A 3-D Integrated Multi-Physics UCG Simulator Applied to UCG Field Tests

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Based on conference presentations in August 2012 and June 2013

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Disclaimer

Auspices Statement

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Preface (2017)

In the late 1980's, Lawrence Livermore National Laboratory (LLNL), developed an outstanding multi-physics two-dimensional model of the underground coal gasification (UCG) process called CAVSIM (c.f. Britten and Thorsness, 1989). From 2009 to 2013, a different LLNL team developed along the same lines a modern high-fidelity multi-physics three-dimensional model of UCG called UCG-SIM3D.

UCG-SIM3D models much the same phenomena as CAVSIM, but takes advantage of modern computational capabilities, algorithms, and software elements from other state-of-art codes. Important advances over CAVSIM include: flexible 3-D geometry that allows for arbitrary spatial variations of geologic properties such as multiple coal seams of different compositions, dip, varying permeabilities, etc.; flexibility to move one or more injection points and production points to locations that can change with time; a sophisticated algorithm that tracks 3-D growth of the cavity and rubble boundaries and rubble composition; an improved 3-D model of flow, reactions, and heat transfer within the rubble bed and in the open void region; a 3-D non-isothermal unsaturated water and gas flow model for both the near- and far-field surroundings. As with CAVSIM, sideward and upward growth of the cavity in coal and overburden rock is by spalling, with user-specified rate coefficients in a temperature-dependent model. The code structure would allow for interface with a geomechanics code that could predict cavity growth by structural roof collapse, but this was not implemented. After fitting some parameters, UCG-SIM3D very accurately calculated the 3-dimensional development of the cavity and its rubble contents, the 3-dimensional temperature, pressure, and composition fields, and product gas composition of the Hoe Creek III and Rocky Mountain 1-CRIP field tests. UCG-SIM3D development ended before being matured into an engineering tool for use by non-experts.

UCG-SIM3D was not fully documented in a technical report, as the last available resources were directed at completing the successful simulation of the Rocky Mountain 1 UCG field test. A 2013 conference presentation (Camp et al., 2013) has been the best overview description of the UCG-SIM3D model. (That 2013 presentation superceded another very similar 2012 conference presentation (Camp et al., 2012)). The 2013 presentation is reproduced here as an LLNL Technical Report to make it easily accessible to a wider audience. This Preface has been added and the cavity sketch in Slide 14 has modified to more properly illustrate the vertical growth of the cavity. Two accessible technical reports that describe the model at earlier stages of development are Nitao et al., 2011 and Nitao et al., 2010. The code itself and its software-level documentation were largely written by John Nitao and reside within LLNL as internal files.

David W. Camp
LLNL UCG program leader, 2009-2014

Preface References:

The proper citation for this document is:

Camp, D.W., J. J. Nitao, J. A. White, J.L. Wagoner, G. C. Burton, T.A. Buscheck, C. M. Reid, S.M. Ezzedine, M. Chen, and S. J. Friedmann. ([2013] 2017). A 3-D Integrated Multi-Physics UCG Simulator Applied to UCG Field Tests. LLNL-TR-738118.

Other documents referenced here-in are:

Britten, J.A. and C.B. Thorsness. (1989). A Model for Cavity Growth and Resource Recovery During Underground Coal Gasification, *IN SITU*, 13(1&2), 1-53.

Camp, D.W., J. J. Nitao, J. A. White, G. C. Burton, C. M. Reid, S. J. Friedmann. (2013). A 3-D, Multi-Physics UCG Simulator Applied to UCG Field Tests. LLNL-PRES-564357, and in: *Proc. 8th UCGA Conf. & Workshop on UCG, June 2013, London*

Camp, D.W., J. J. Nitao, J. A. White, G. C. Burton, C. M. Reid, S. J. Friedmann. (2012). A Fully Integrated 3-D Multi-Physics UCG Simulator Applied to UCG Field Tests. LLNL-PRES-564357-DRAFT, and in: *Proc. UCG Workshop, IEA Clean Coal Centre, Banff, Aug. 2012*

Nitao, J.J., D.W. Camp, T.A. Buscheck, J.A. White, G.C. Burton, J.L. Wagoner, and M. Chen. (2011). Progress on a New Integrated 3-D UCG Simulator and its Initial Application. LLNL-CONF-50055, and In: *Proc. Int. Pittsburgh Coal Conf., Pittsburgh, Sept 2011*.

Nitao, J.J., T.A. Buscheck, S.M. Ezzedine, S.J. Friedmann, and D.W. Camp. (2010). An Integrated 3-D UCG Model for Predicting Cavity Growth, Product Gas, and Interactions with the Host Environment. LLNL-CONF-459611, and in: Proc. 27th An. Int. Pittsburgh Coal Conference, October 11-14, 2010, Istanbul.

The slides that follow in this 2017 TR document are nearly identical to a June 2013 presentation prepared for the UCGA Conference in London

A 3-D, Multi-Physics UCG Simulator Applied to UCG Field Tests

8th UCGA Conference and Workshop on Underground Coal Gasification

June 5-6, 2013 • London

Lawrence Livermore National Laboratory

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LLNL-PRES-564357

This work was performed under the auspices of the U.S. Department of Energy by Lawrence Livermore National Laboratory under contract DE-AC52-07NA27344. Lawrence Livermore National Security, LLC

The June 2013 presentation prepared for the UCGA Conference followed a very similar presentation made at the August 2012 IEA Clean Coal Centre's UCG Workshop

A Fully Integrated, 3-D, Multi-Physics UCG Simulator Applied to UCG Field Tests

IEA Clean Coal Centre
2nd Underground Coal Gasification Network Workshop

August 22-23, 2012 • Banff, Alberta, Canada

Lawrence Livermore National Laboratory

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LLNL-PRES-564357

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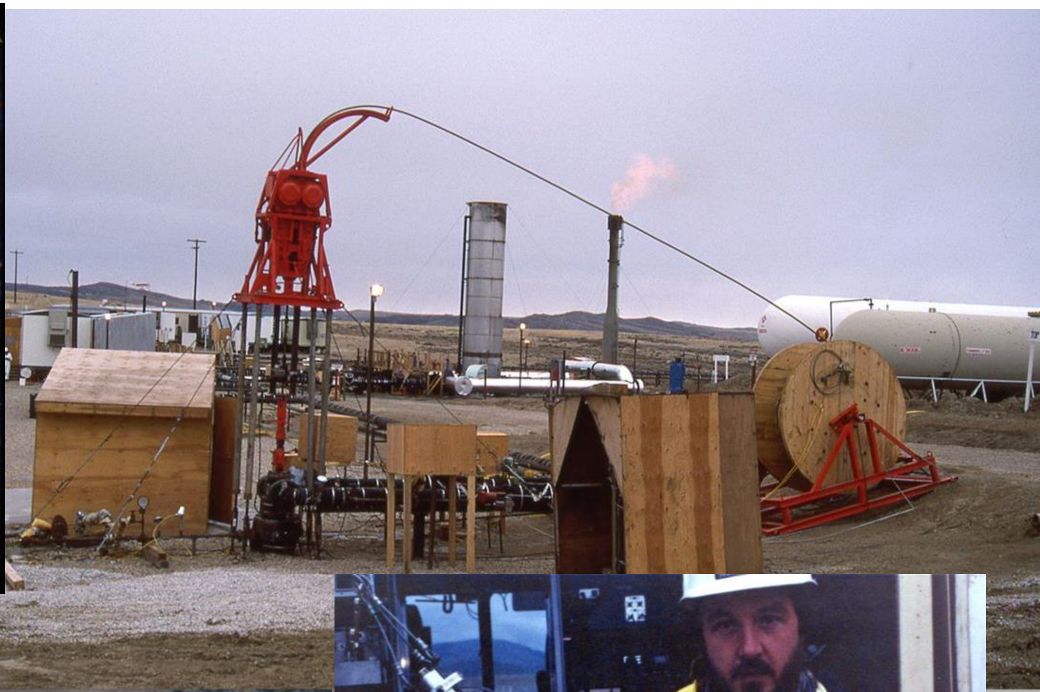
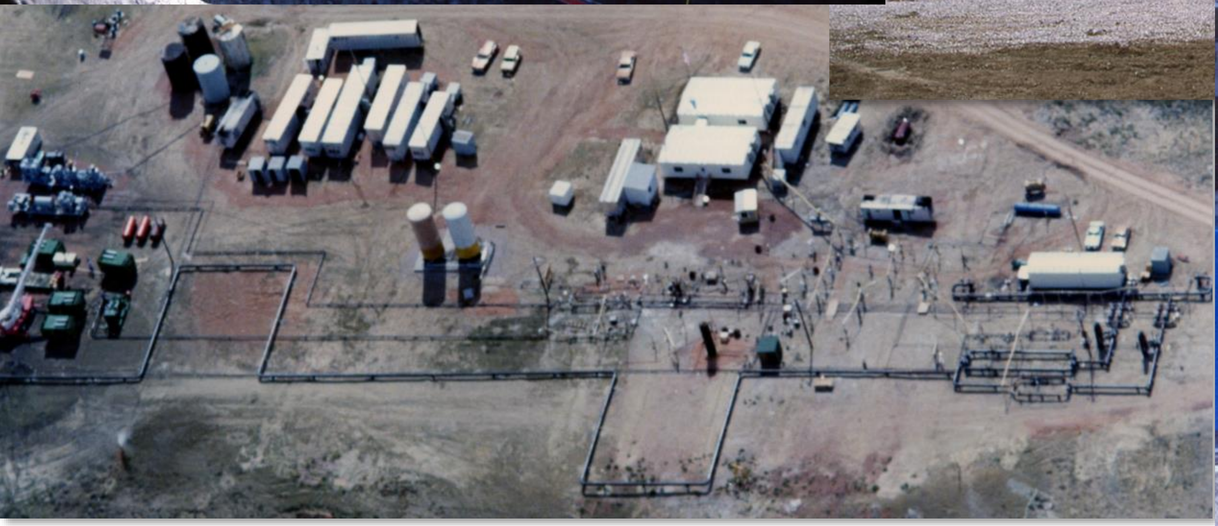
- Approximately 6,000 employees
  - Scientists, engineers, technicians, and support staff
- World class experimental and computational facilities, capabilities
- Multidisciplinary project approach
- Worldwide reputation in supercomputing

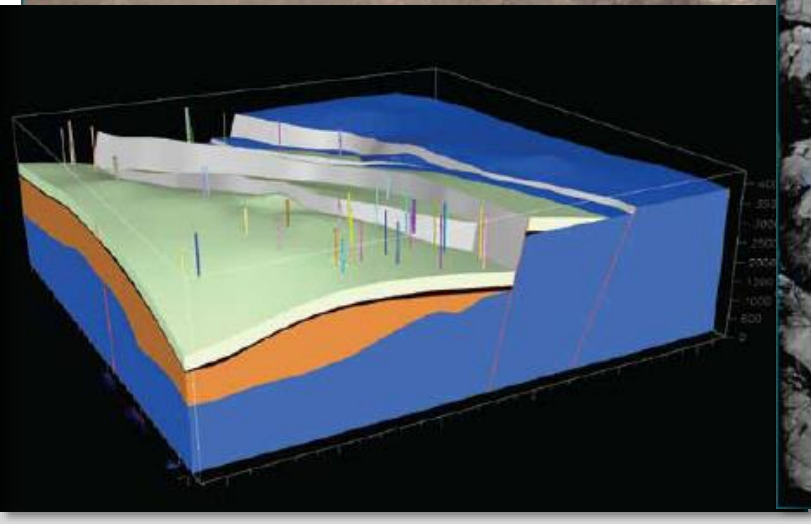
LLNL was a UCG leader in the 1970's and 1980's - only US institution still active in UCG

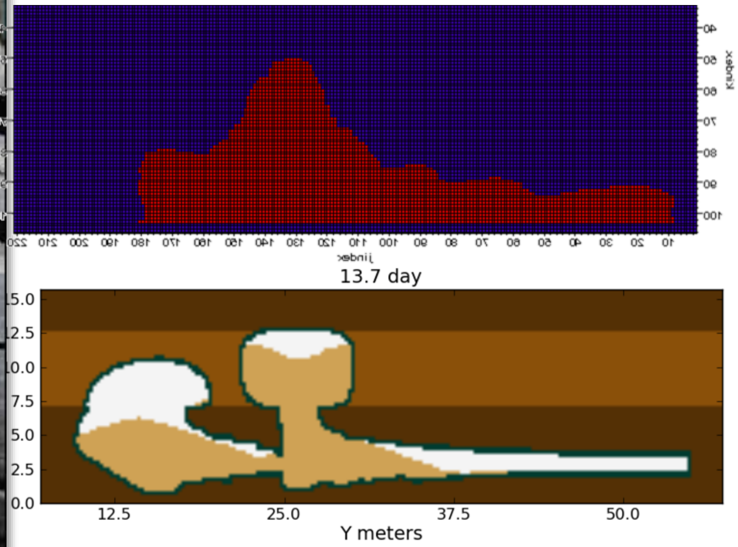




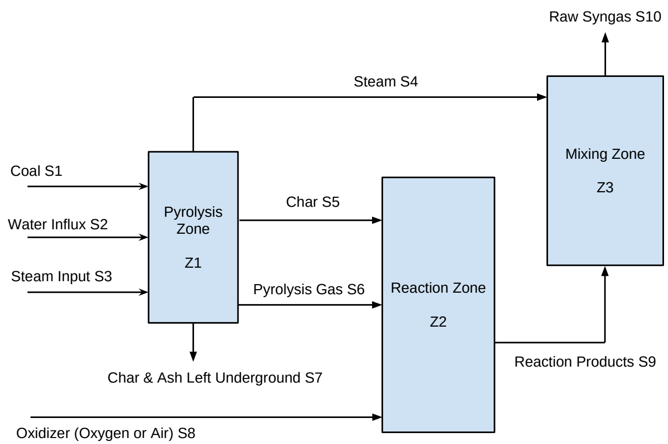
We continue with state-of-art analyses and practical support for projects

- Site Selection
- Site Characterization
- Design
- Simulation
- Environmental Analyses
- Critical Reviews
- Process engineering and economics
- Monitoring
- Program planning

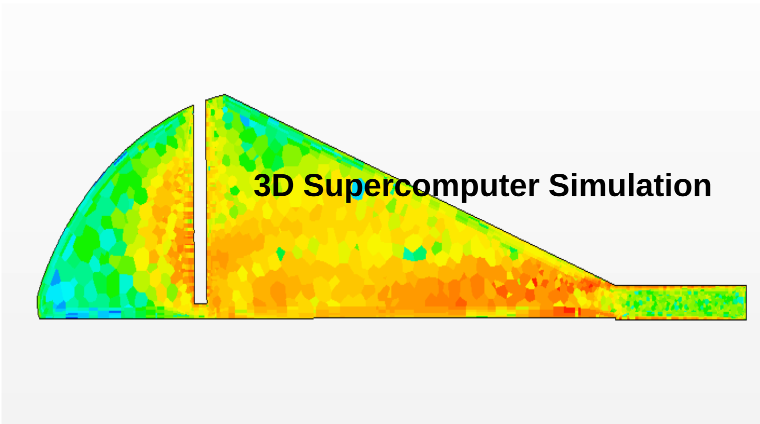


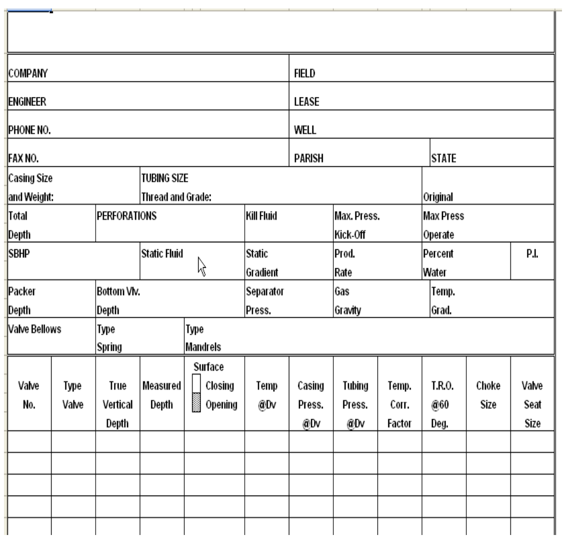


We have a multidisciplinary UCG team of ~20, and a suite of UCG modeling tools, from simple to simulator



