SAND2018-11819C

Fire Science & Technology

40th Tritium Focus Group Meeting
Albuquerque, New Mexico, USA
October 23-25, 2018

Hazardous Material Assessments with SIERRA/Fuego

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U.S. DEPARTMENT OF ENERGY
NNSA National Nuclear Security Administration
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Outline

- Code Overview—What is SIERRA/Fuego
- NSRD Contaminant (Hdbk 3010) Project Results
  - Beaker Fire Tests Revisited
  - Gasoline Fire Tests Revisited
- NSRD Rubble Fire Project
- Plumes
- Spent Fuel Refining Accidents
- Summary

Sierra Mechanics

Covers the breadth of physics and numerics required to support Sandia Engineering mission needs

Systems and component functions in normal, abnormal, and hostile environments

Aero

Solid Mechanics

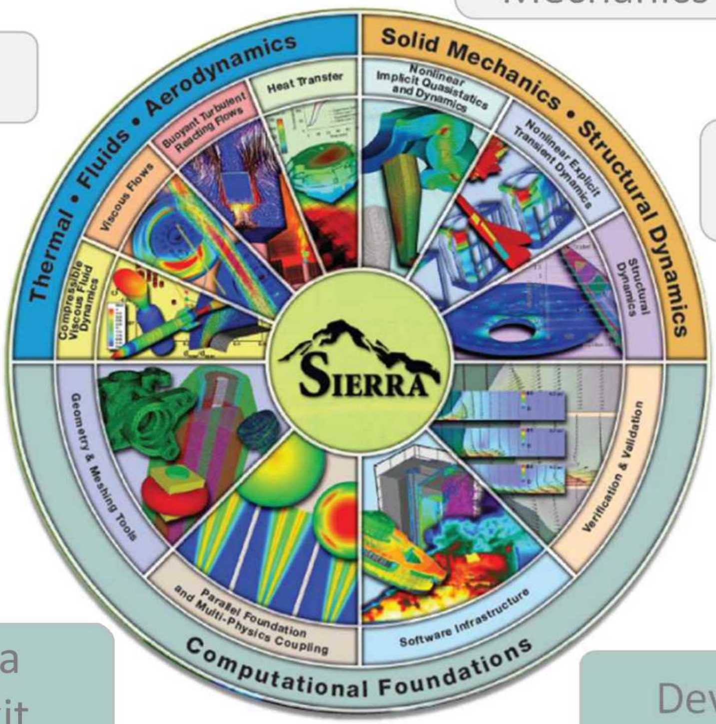
DOE O 414.1D

SAND 2008-5517

Fluid

Thermal

Structural Dynamics



Meshing

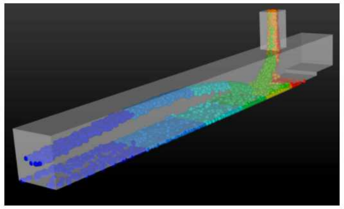
V&V Tools, Methodologies

Sierra Toolkit

DevOps

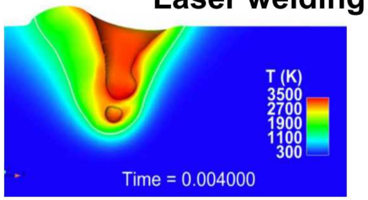
Sierra : Thermal/Fluid, Fire

Particles in crossflow



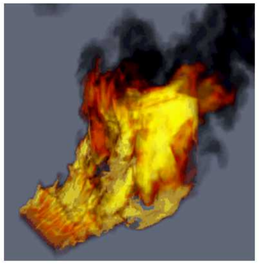
low-mach flows (thermal, fluids, participating media)

Laser welding

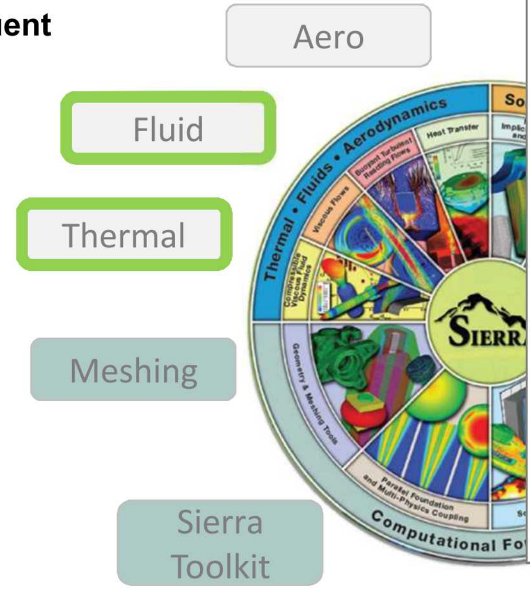


Manufacturing (thermal, fluids)

Fire modeling for subsequent weapon thermal response



Abnormal Fire env (thermal, fluids, participating media)



