End-to-end numerical simulation of explosion cavity creation & circulation processes, subsurface gas venting & transport, and prompt atmospheric releases

S. Ezzedine, O. Vorobiev, C. Velsko, S. Myers, & E. Herbold

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INTRODUCTION AND MAIN RESULTS

LLNL is building a comprehensive Cavity SIMulator (`**CASIM**') that includes the following processes, but not limited to, physico-chemical processes that lead to the formation of the cavity, the puddle melt, creation of the radiochemical species, their fractionation and evolution within the cavity, and the eventual creation & collapse of the chimney using state-of-the-art HPC numerical models. CASIM is being coupled to LLNL GEODYN hydrocode and produces a source term to LLNL long- term gas seepage code NUFT, LLNL non-isothermal variably saturated subsurface flow and transport code. Source of leakages at the ground surface is then used to initiate atmospheric transport. The end-to-end modeling capability is operational in 2 & 3 dimensions.

This work was done by Lawrence Livermore National Laboratory (LLNL) under award number DE-AC52-06NA25946. The views expressed here do not necessarily reflect the opinion of the United States Government, the United States Department of Energy, or Lawrence Livermore National Laboratory.

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T2.3-476

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Introduction

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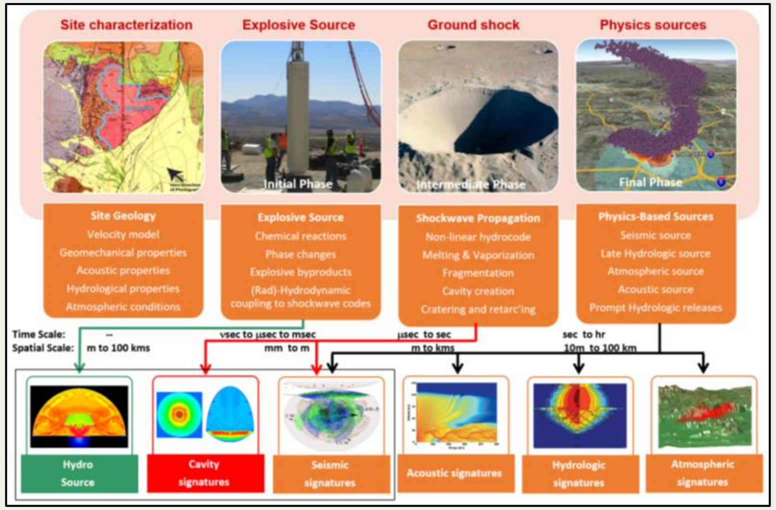
Methods

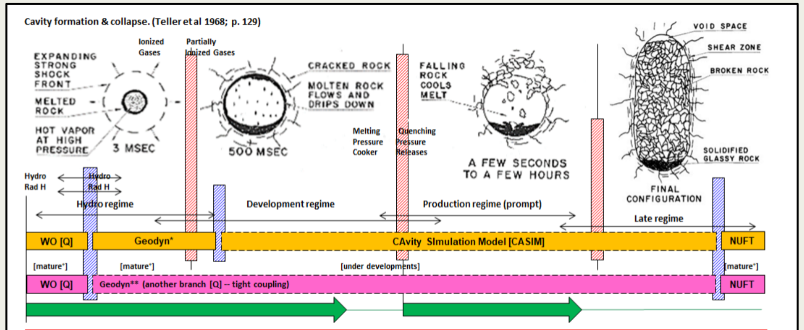
To goal is to simulate underground chemical explosion from end-to-end, source-to-receiver. LYNM program encompasses four thrusts: 1/ Explosive Source, 2/ Containment, 3/ Instrumentation and 4/ Far-field seismic and acoustic networks. An end-to-end simulation involves several disparate spatial and temporal scales.



Main physics-based building blocks for the end-to-end, source-to-receiver, numerical simulation

Our approach is to de-construct the problem into building blocks and use the best available state-of-the-art codes for solving the building block physics then reconstruct the end-to-end final solution. This approach has been proven very efficient to solving several DOE sponsored projects and more recently was applied successfully to the Source Physics Experiment (SPE) Phase I (SPE) and Phase II (DAG) projects and it is being refined to support the design and predictions of SPE Phase III (RVDC)..