UCG-MEEE

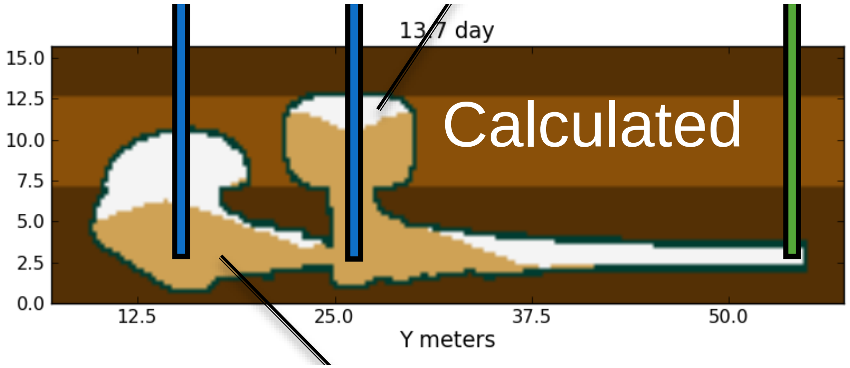




COMPANY		FIELD	
ENGINEER		LEASE	
PHONE NO.		WELL	
FAX NO.		PARISH	STATE

Casing Size and Weight:	TUBING SIZE Thread and Grade:				Original	
Total Depth	PERFORATIONS		Kill Fluid	Max. Press. Kick-Off	Max Press Operate	
SBHP	Static Fluid		Static Gradient	Prod. Rate	Percent Water	P.I.
Packer Depth	Bottom Vlv. Depth		Separator Press.	Gas Gravity	Temp. Grad.	
Valve Bellows	Type Spring	Type Mandrels				

Valve No.	Type Valve	True Vertical Depth	Measured Depth	Surface Closing Opening	Temp @Dv	Casing Press. @Dv	Tubing Press. @Dv	Temp. Corr. Factor	T.R.O. @60 Deg.	Choke Size	Valve Seat Size



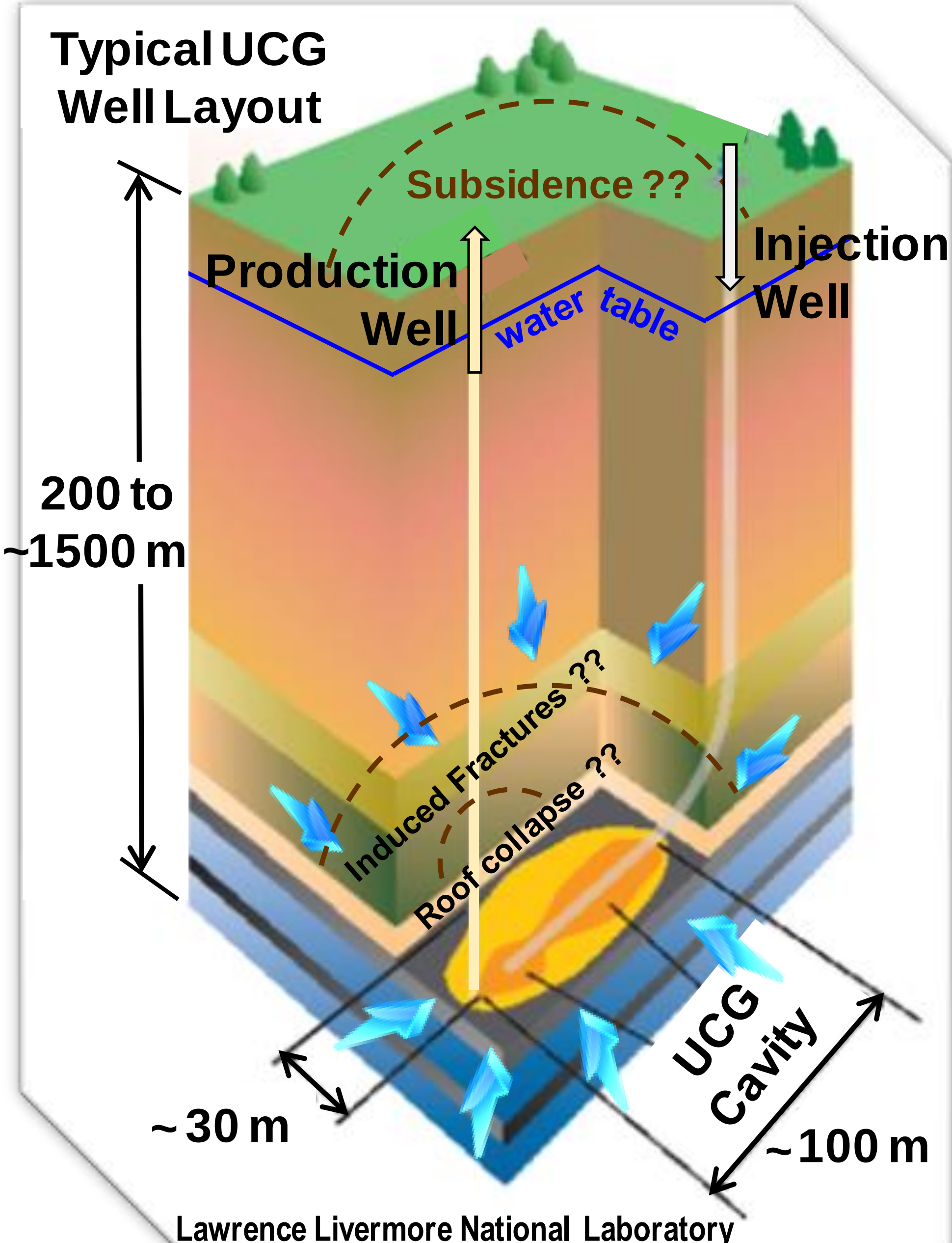
Simulator Goal:
A Full-physics, flexible 3-D UCG simulator

- **Models all necessary physical domains**
  - **Near-field cavity, wall, and rubble zones**
  - **Far-field hydrologic and geomechanic domains**
- **Flexible and powerful**
  - **Complex geology**
  - **Any module design**
- **Predictive**
  - **Cavity shape is predicted, not specified**
  - **Product composition, hydrologic pressure field, overburden changes**
  - **Process details such as T, P fields**

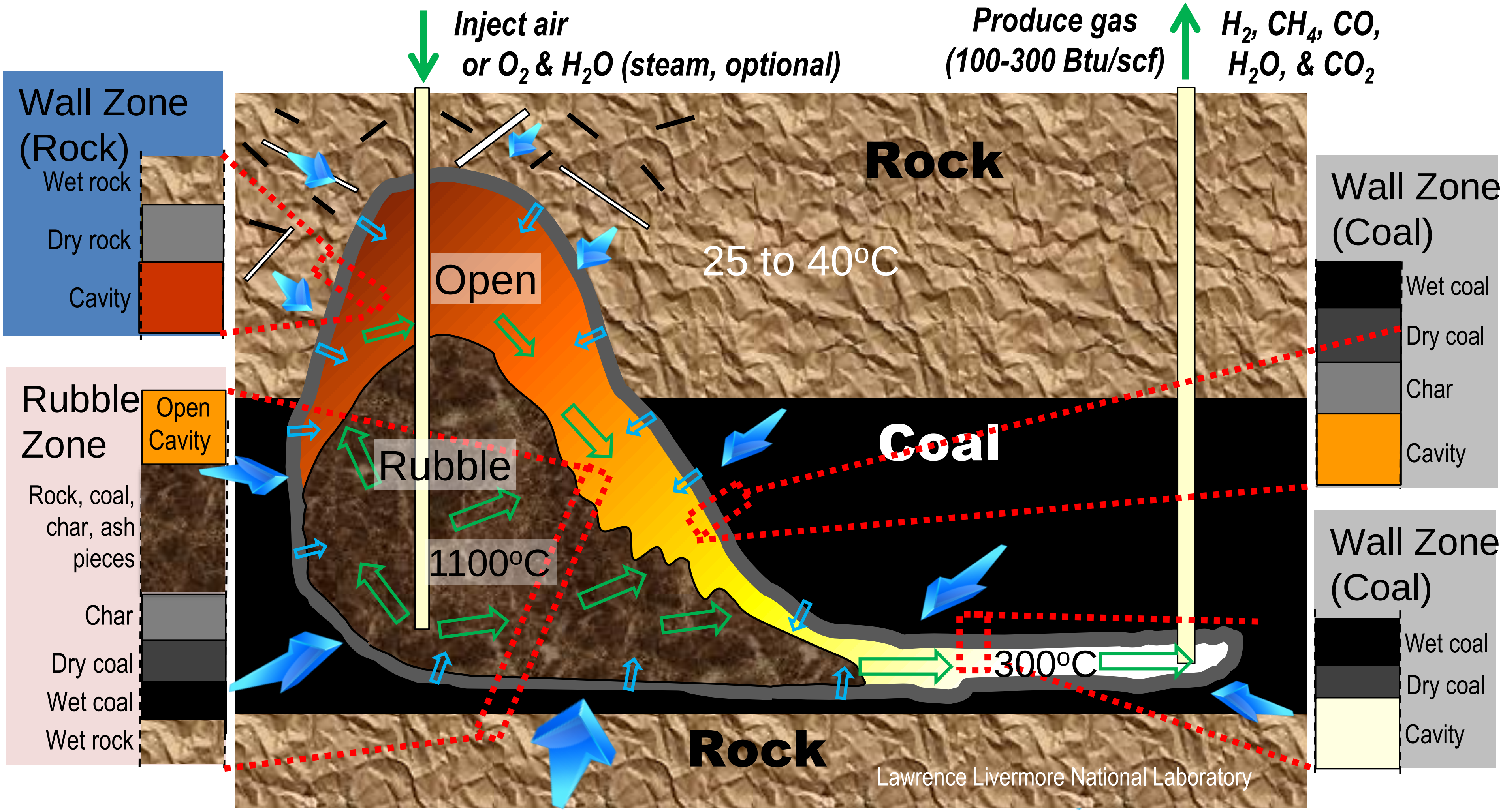
LLNL's Simulation Philosophy

- Model the right physics
- Assure the model is consistent with observations and the best understanding of how UCG works
- Stand on the shoulders of past giants
- Employ modern computational capabilities

Hydrology and geomechanics are important far-field domains

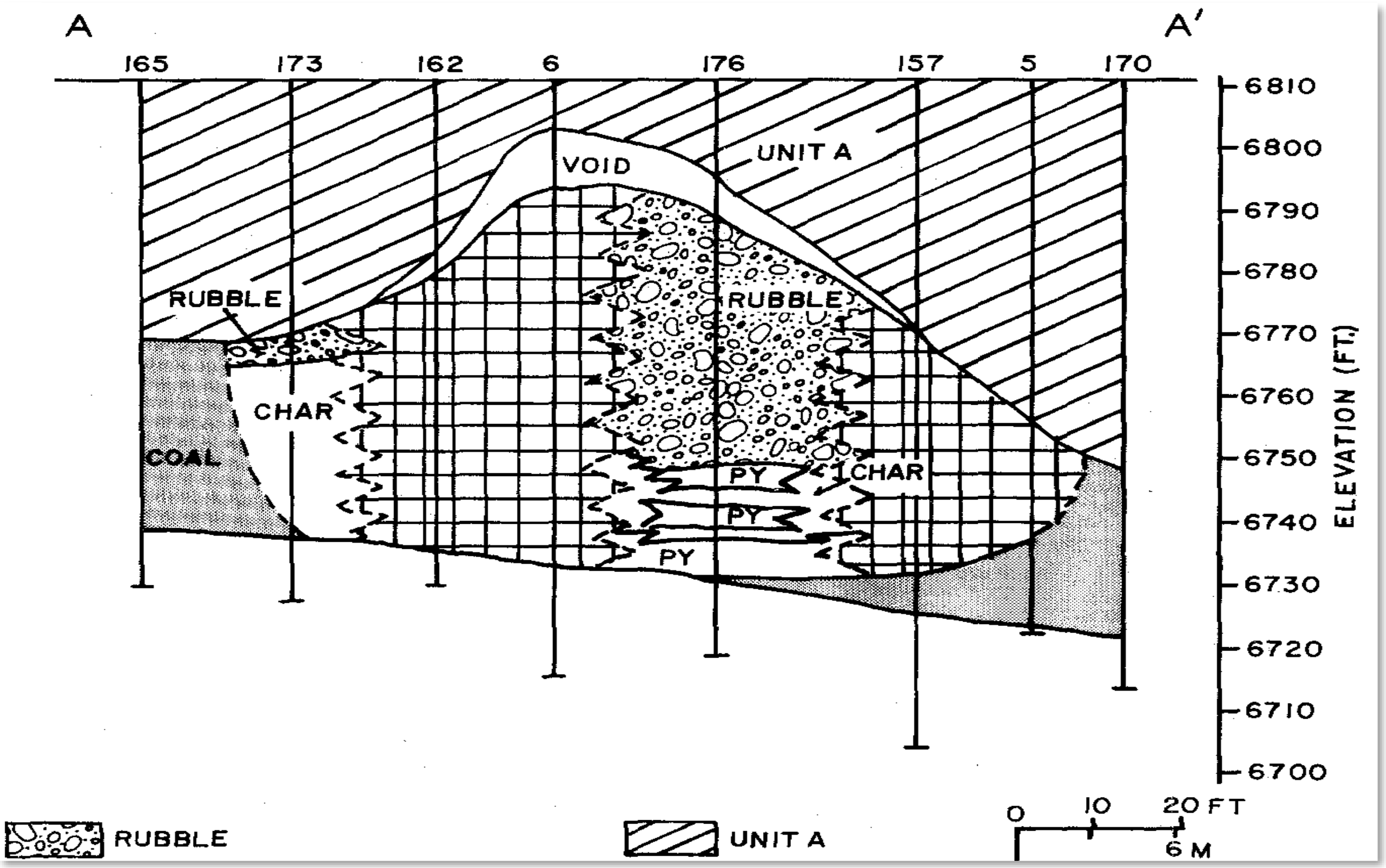


Near-field domains include open cavity, rubble cavity, coal wall zone, rock wall zone, and near surroundings.



$$\text{Coal } (\sim C\,H_{0.8}\,O_{0.2}) + O_2 + H_2O_\ell \longrightarrow CO + H_2 + CH_4 + HC\text{'s} + CO_2 + H_2O_g$$

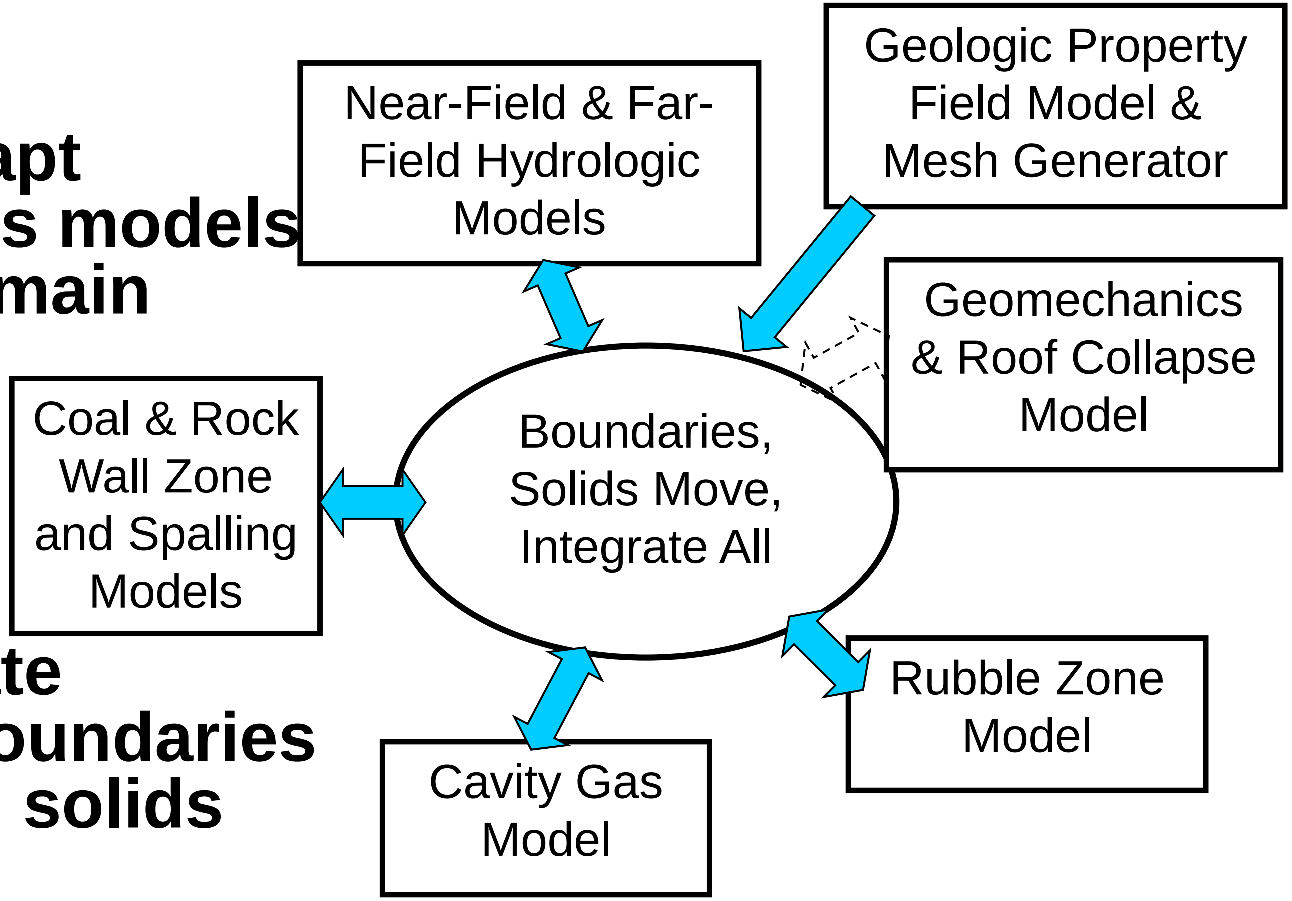
Cavities often grow up in the coal and into the overburden by small-scale spalling and/or mechanical collapse. Collapsed solids form a packed bed that allows gas flow, dries, reacts, moves, and transfers heat.



