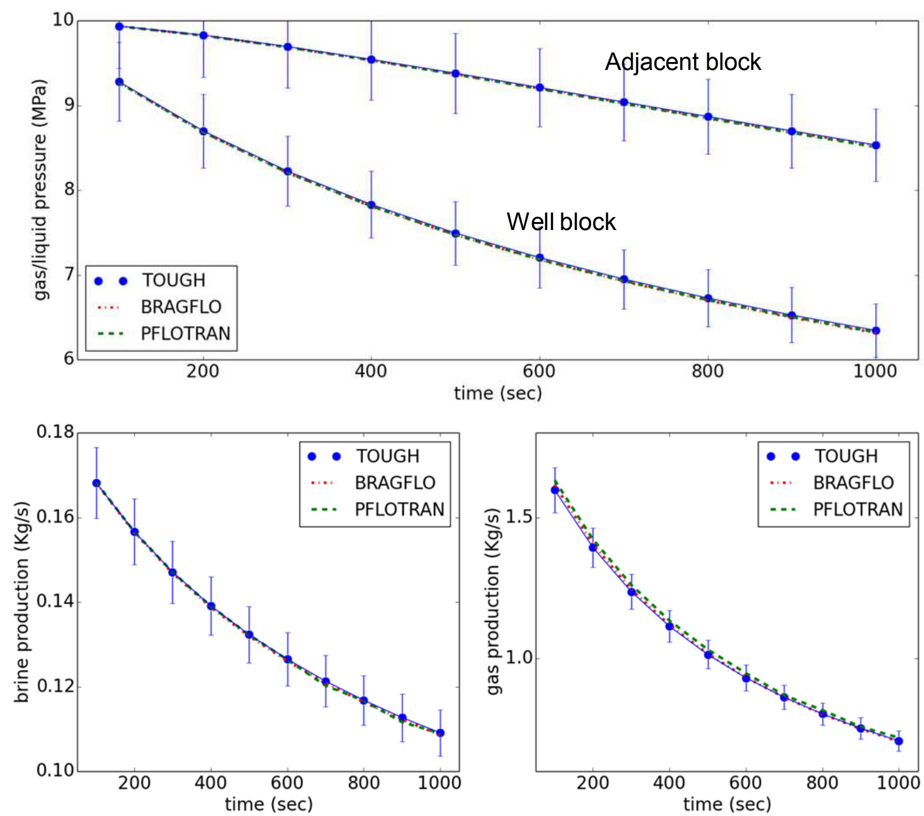
- Two 10 meter cubes
- Initially at 10 MPa
- Saturation of 0.5
- Well is created on the left block
- Fluids consist of pure water and hydrogen gas
- Well production will continue for 1000s



Figures by Heeho Park

Well Production

- Production at the well block decreases as it loses pressure over time
- Well block has lower pressure than the adjacent block during 1000 seconds
- All three codes agree very well within **5% relative error**.



Figures by Heeho Park

Klinkenberg Effect

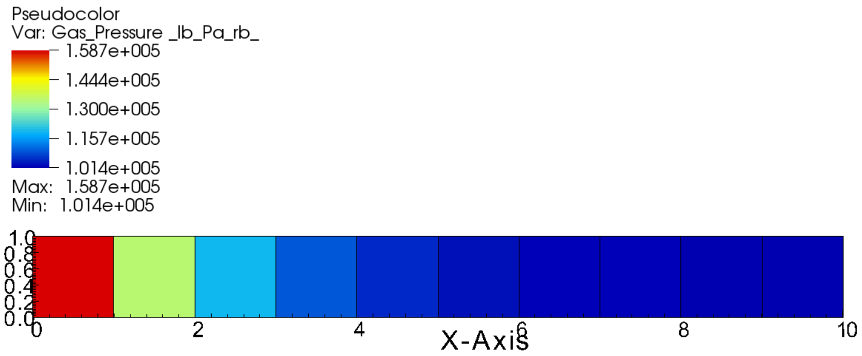
- Gas flow in porous media differs from liquid flow because of the large gas compressibility and pressure-dependent effective permeability
- Klinkenberg noticed the latter to have significant impact on gas behavior especially in low permeability media.
- BRAGFLO calculates the Klinkenberg effect on gas permeability’s using the following equation:

$$k_g = k_w \left(1 + \frac{b k_w^a}{p} \right)$$

where
k_g = intrinsic permeability to gas [m^2],
k_w = intrinsic permeability to brine [m^2],
a = rock formation-dependent constant,
b = rock formation-dependent constant,
p = gas pressure [Pa]

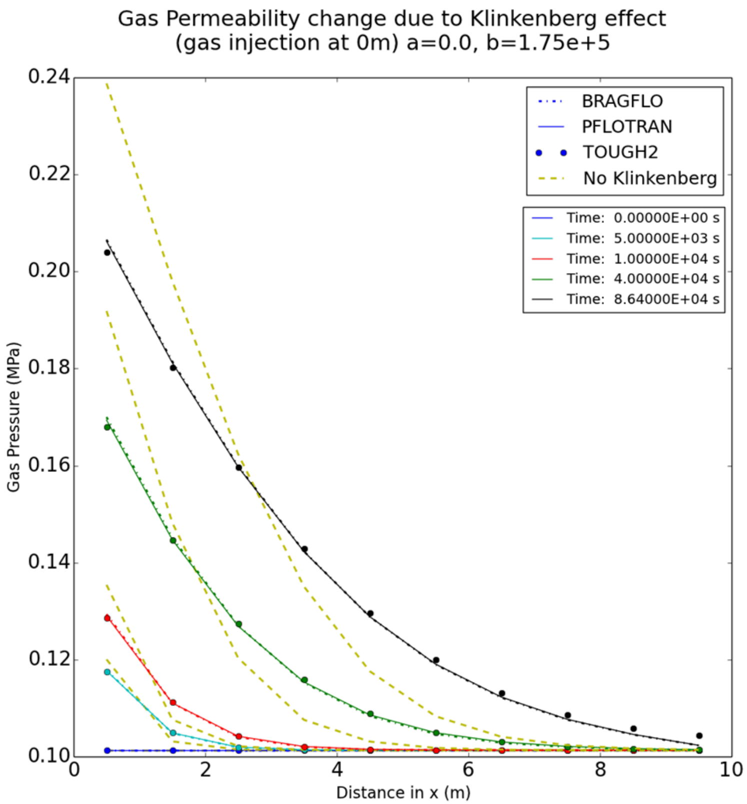
Klinkenberg Effect

- Ten 1m cells in x-direction
- No-flow left boundary
- 1 atm with 100% gas saturation boundary on the right
- Gas injection at the rate of 1.0e-6 kg/s at the left most cell



Klinkenberg Effect

- Gas pressure propagates to right quicker with Klinkenberg effect
- All three codes agree within 1% relative error.



Questions? (References)

- 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).
- HDF Group. HDF5, *Hierarchical Data Format*, URL: http://www.hdfgroup.org/HDF5 (2013).
- C. CAMPHOUSE, *Requirements Document & Validation and Verification Plan for BRAGFLO Version 6.02 ERMS# 558659*, Sandia National Laboratories, Albuquerque, NM (2012)
- YU-SHU WU, KARSTEN PRUESS, and PETER PERSOFF, *Gas Flow in Porous Media with Klinkenberg Effects, Earth Sciences Division*. Lawrence berkely National Laboratory, Berkeley, CA 94720, USA (1998)
- S. BALAY, W. GROPP, L. C. MCINNES, and B. F. SMITH*, PETSc, the portable, extensible toolkit for scientific computation*, Argonne National Laboratory (1998).