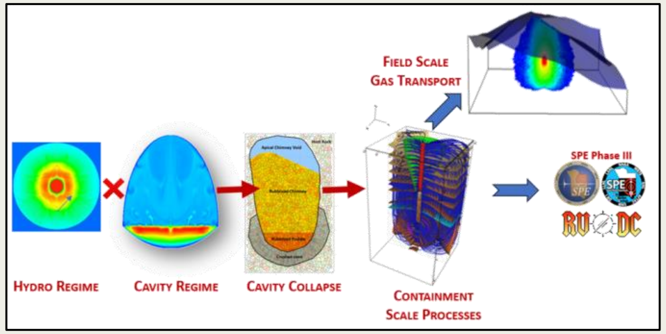
Cavity Processes Physics & 'CASIM'



1. ULTIMATELY CREATE "SOURCES/TRACERS" FOR SUBSEQUENT ANALYSES (LONG-TERM RELEASES, SEISMO-ACOUSTICS, ATM…)
2. Predictively assess what does really matter as function of yield w/o ad-hoc assumptions.
3. Capabilities are for NE & HE. Both bring different (& similar) characteristics signatures & physics.
4. NEW: CASIM is extended to ATM (~1-2km) for prompt releases.
5. NEW: High temperature, high strain Cavity Instrumentations

Numerical developments & simulations

LLNL is developing: 1) a physics-based cavity formation & processes, 2) an efficient damage-to-permeability interface in the vicinity of the cavity, and 3) a library of prototypes of cavity for production runs



Execution of the end-to-end simulation framework

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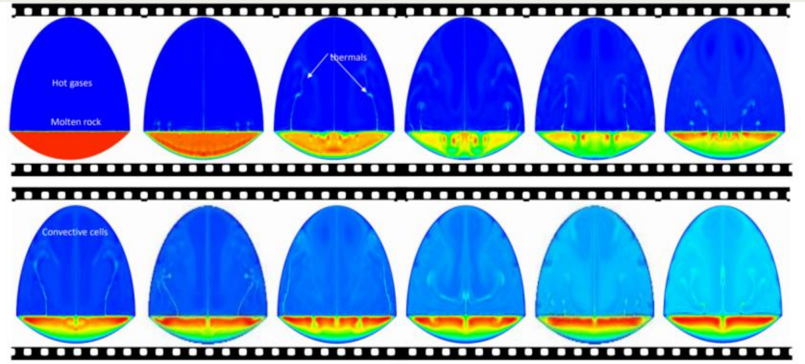
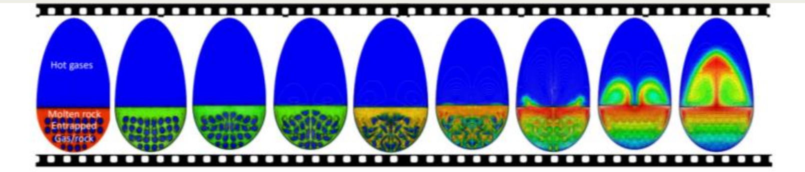
'CASIM' Numerical Simulations

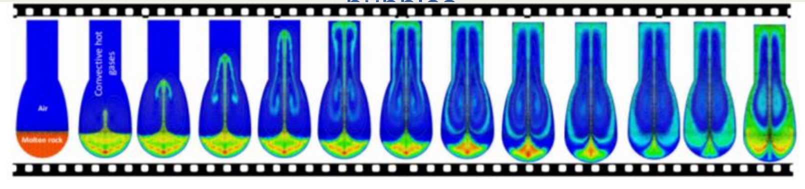
We have exercised CASIM to simulate the relevant physical process within a contained cavity. The scenario involves multiphase flow, heat and mass transport, fractionation, to name a few.



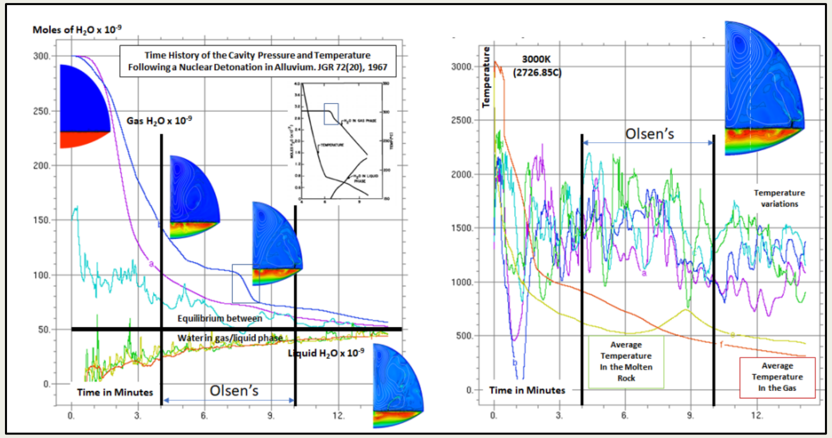
Simulation of thermal transport within a partially gas filled chamber with settled molten granitic rock puddle



Simulation of thermal transport in a partially gas filled chamber with viscous molten rock puddle & gas filled bubbles