Hanna Test Cross-Section

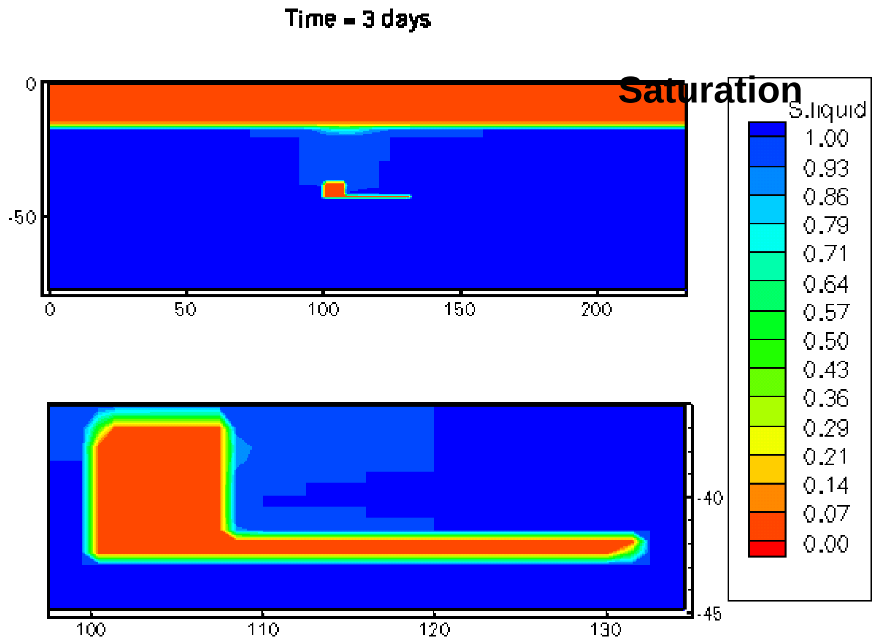
Models of key domains are coupled

- **Build or adapt best-in-class models for each domain**
- **Track and communicate changing boundaries and moving solids**
- **Couple and integrate**

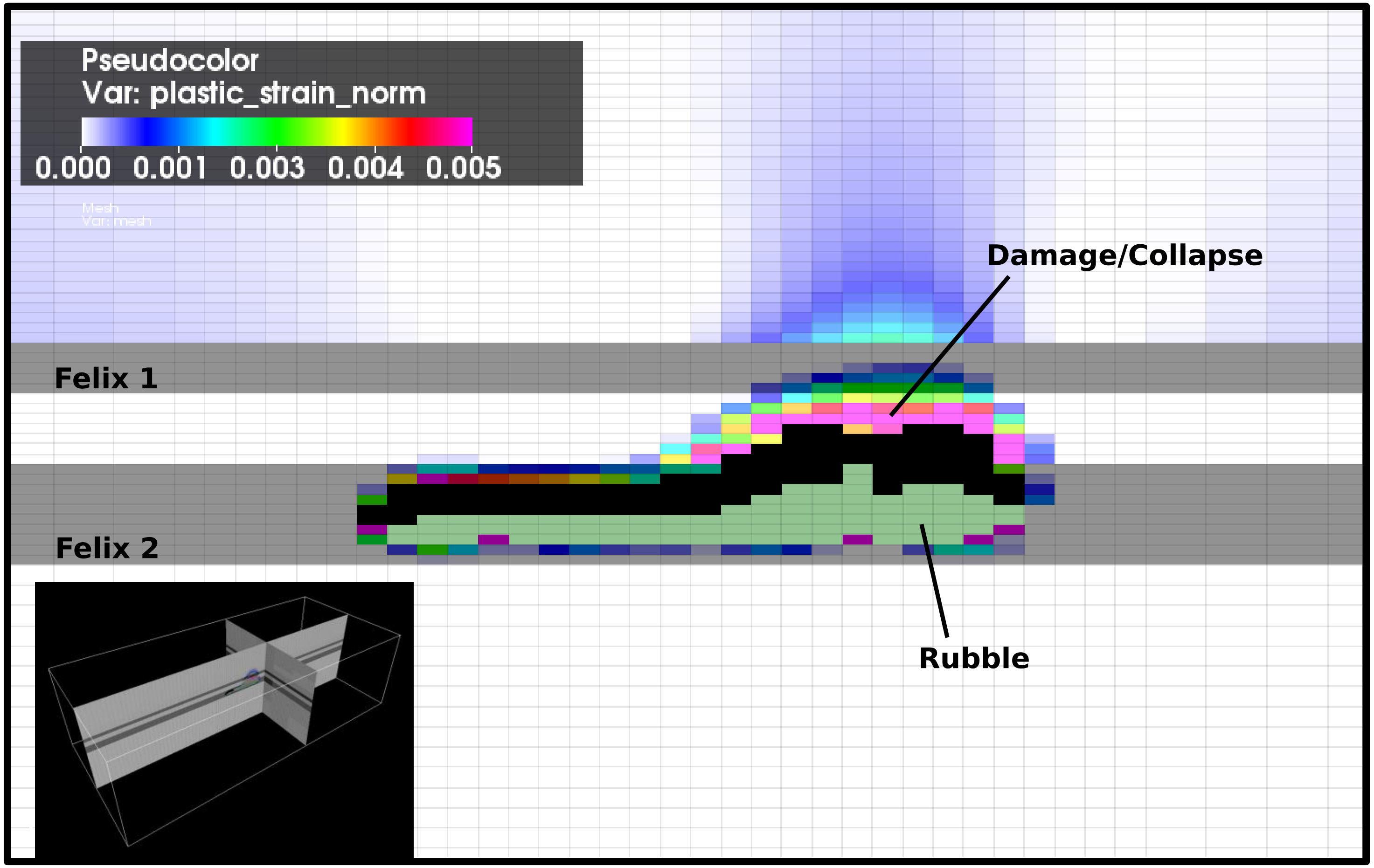


Far-field and near-field transport of fluids and heat outside the cavity use LLNL's NUFT code (NonIsothermal Unsaturated Flow & Transport)

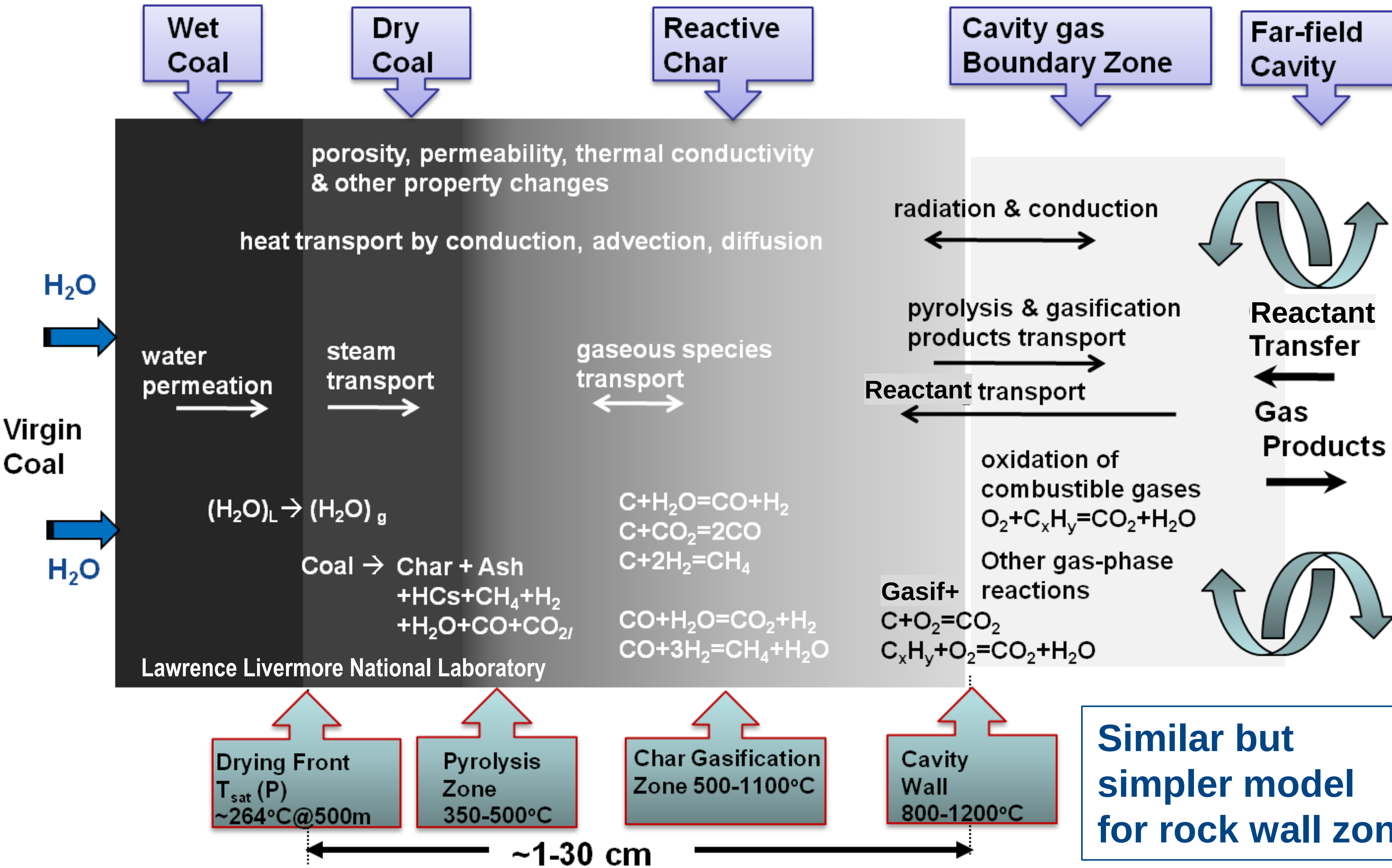
- Porous media flow and transport
- Thermal and chem transport
- Saturated and unsaturated
- Matrix and fracture flow and transport
- Meshing from geomodel
- Handles active aquifer management activities
- Usually we use:
- Near-field is unsaturated nonisothermal
- Far field is saturated isothermal



For geomechanics we use a streamlined version of state-of-art Geocentrics code

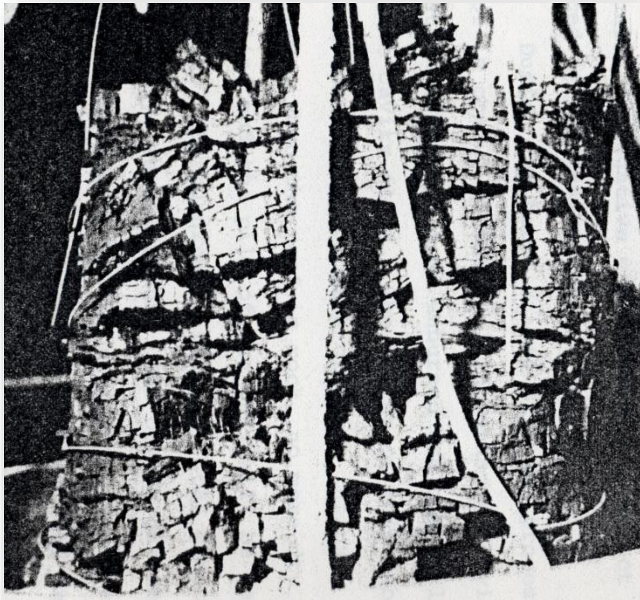


Coal wall zone model includes transport and reactions at fine spatial resolution. With spalling.



Similar but simpler model for rock wall zone

Spalling can be a major mechanism of vertical and sidewards cavity growth



Photos of heated cores

(Oak Ridge National Laboratory, ca 1978)

Wilcox Lignite 15 cm heated to 800°C

Hoe Creek Overburden 5 cm heated to 1000°C

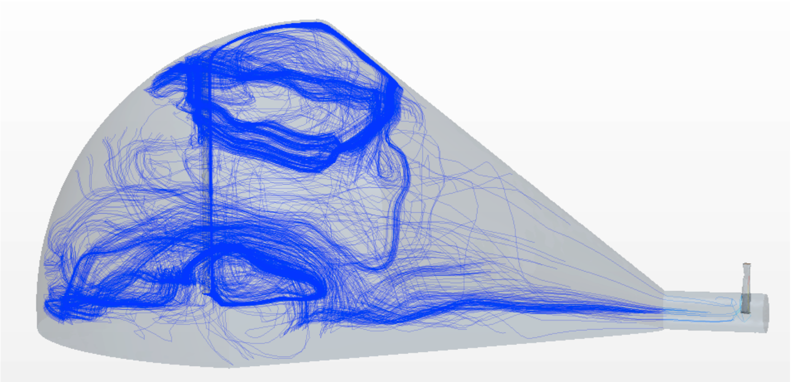
- **Spalling is the localized fracture and falling of coal or rock, typically:**
  - **scale of a few millimeters up to a meter**
  - **at or near drying front or zones of high local gradients**
  - **due to steam escape pressure, thermo-mechanical stresses, …**

Our wall-zone models for coal and roof rock include spalling

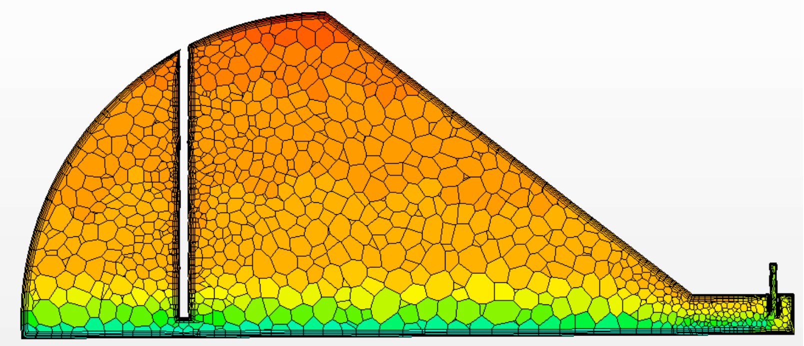
For the open cavity domain, we use a 3-D advection dispersion model with reactions and radiation. Advised by CFD runs.

- 3-D Advective-Dispersive
  - Potential flow with or without gravity
  - Dispersivities f()
  - Full reactions
  - Radiative and convective heat transfer
  - Advised by CFD runs
- 3-D CFD (STAR)
  - Too slow
- 2-D CFD (STAR)
  - Inadequate

3-D CFD simulation of 75 x 60 x 40 m cavity. With heat, buoyancy, turbulence, radiation, but no chemistry



Streamline trace through center plane



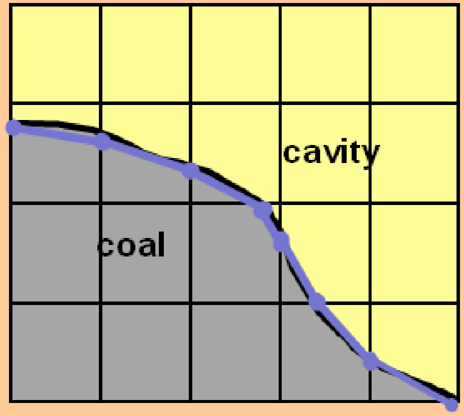
Temperature profile through center plane

Rubble Zone Model is a 3-D extension of the Britten-Thorsness model, + extra physics & chemistry

- **Accumulations from falling ash; spalled char, coal, and roof rock; collapsed roof rock**
- **Solids move due to gravity, angle of repose, and settling (from reaction-caused volume reduction)**
- **3-D fluid flow (gas and liquid) within rubble with radiative and convective heat transport, & dispersive mass transport**
- **Full set of gas, solid, and heterogeneous reactions**
- **Tracks rubble composition (Char, VM, Ash, Rock) & energy**

The Boundary and Rubble Tracking Module uses a sophisticated algorithm to move material and boundaries

- **Algorithm tracks wall boundaries within a 3-D lattice of small cubes**

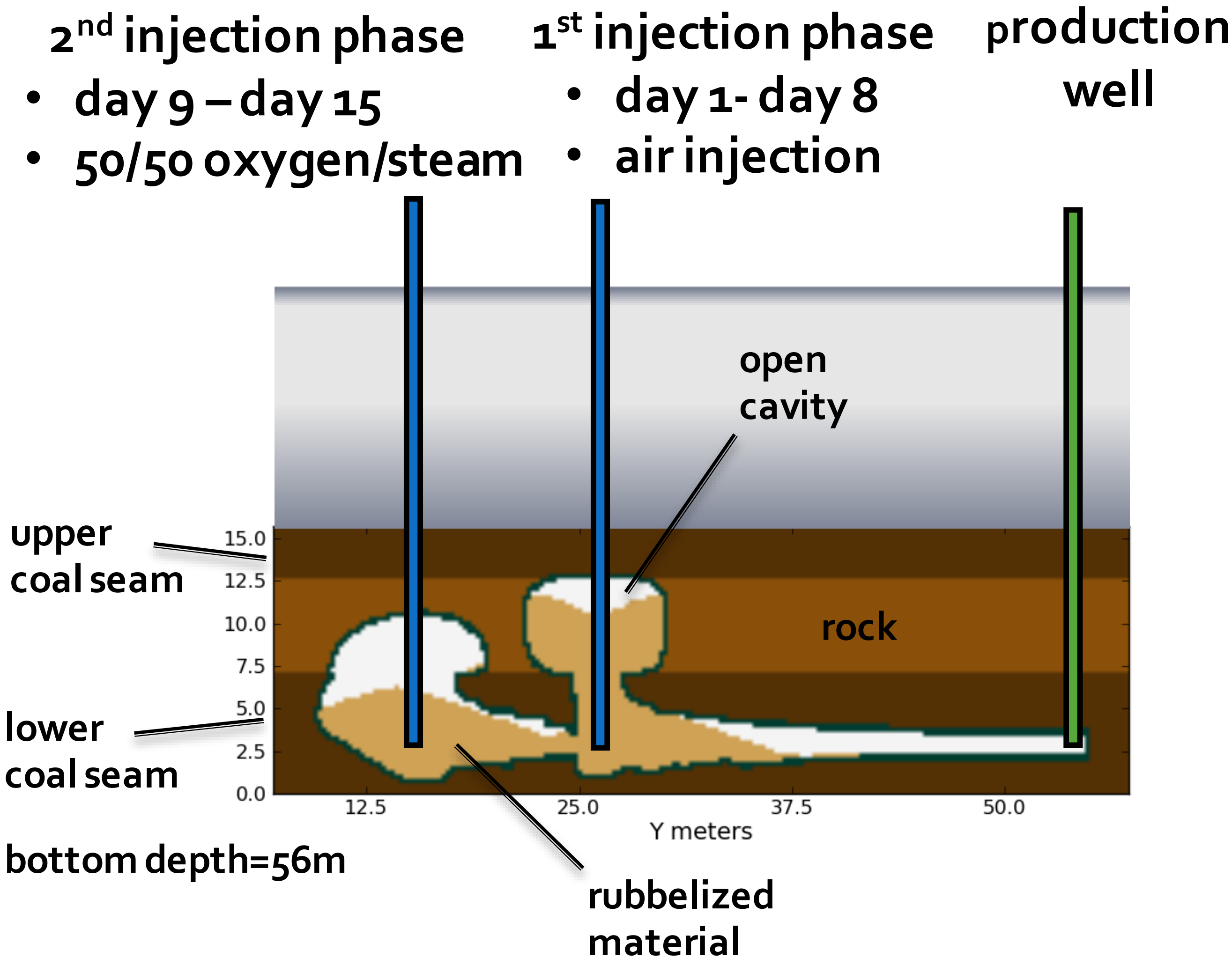


- **Conserves mass exactly**
- **Handles convex and concave curvature**
- **Accommodates small-scale spalling and large-scale block collapse**
- **Simplifies computational geometry**

Simulation of our old field tests

- **Version 1 applied to Hoe Creek III Days 1-13**
- **Version 2 modeling Rocky Mountain 1 CRIP Days 1-35**

The Hoe Creek III test (1979, Powder River Basin, WY) had two coal seams, two injection points, two injection compositions, and changing injection rate and pressure



Hoe Creek III observed cavity growth

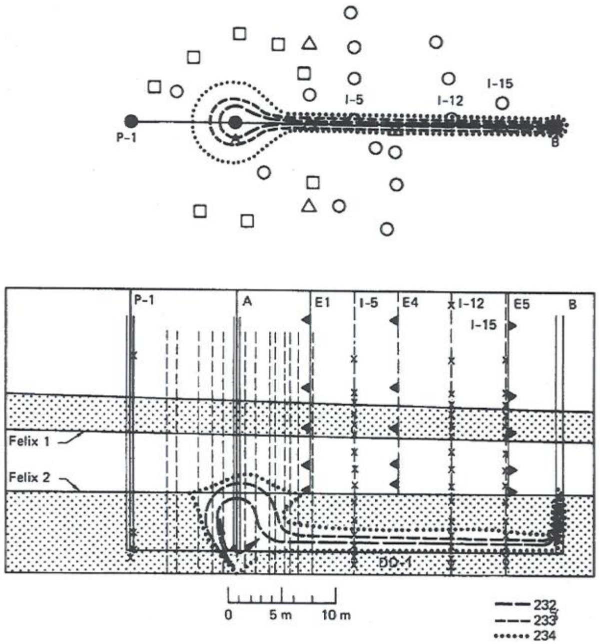


FIG. 8. Plan and elevation views of the Hoe Creek No. 3 burn cavity on days 232, 233, and 234.

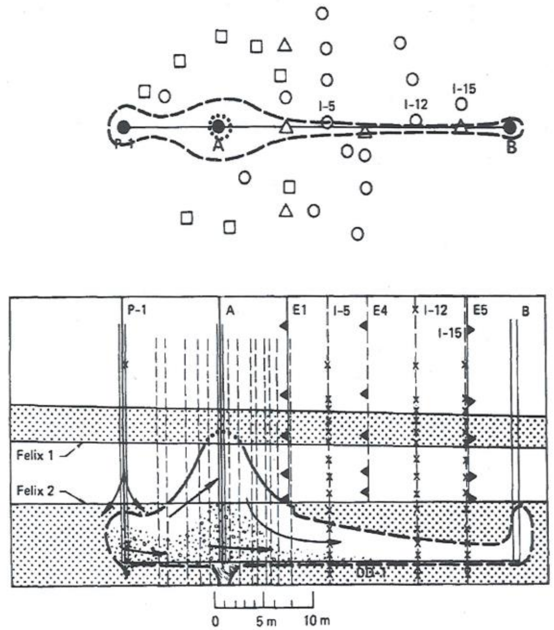


FIG. 12. Plan and elevation views of the Hoe Creek No. 3 burn cavity on day 238 of 19

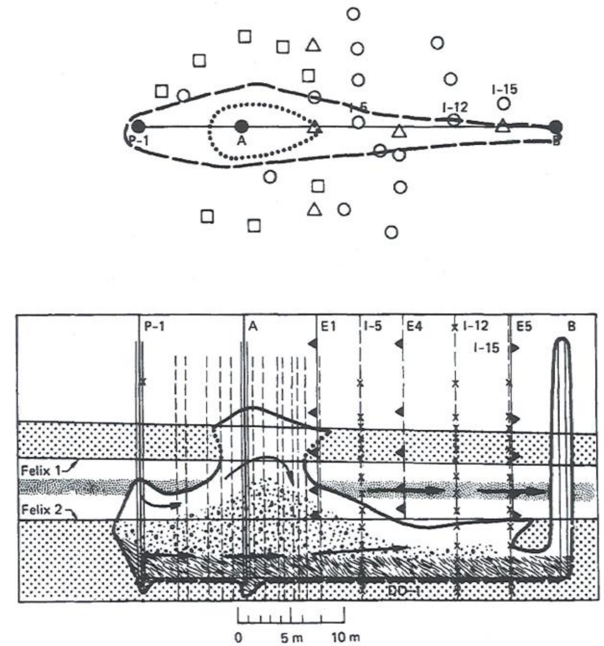
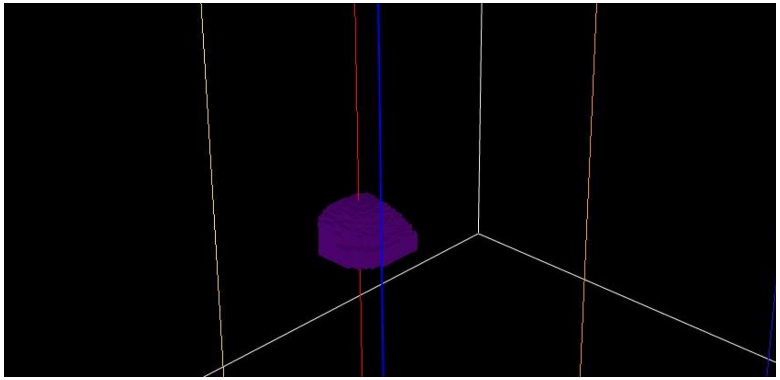


FIG. 14. Plan and elevation views of the Hoe Creek No. 3 burn cavity for day 242.

Observed Cavity Growth for Hoe Creek III

Frames from a 3-D visualization of reported cavity boundary locations

1



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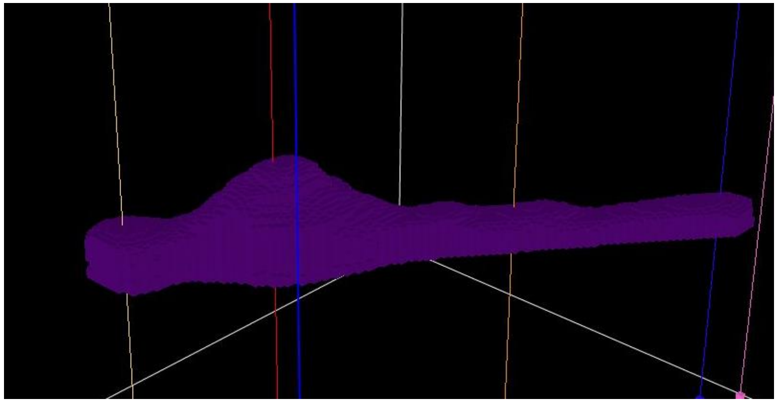

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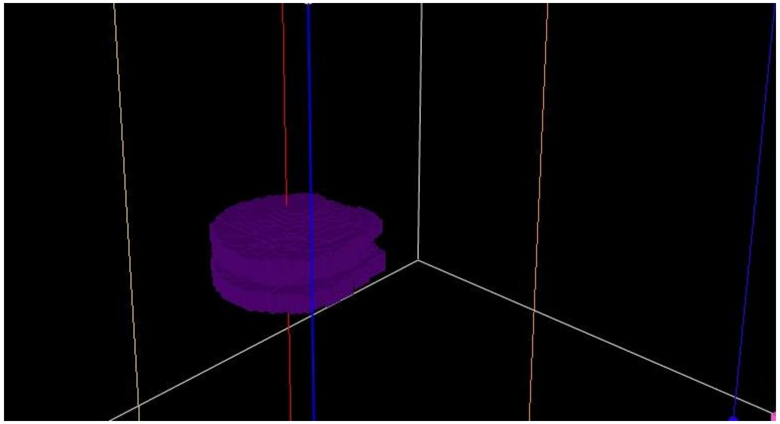

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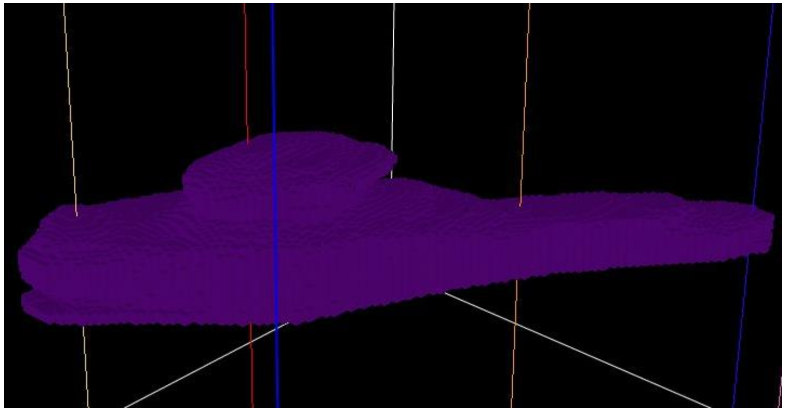
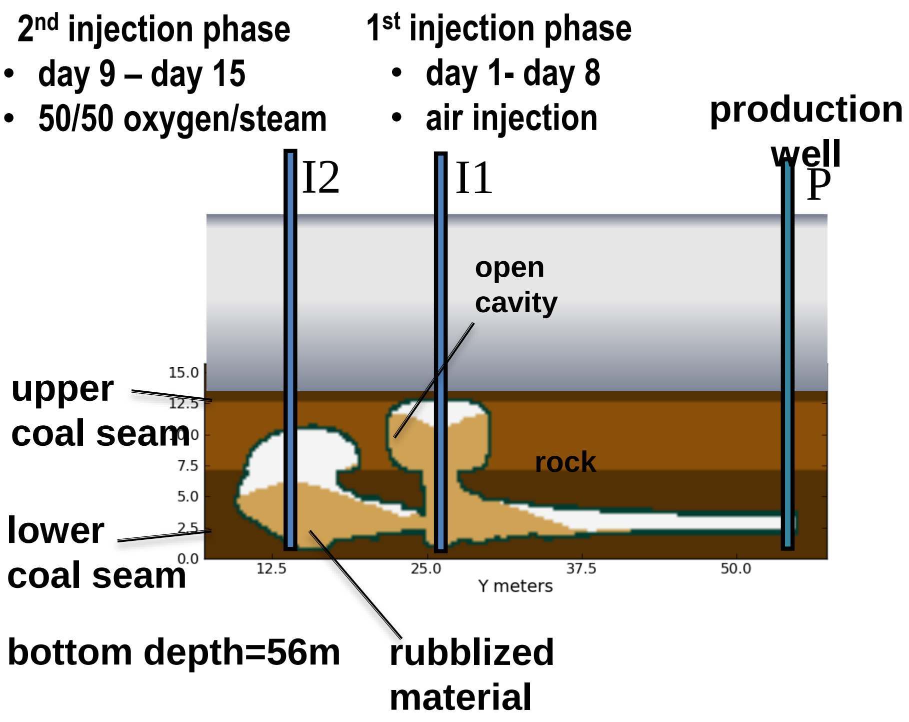
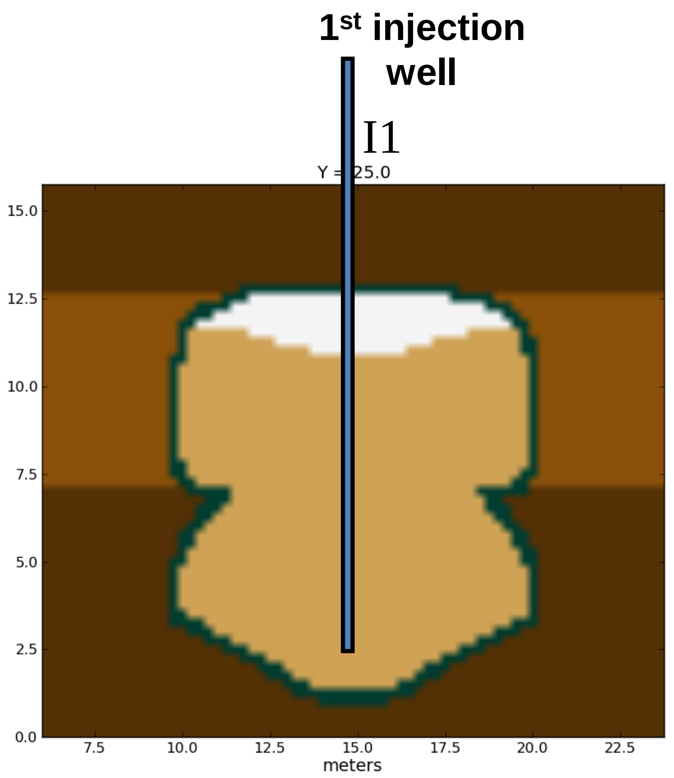


The following movie shows simulation results for cavity growth and rubble accumulation