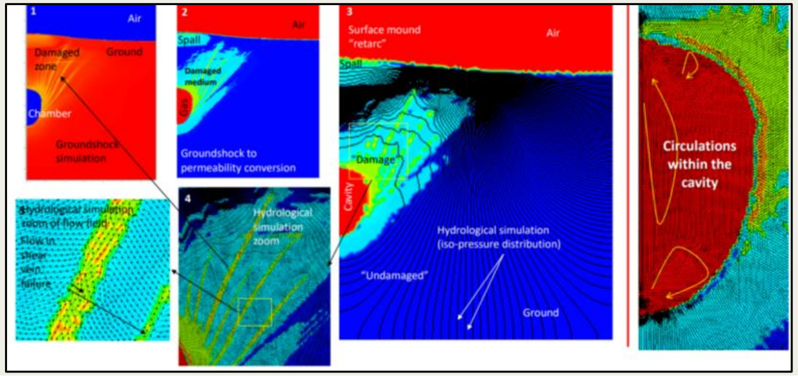
Simulation of thermal transport within a partially gas filled volcanic chamber & chimney



Example of Olsen 1967 UNE cavity cooling problem

Damage-to-Permeability

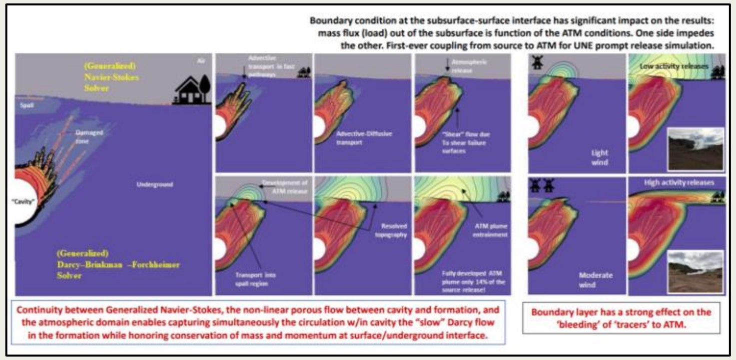
We developed an integrated physics-based scheme to convert the damaged properties in the groundshock simulation into physical hydrological permeability for subsurface simulation of the gas transport.

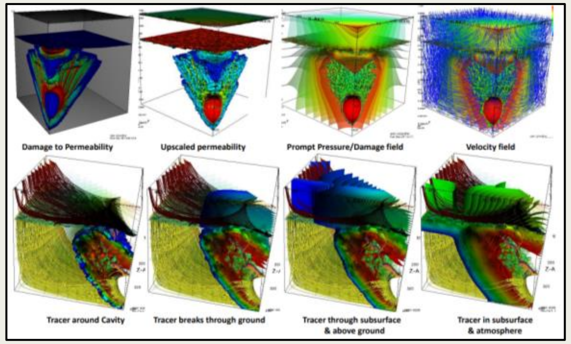


High resolution conversion of damage (1) into hydraulic permeability (2). (3) Pressure distribution in the underground. (4) a zoom of permeable shear damage. Right frame: zoom of the cavity mixing

Subsurface to surface gas transport

Subsurface gases eventually leak into the atmosphere. A full implicit coupling between the atmospheric and the subsurface transport conditions is required. A fully coupled model for both domain as illustrated hereafter. Has been developed This approach eliminate any ad-hoc assumptions and eliminate any dilution factors at the ground surface.





Implicit coupling between the subsurface and the atmospheric mass and heat transport under different ATM wind speed (top: slow, bottom: fast) for a sensitivity study.

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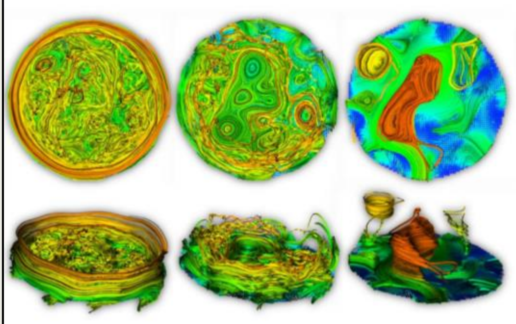
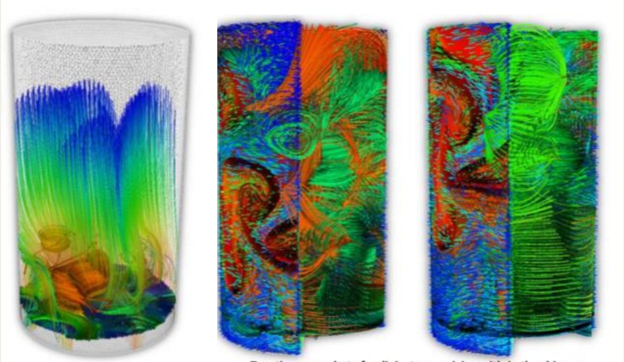
Fully coupled cavity-chimney simulation

To further study the complicated implicit fully coupled transport processes within the cavity and the chimney, we proceeded with a high-resolution numerical simulation of a hemispherical molten rock source releasing heat and mass to the cylindrical chimney as shown hereafter.