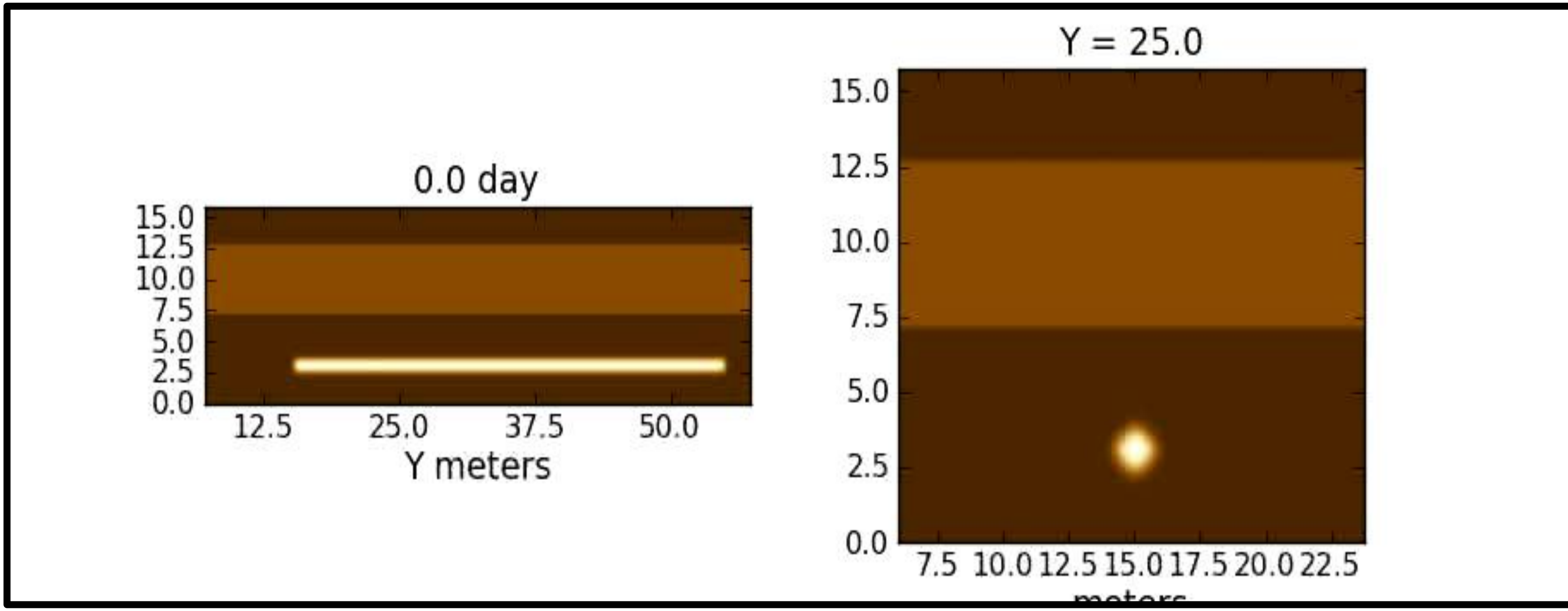
side view



cross-section at 1st injector

Simulation* of HC-III Cavity Growth

Movie of model-calculated zone locations in .ppt file



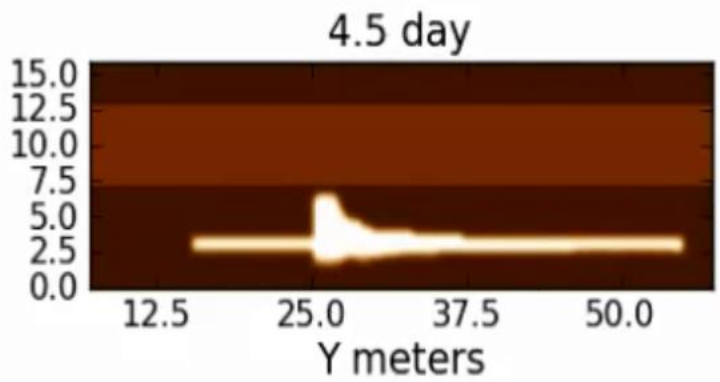
side view

cross-section at 1st injector

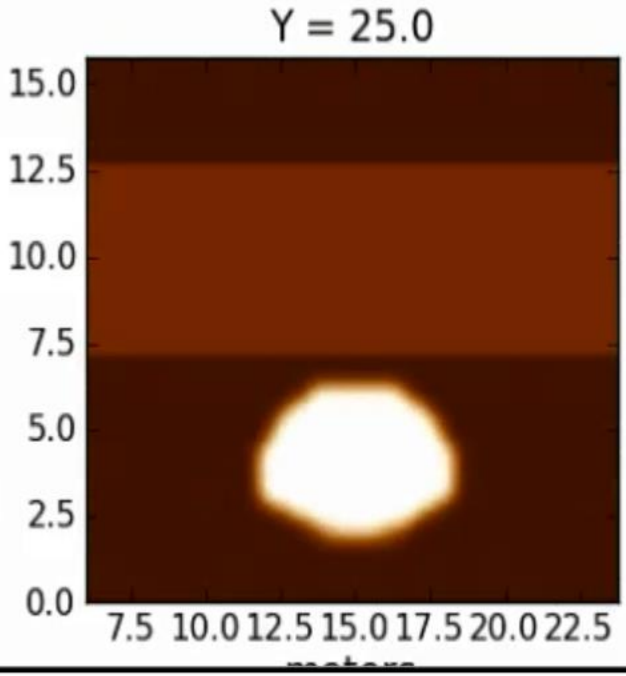
* Hoe Creek III simulations used the 2011 version of UCG-SIM3D

Simulation* of HC-III Cavity Growth

Snapshots at progressing time, 4.5 days; injecting into well I-1



side view

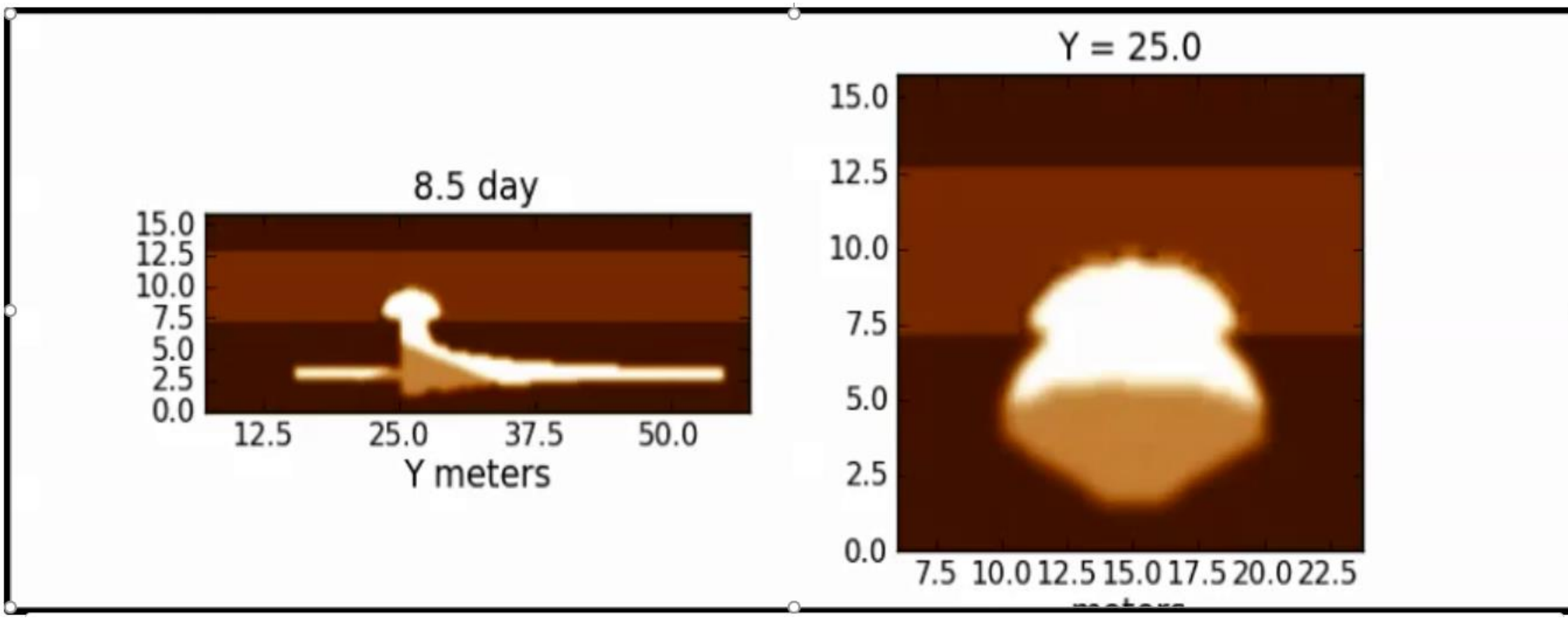


cross-section at 1st injector

* Hoe Creek III simulations used the 2011 version of UCG-SIM3D

Simulation* of HC-III Cavity Growth

Snapshot at progressing time, 8.5 days; still injecting into well I-1



side view

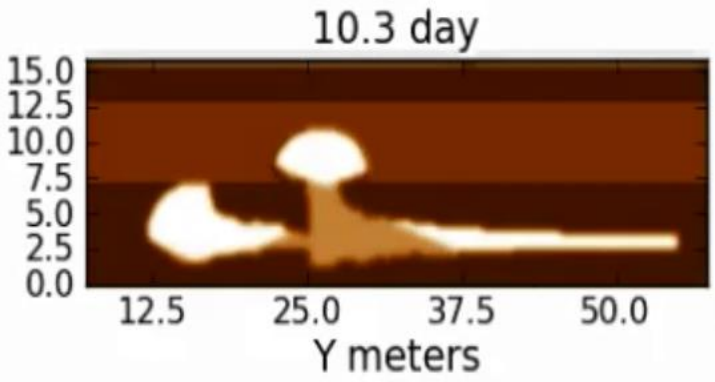
cross-section at 1st injector

* Hoe Creek III simulations used the 2011 version of UCG-SIM3D

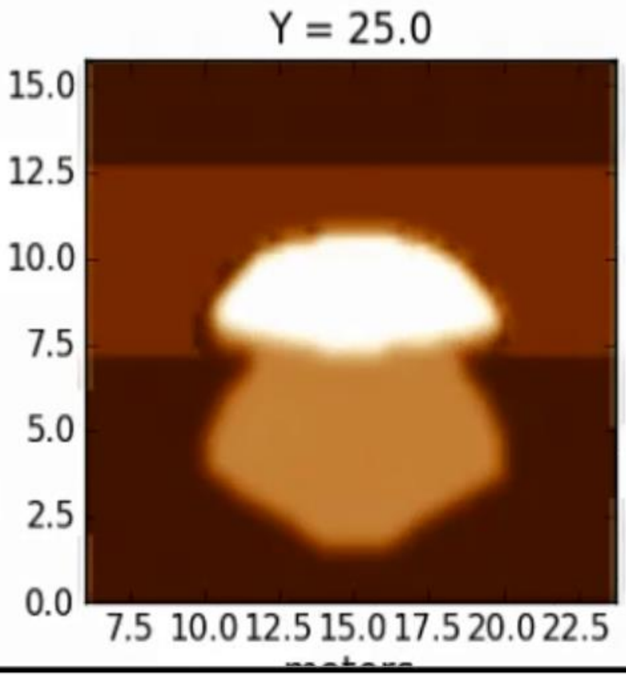
The lack of backward burn within the coal was fixed before the Rocky Mountain 1 simulations

Simulation* of HC-III Cavity Growth

Snapshot at 10.3 days; after switching injection to I-2



side view

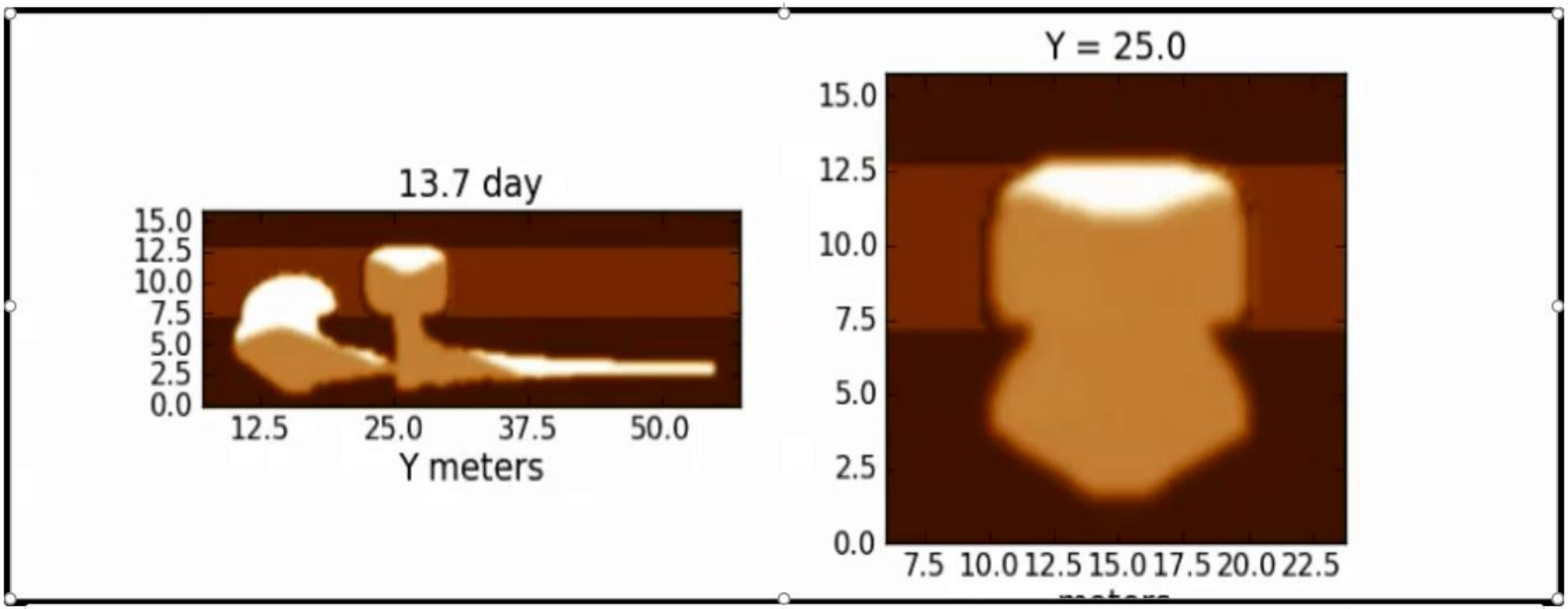


cross-section at 1st injector

* Hoe Creek III simulations used the 2011 version of UCG-SIM3D

Simulation* of HC-III Cavity Growth

Snapshot at 13.7 days; spalling had penetrated up to the upper seam



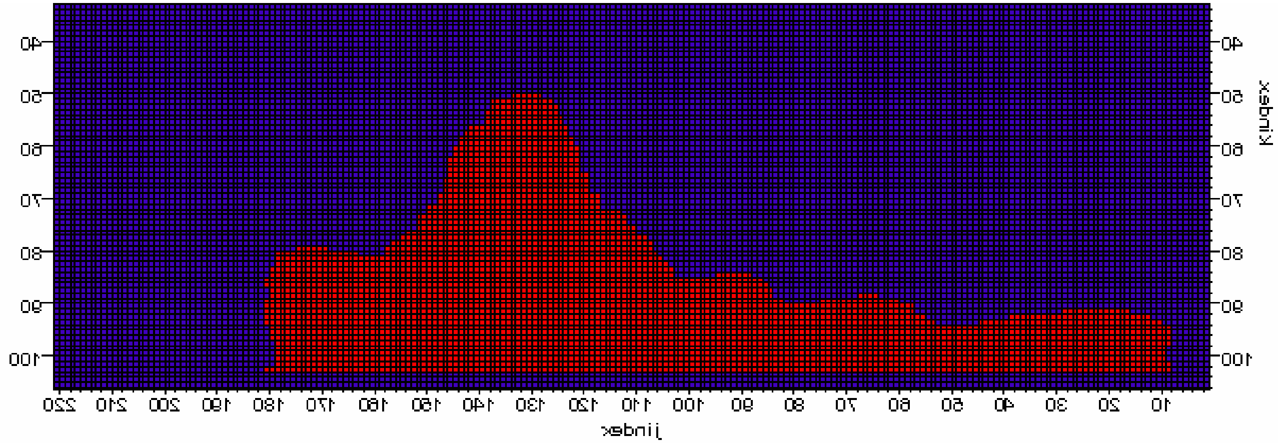
side view

cross-section at 1st injector

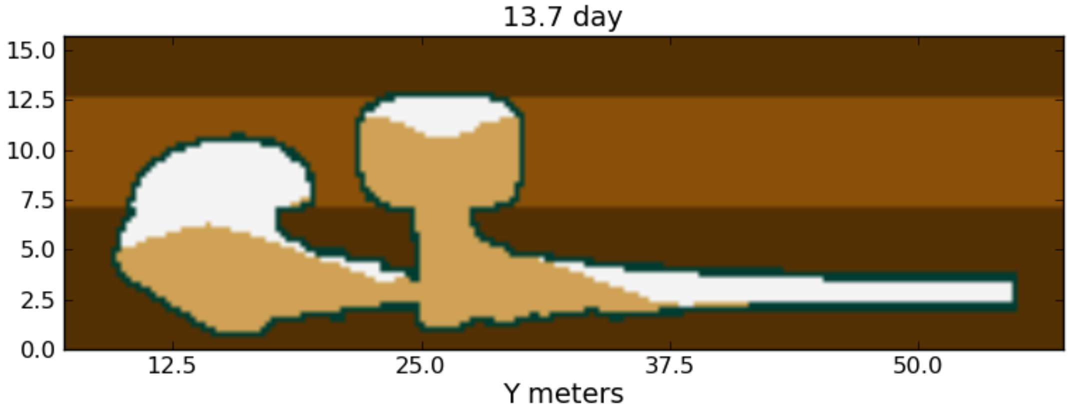
* Hoe Creek III simulations used the 2011 version of UCG-SIM3D

In 2011, the model rubble included ash from consumed coal, and spalled roof rock, but not coal/char from spalled coal

Comparison of cavity shape for HC-III



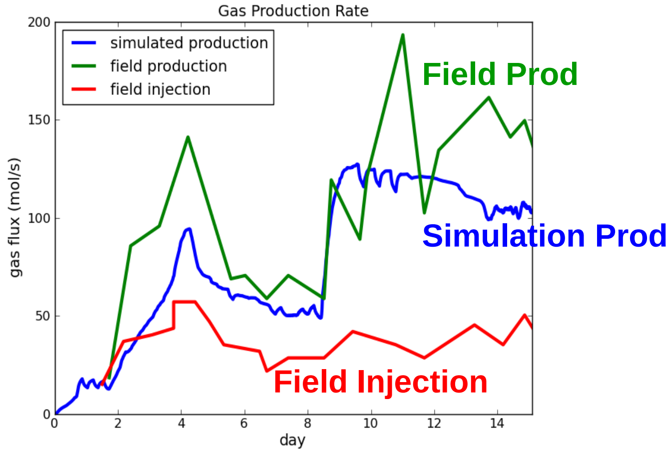
Observed



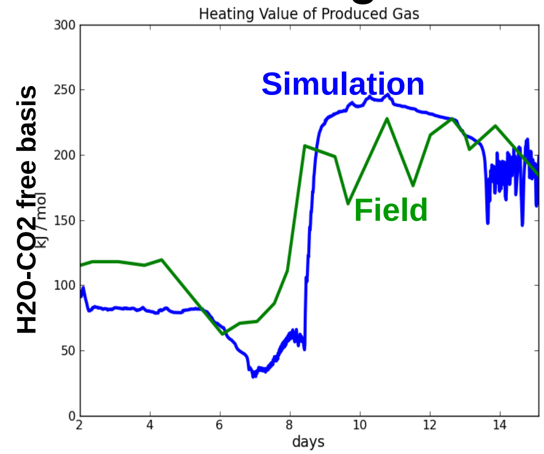
Simulation

Comparison of product histories for HC-III

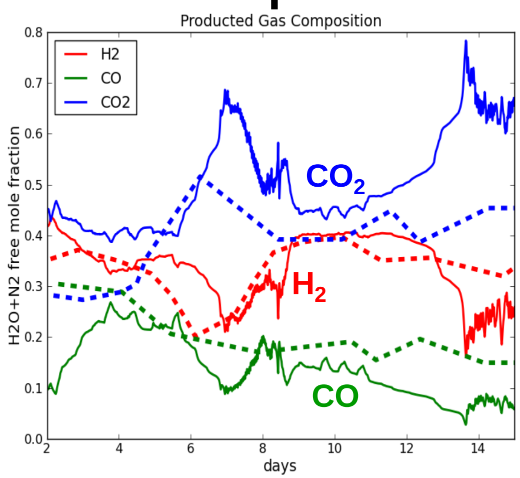
Gas production rate



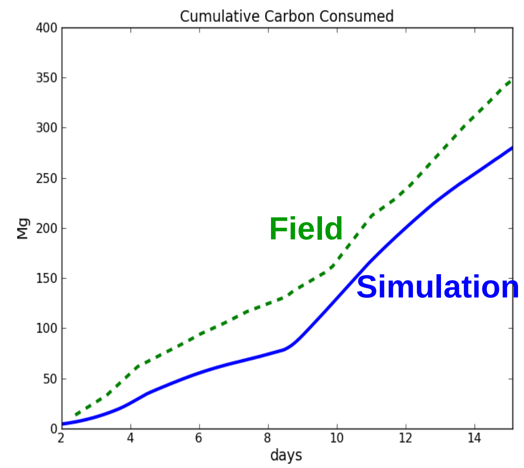
Gas Heating value



Gas Composition

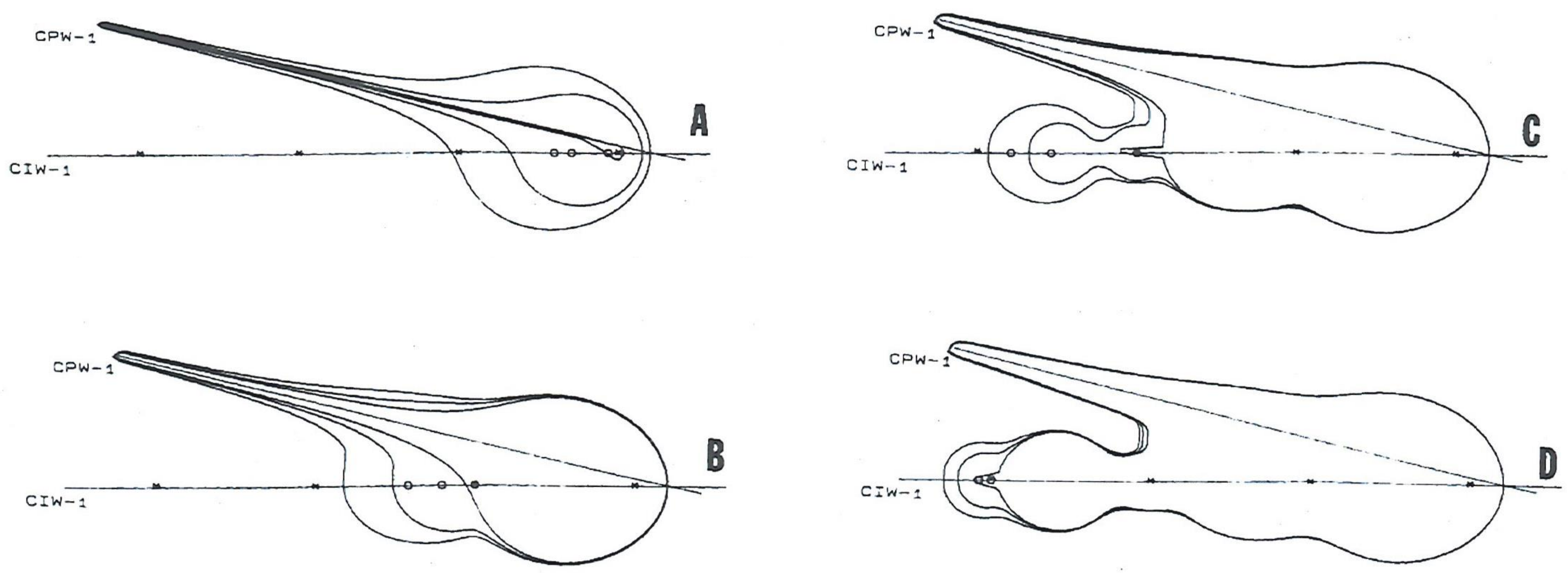


Cumulative carbon consumption



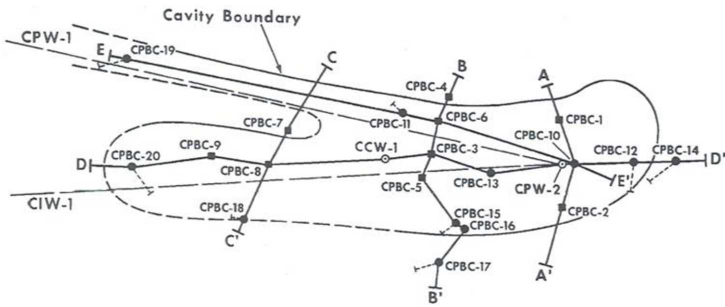
The Rocky Mountain I CRIP test (Hanna Basin, WY, 1987-88) had intersecting horizontal injection and production wells, and changing injection location, composition, rate, and pressure.

Plan views of growing cavity and moving injection points

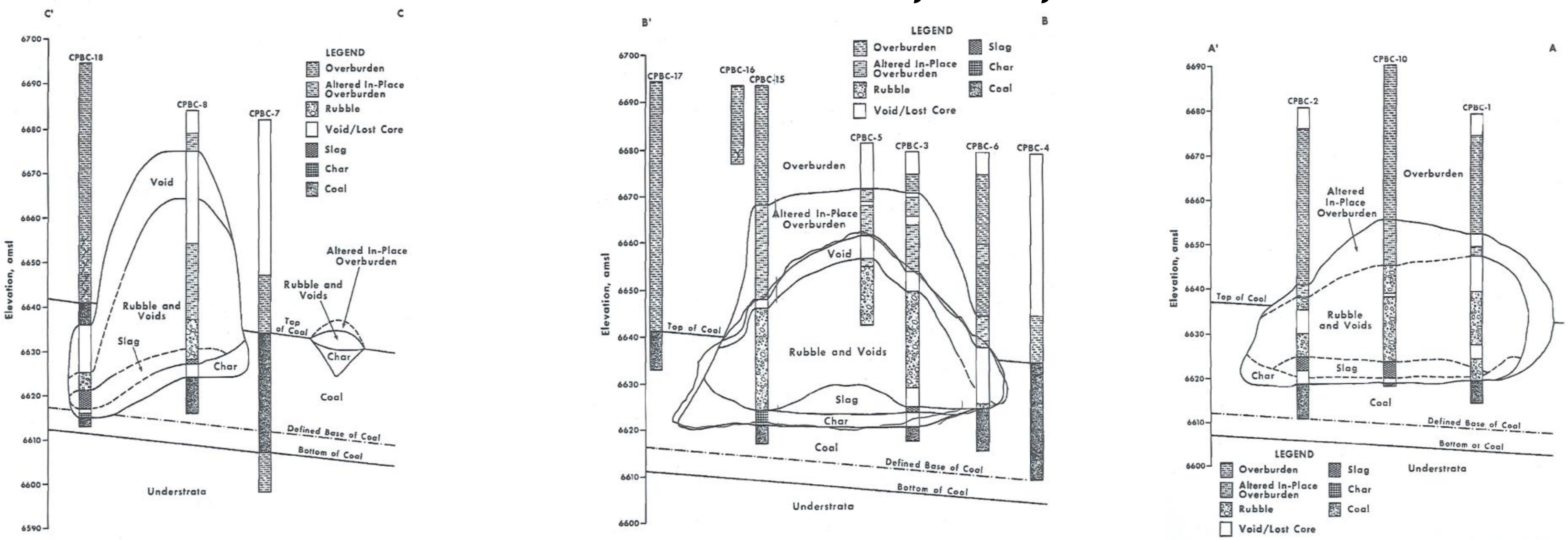


RM I post-burn coring showed much roof spall/fall, rubble, and a complex cavity shape

Plan view



Cross sections CC', BB', AA'

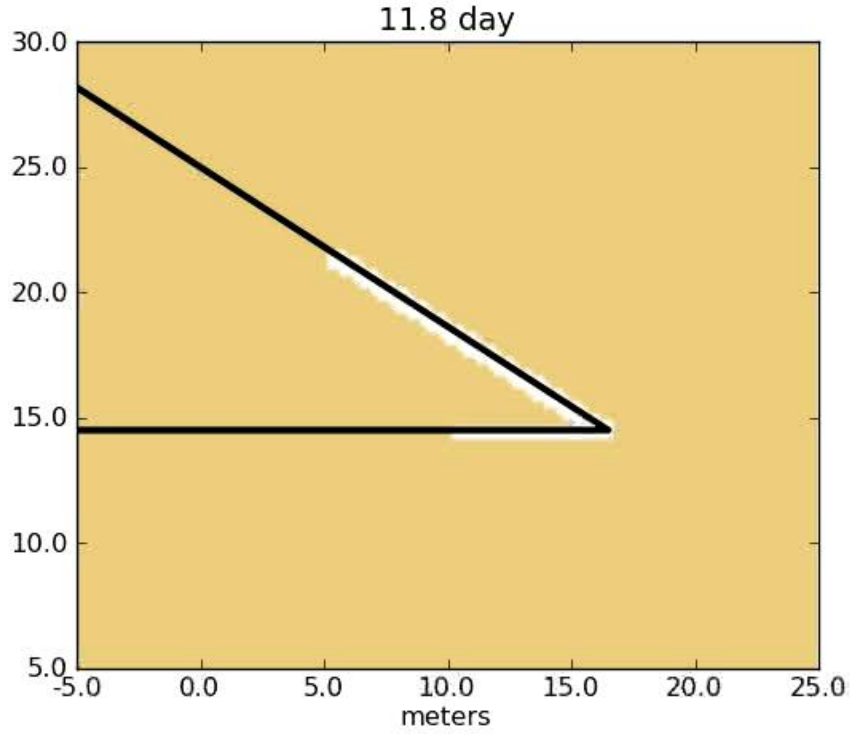


Note: corings were months? after the test

Plan View of Simulated RM1 Cavity Growth
First 35 Days

B

A



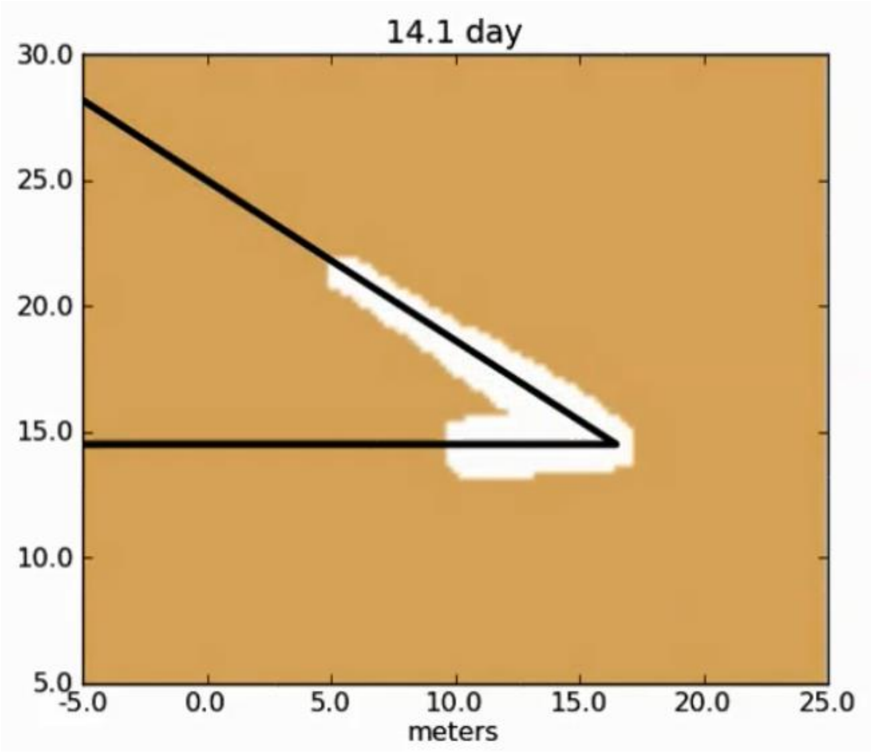
A'

B'

Plan View of Simulated RM1 Cavity Growth First 35 Days

B

A



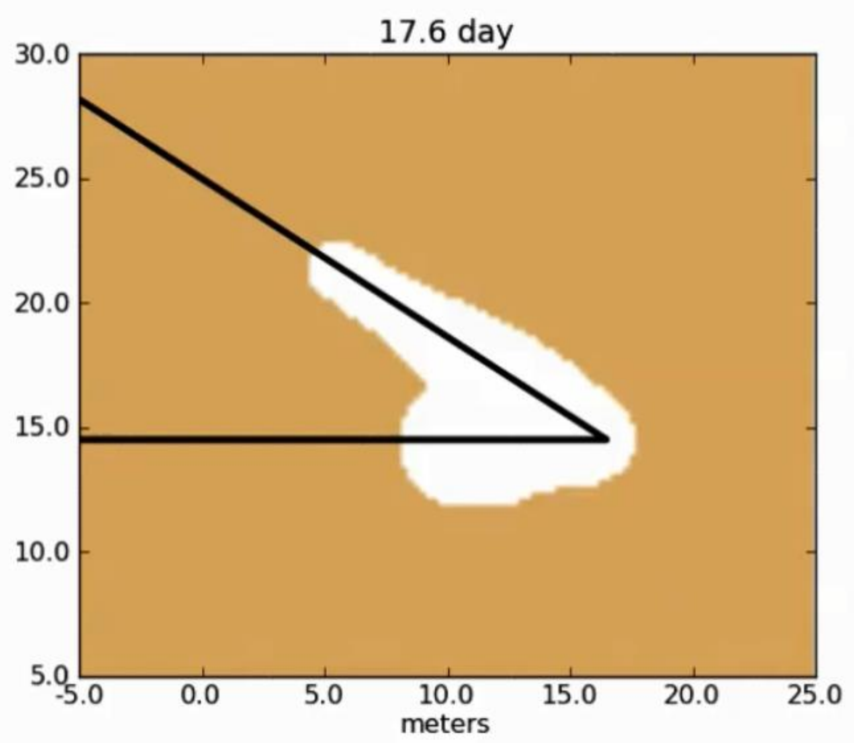
A'

B'