Areal view of mixing within top cavity.
Time varies from left to right: early-, mid-, and late-time.

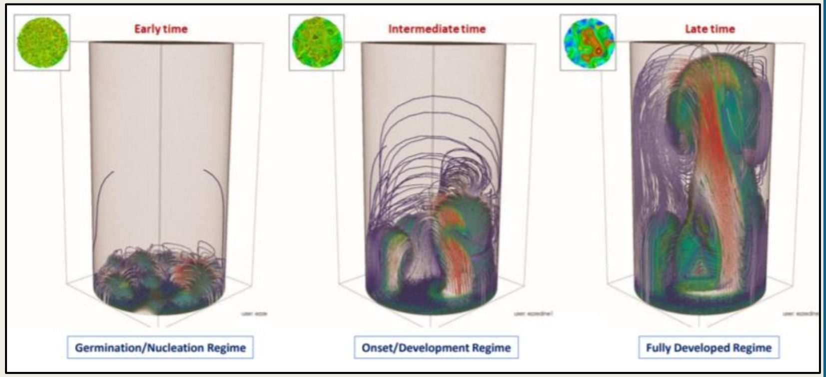


Two time-snapshot of radioisotopes mixing with-in the chimney

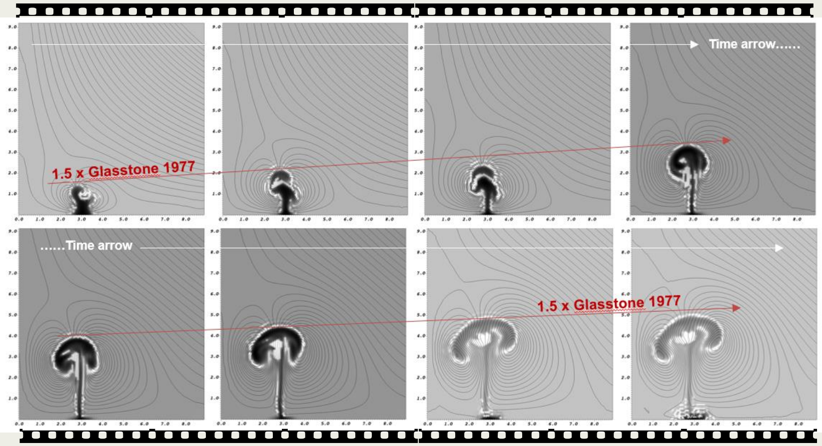
(Top) 3 Time-history of the convective mixing at the molten-rock/chimney interface.
(Bottom) 3 frames show the correspondent gas circulation and mixing in the chimney.

Large Scale Cloud Transport Simulation

Once the cloud development reaches stability the cloud transport can extend to regional and even global scales. We have developed tools to fill those gaps as shown in the subsequent figures.



Full 3D coupled conjugated flow and transport in the cavity-chimney which is relevant to source signature discoveries and even forensics.



Regional cloud rise and the development of stable cloud

Summary

- **Physics includes, but not limited to,**
  - Conjugated heat and transport of species & phases
  - Geomechanics (gravity, tectonics, and thermal stress)
  - Seepage through the hosting rock or fast pathways
  - Condensation of gases and (re)vaporization of liquids
  - Non-linearities of physical properties (density, viscosity, …)
  - Instabilities & multiphase effects (Rayleigh, Helmholtz, …)
  - Radiation transport
- **Chemistry includes, but not limited to,**
  - Radiochemistry, decay chains
  - Fractionization in solid/liquid/gas
  - Partially ionized gases
  - Electrochemical transport
  - Geochemistry of Silica and Carbonate systems
- **Damaged zones is converted to permeability**
  - Weak coupling between Geodyn & Cavity
  - Stochastic generation of rock properties & fragments
  - Weak coupling between rubbles & surrounding phases
- **Future extensions**
  - Highly ionized gases & their consequences
  - Seismo-acoustic responses
  - Chimney and cavity collapses
  - Surface expressions

Acknowledgements & Auspices

Acknowledgements & Auspices: The LYNM would not have been possible without the support of many people from several organizations. The authors wish to express their gratitude to the National Nuclear Security Administration (NNSA), Defense Nuclear Nonproliferation Research and Development (DNN R&D), and the Containment ventures and working group, a multi-institutional and interdisciplinary group of scientists and engineers. This work was done by Lawrence Livermore National Laboratory (LLNL) under award number DE-AC52-06NA25946.