Plan View of Simulated RM1 Cavity Growth First 35 Days

B

A

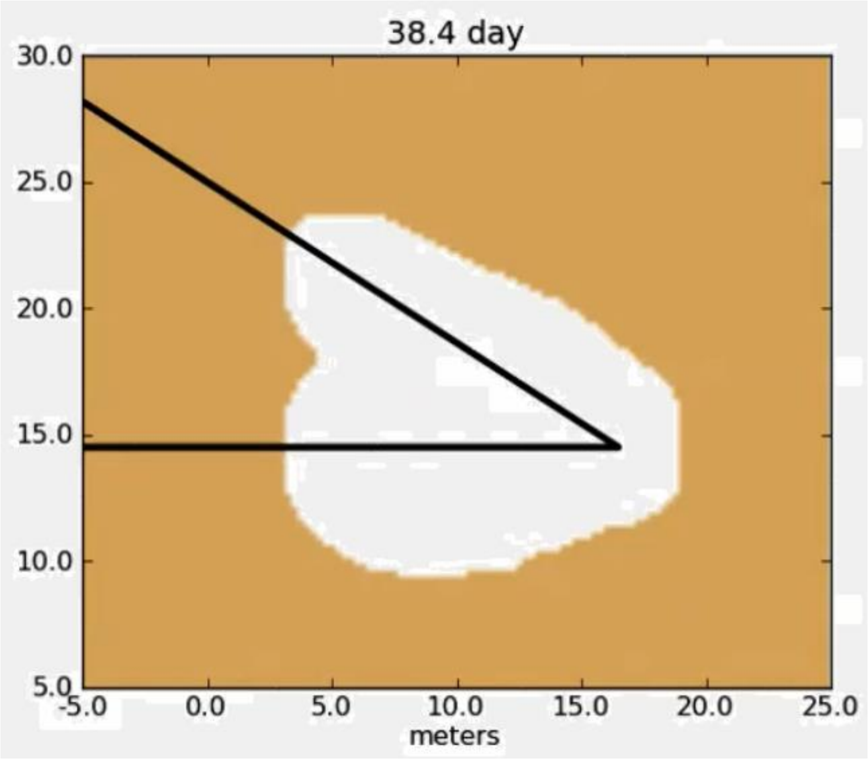


A'

B'

Plan View of Simulated RM1 Cavity Growth First 35 Days

B

A  A’

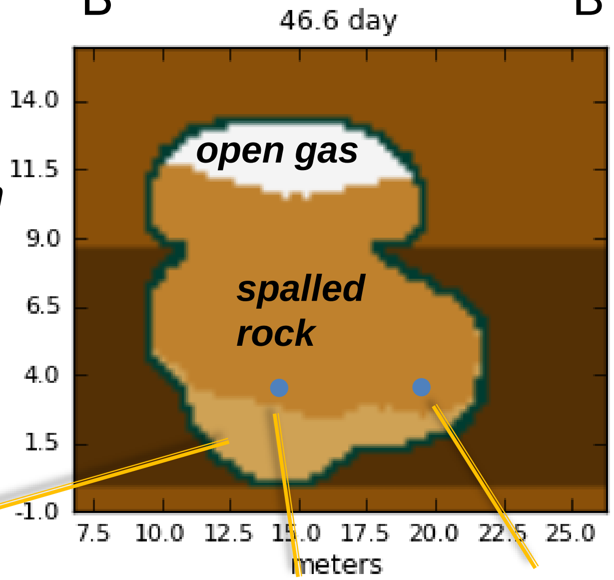
B’

Cross sections of simulated RM 1 cavity growth First 35 days

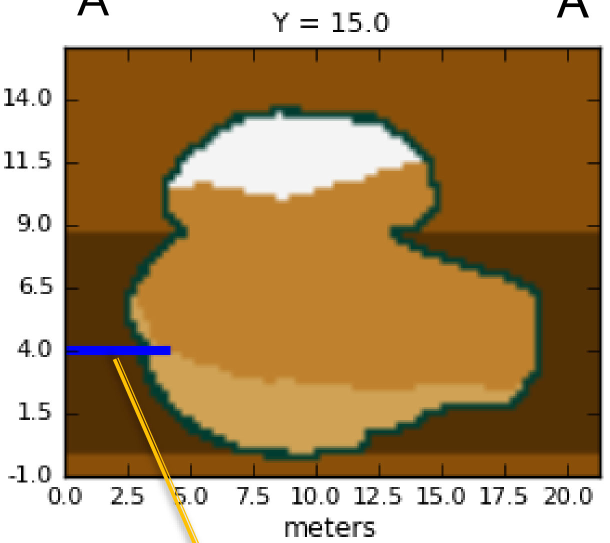
Cross section perpendicular to injection borehole through initial injection point

Cross section along injection borehole

B’ B



A A’



rock overburden

coal seam

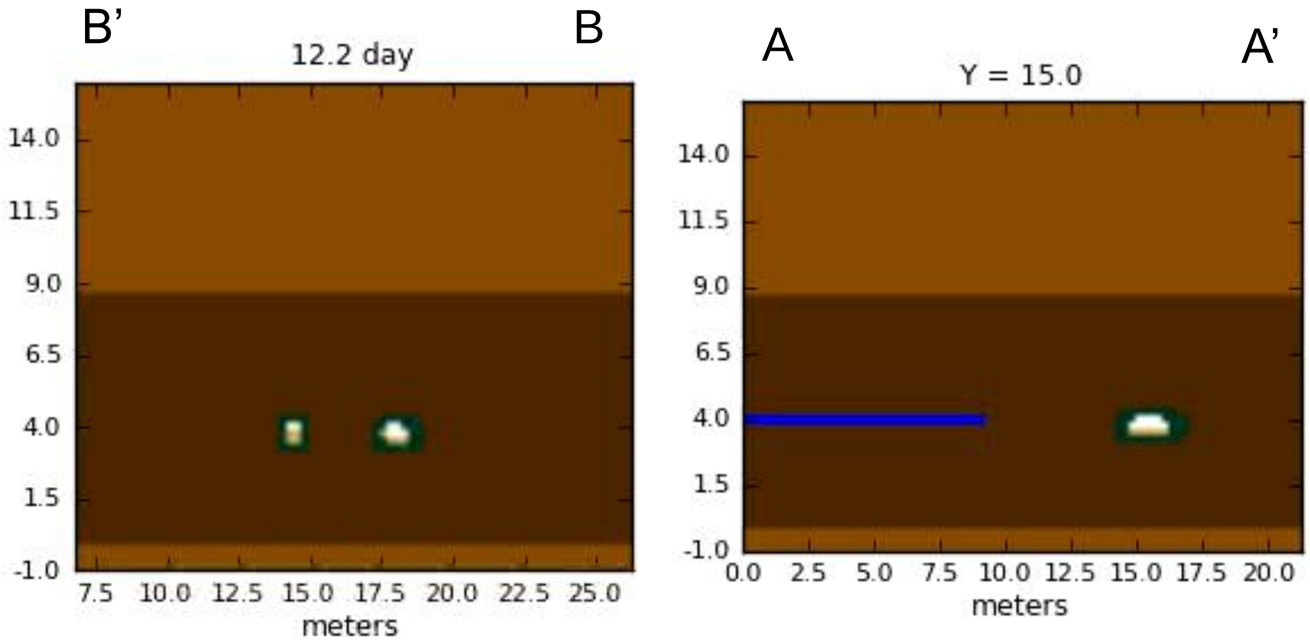
ash+char

init. inject. borehole

init. prod. borehole

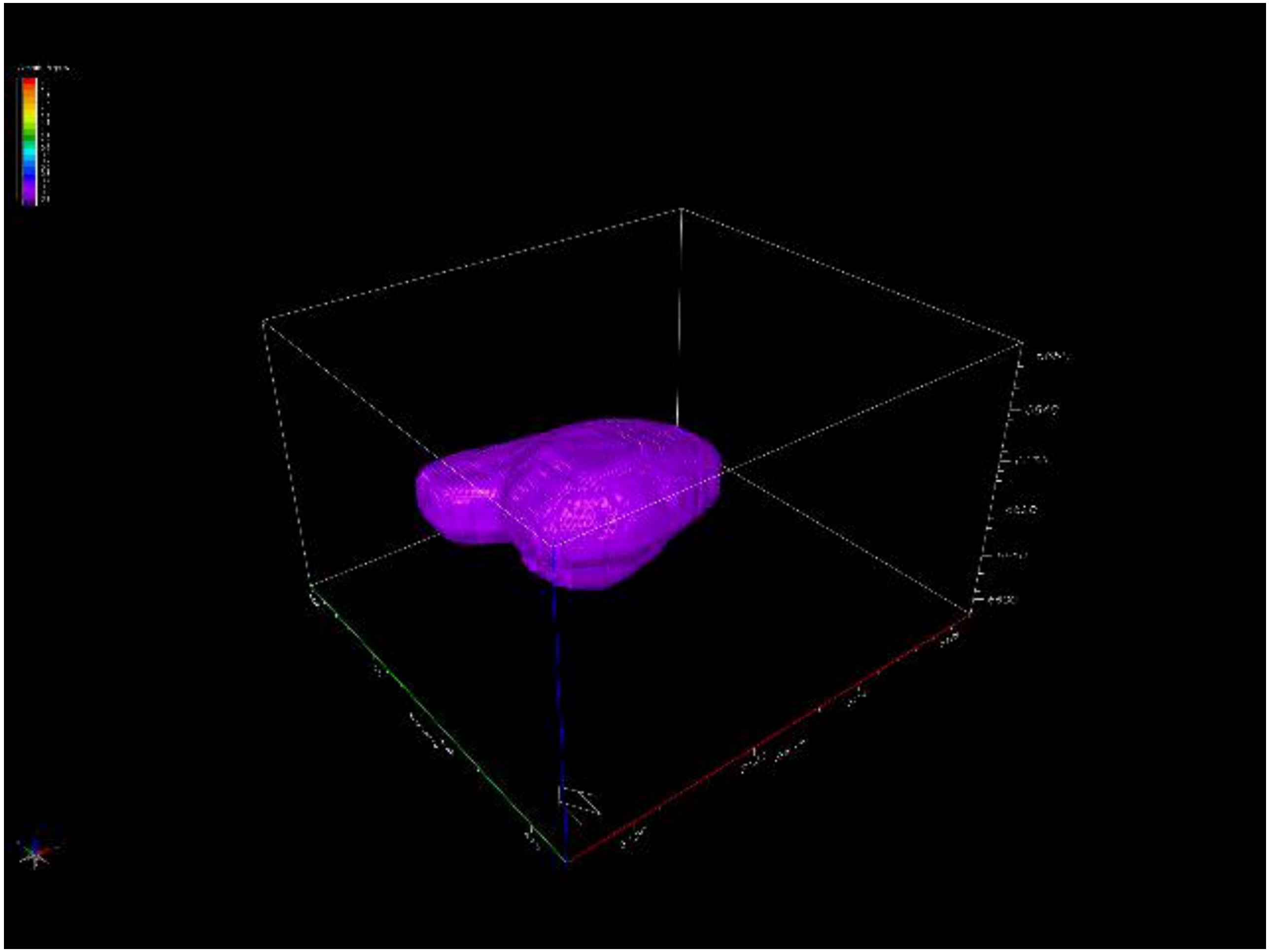
lined portion of inject. borehole

Simulation Cross-section movie Showing Cavity Growth, Coal and Rock Spalling



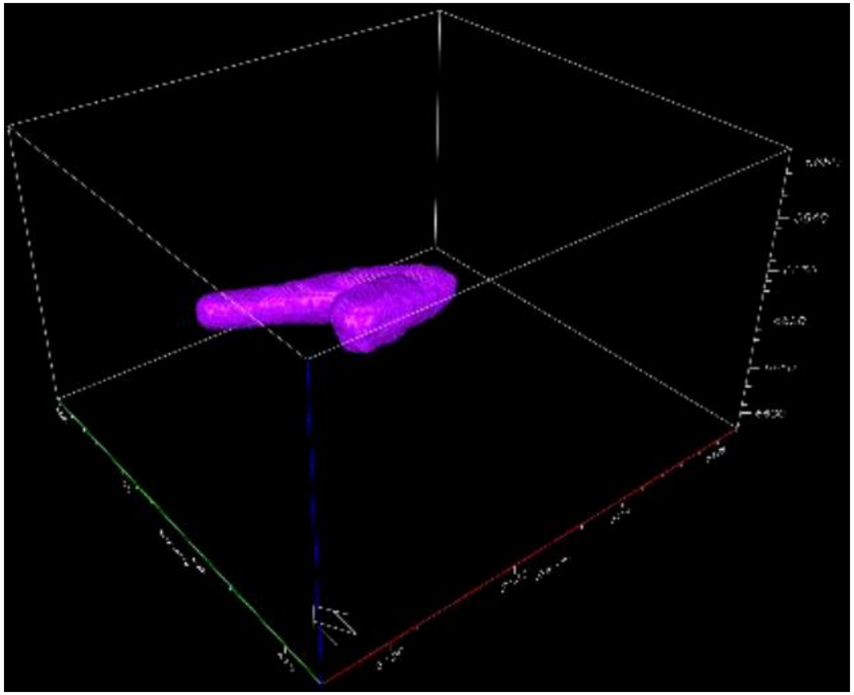
RM I cavity growth animation from simulator (days 14-46)

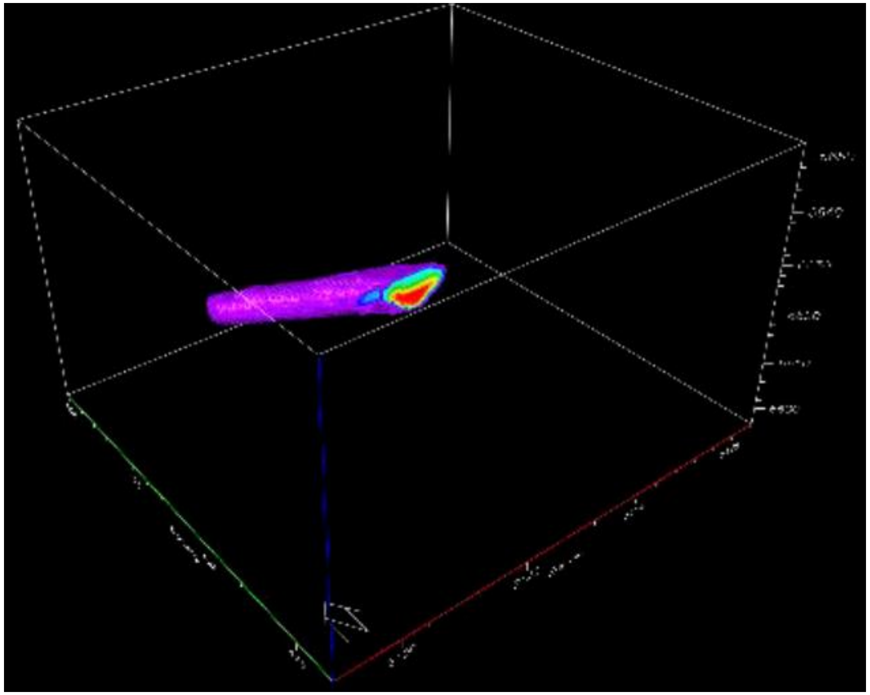
Animation file in .ppt



RM I cavity growth animation from simulator (days 14-46)

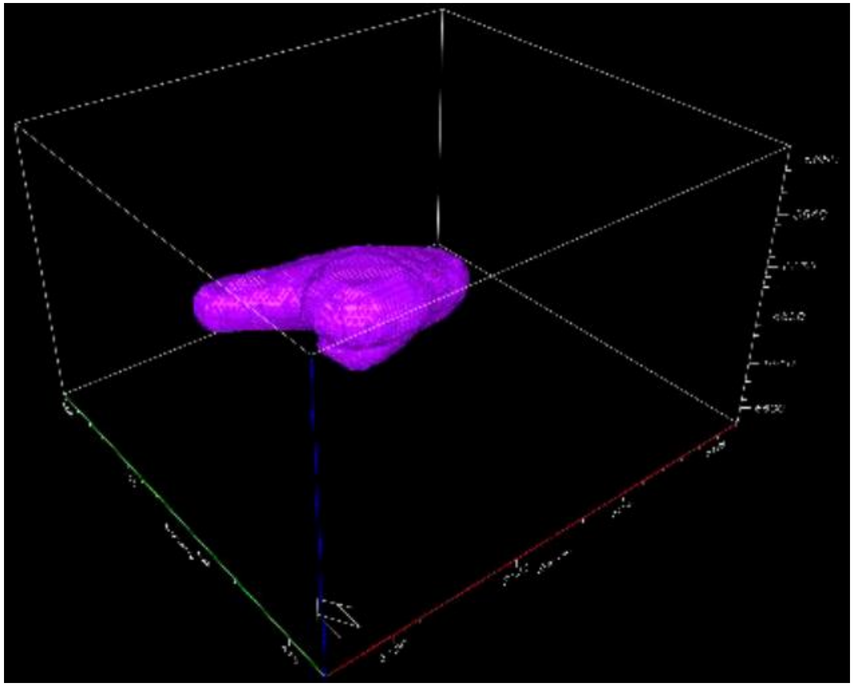
Still frames

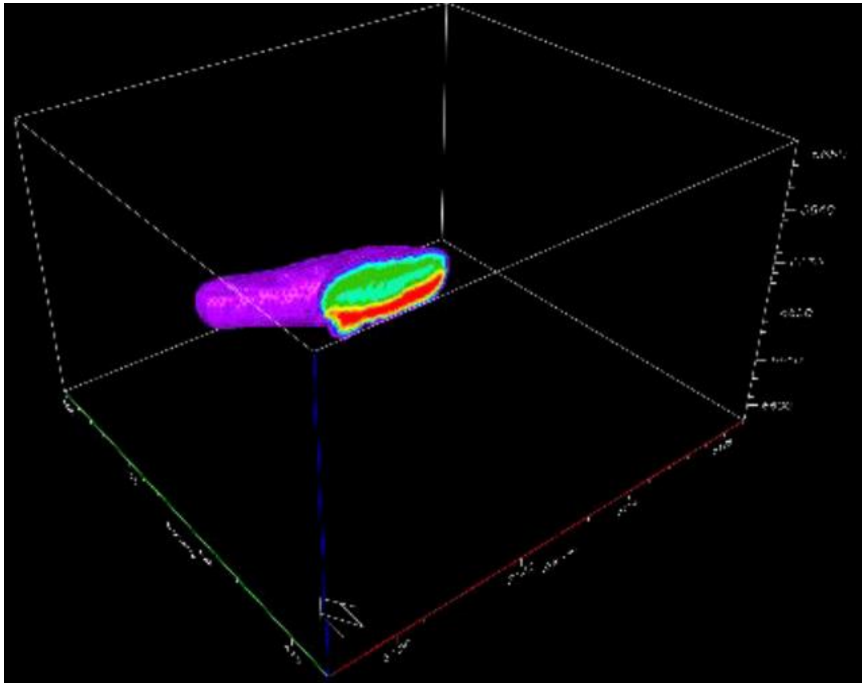




RM I cavity growth animation from simulator (days 14-46)

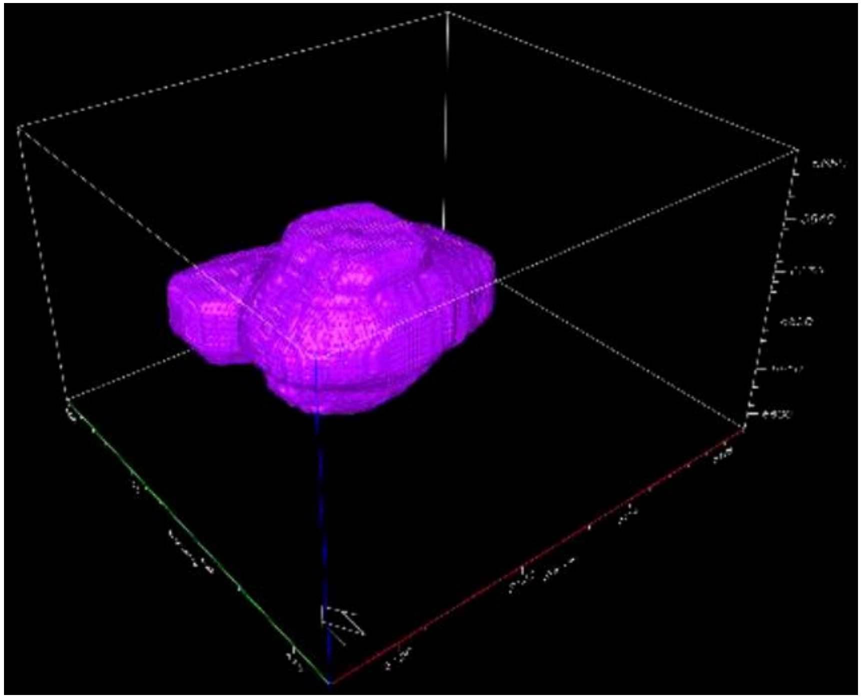
Still frames

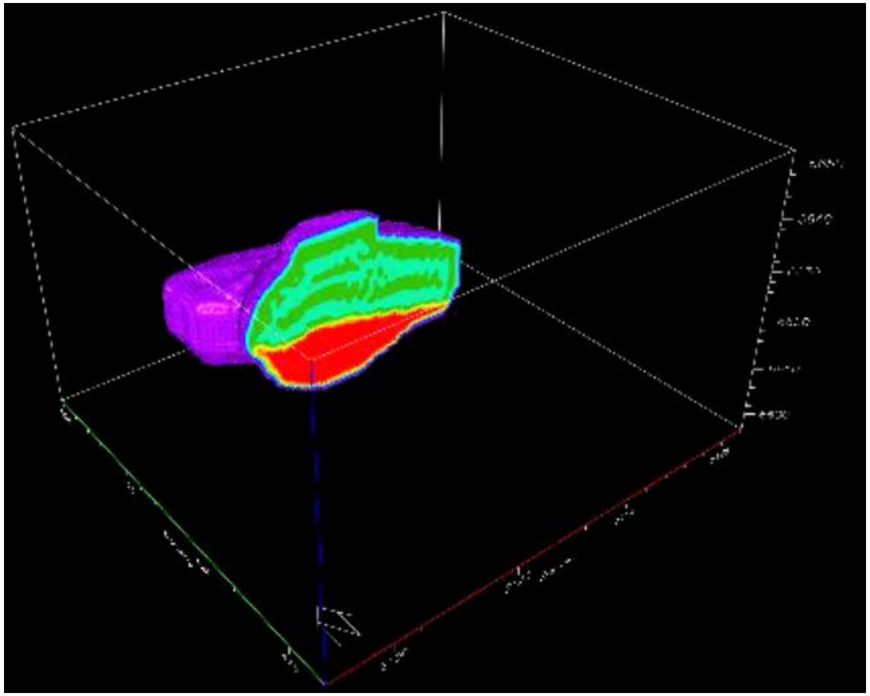




RM I cavity growth animation from simulator (days 14-46)

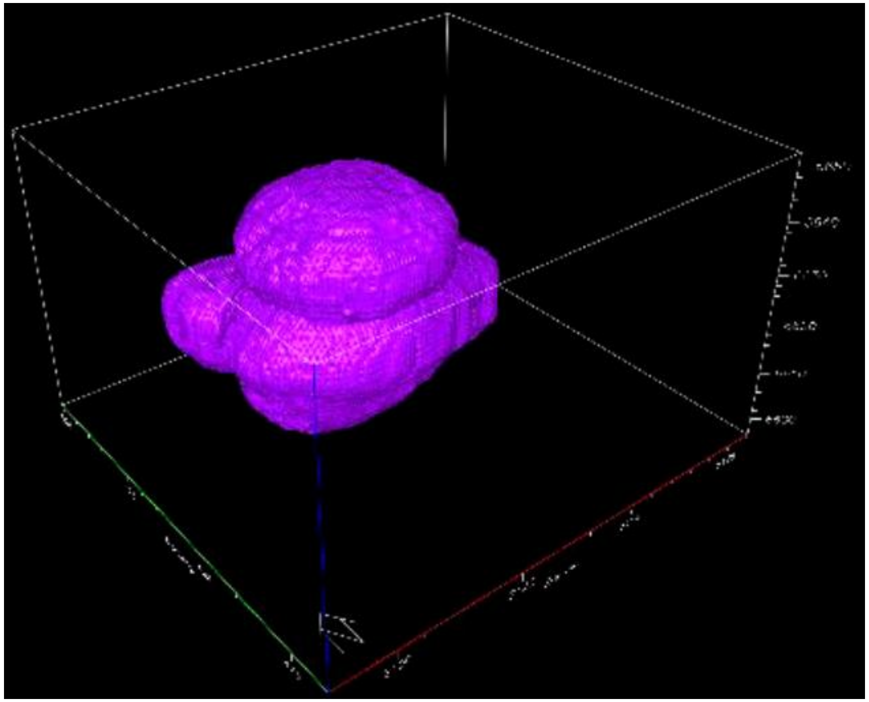
Still frames

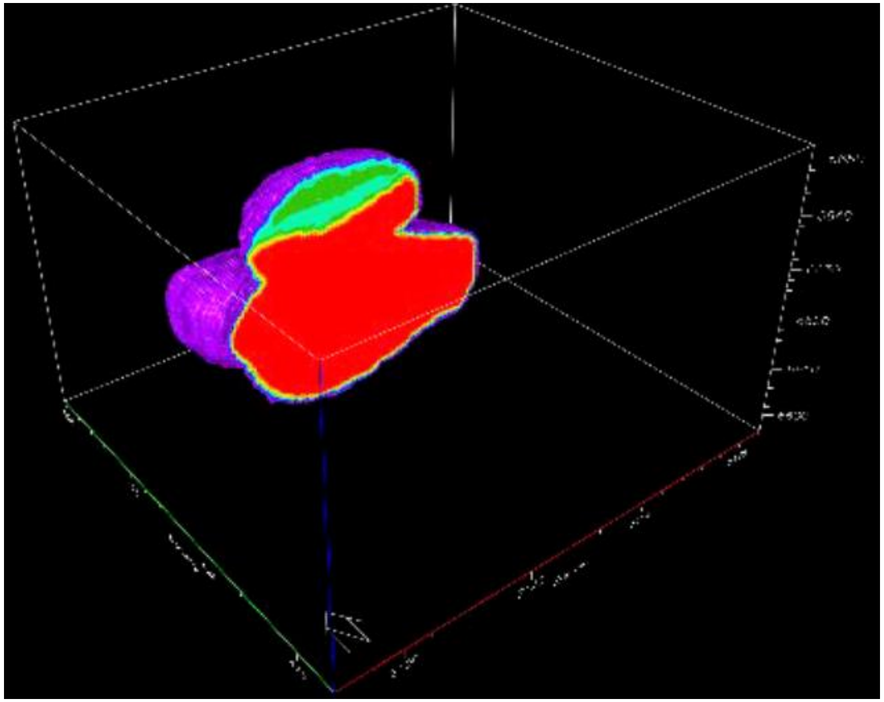




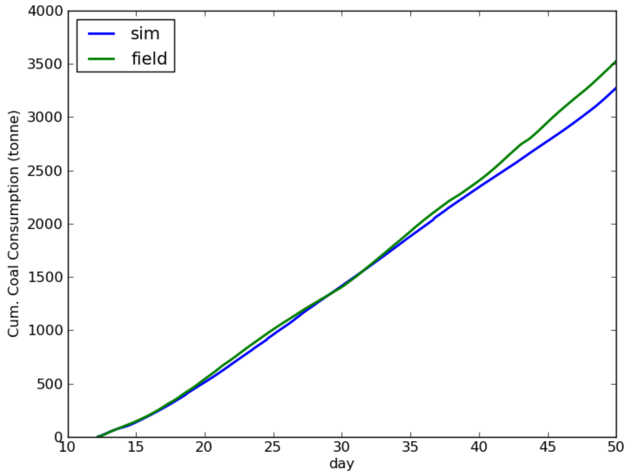
RM I cavity growth animation from simulator (days 14-46)

Still frames



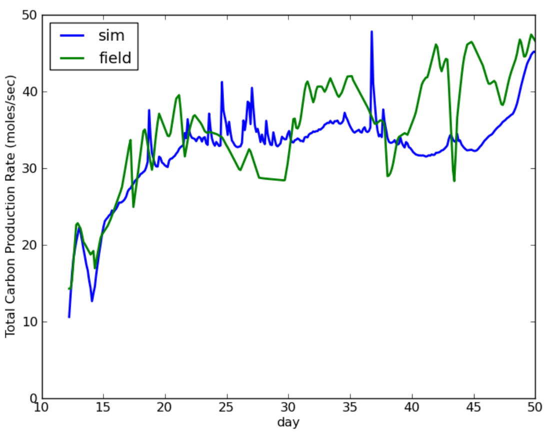


Comparison of Predicted Production Rates with Rocky Mt. I Field Test Data

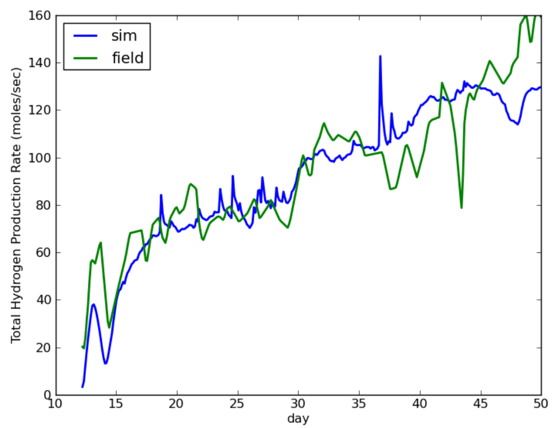


Cum. metric tons of coal consumed

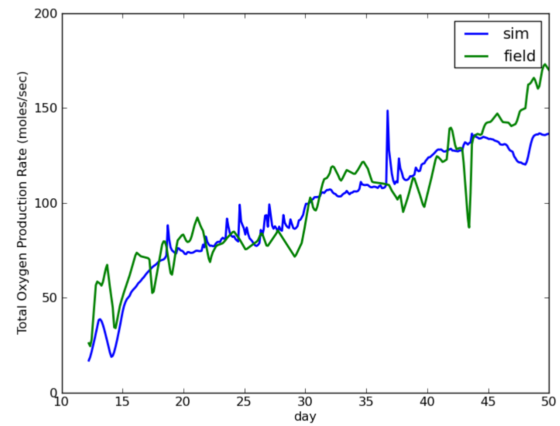
Total Carbon Mole Rate



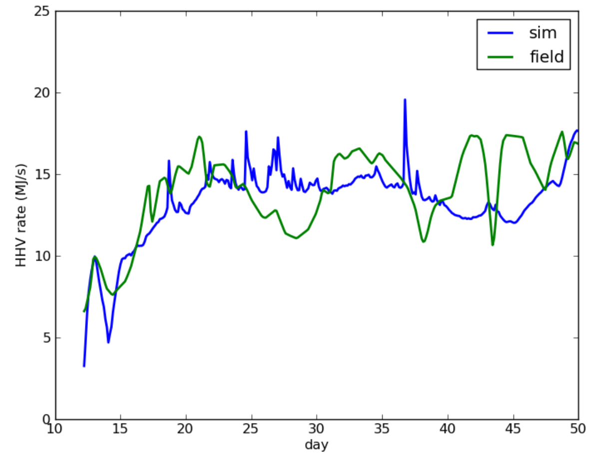
Total Hydrogen Mole Rate



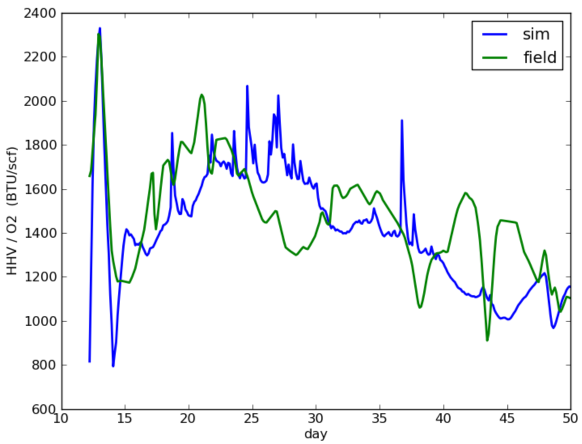
Total Oxygen Mole Rate



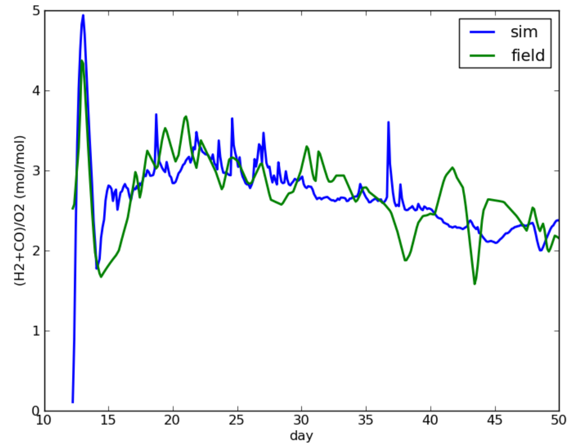
Comparison of Predicted Heating Value Rate with Rocky Mt. I Field Test



Higher Heating Value (HHV) Rate



HHV / O_2 (BTU/scf)



(H2+CO) / O_2 (mol/mol)

UCG-SIM3 can accurately model UCG

- **UCG-SIM3 is a full-physics, flexible, 3-D UCG simulator**
  - Correct physics & chemistry
  - Handles complex geology and design/operation configuration
  - Predicts cavity growth, water, products, T, P, y_i fields, …
- **It is still a research code**
  - Requires expert to set up, troubleshoot, and run
  - Each new case will require effort
  - Not yet mature engineering tool