Thermal – Heat Transfer, Enclosure Radiation and Chemistry

- Conduction, Radiation, Convection
- Dynamic thermal radiation enclosures
- Element birth death, Contact

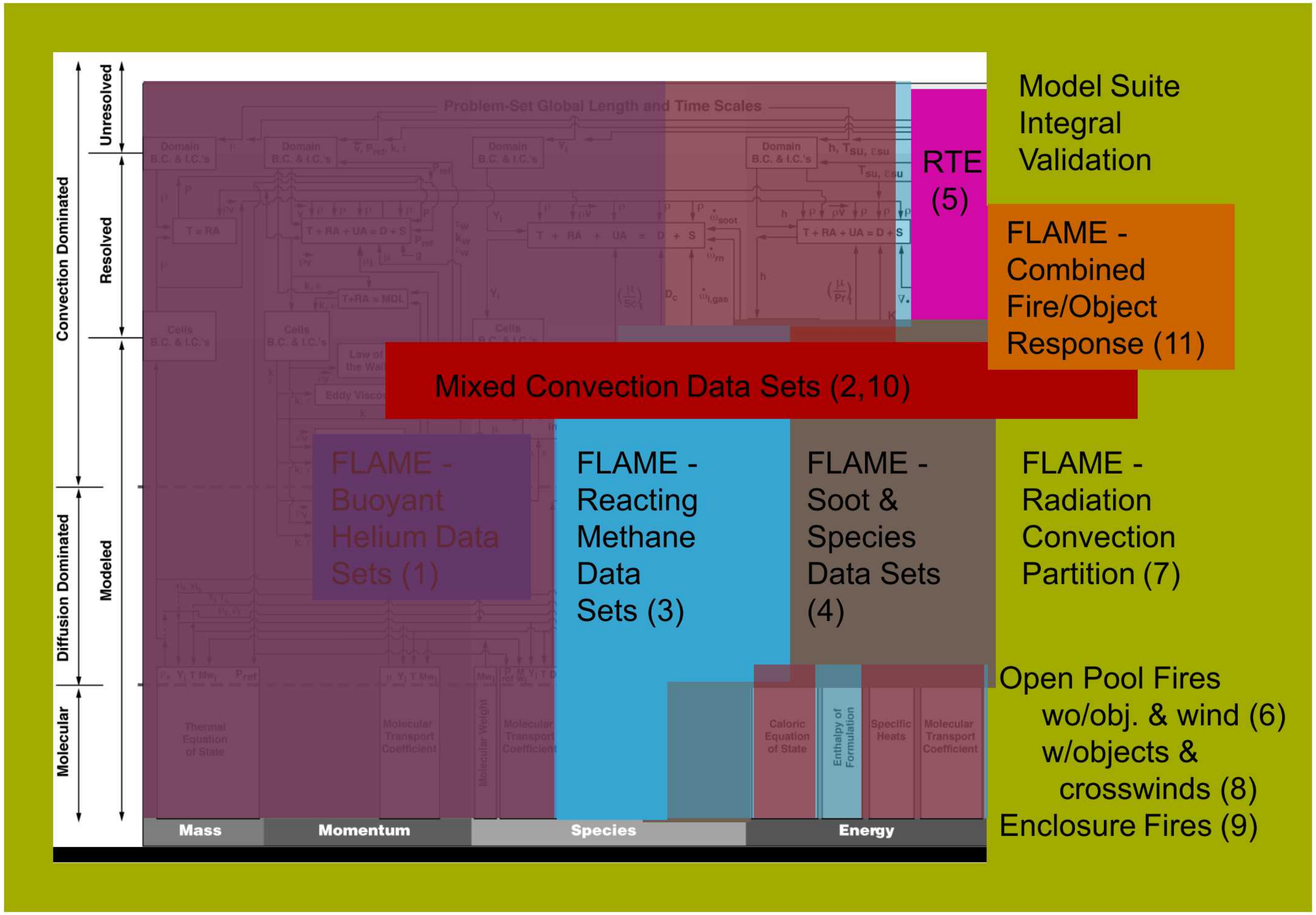
Multiphase – Non-Newtonian, Multi-physics, and Free Surface Flows

- Complex material response, Flexible coupling schemes
- Level sets, VOF for surface tracking

Fire/Combustion – Low Speed, Variable Density, Chemically Reacting Flows

- Eddy dissipation and mixture fraction reaction models,
- Variable density
- RANS and LES based turbulence models, Unstructured Mesh, Pressurization models
- coupling to Radiation transport code

Historic Validation



This was from the SIERRA/Fuego validation plan conducted 10-15 years ago
Urban plume not represented in this matrix, so we are conducting validation exercises

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DOE Handbook 3010

- What does 3010 mean to us with regard to haz cats?
  - Provides a consistent and uniform basis for bounding hazards
- Used primarily as a look-up reference
  - Basis?

NOT MEASUREMENT SENSITIVE

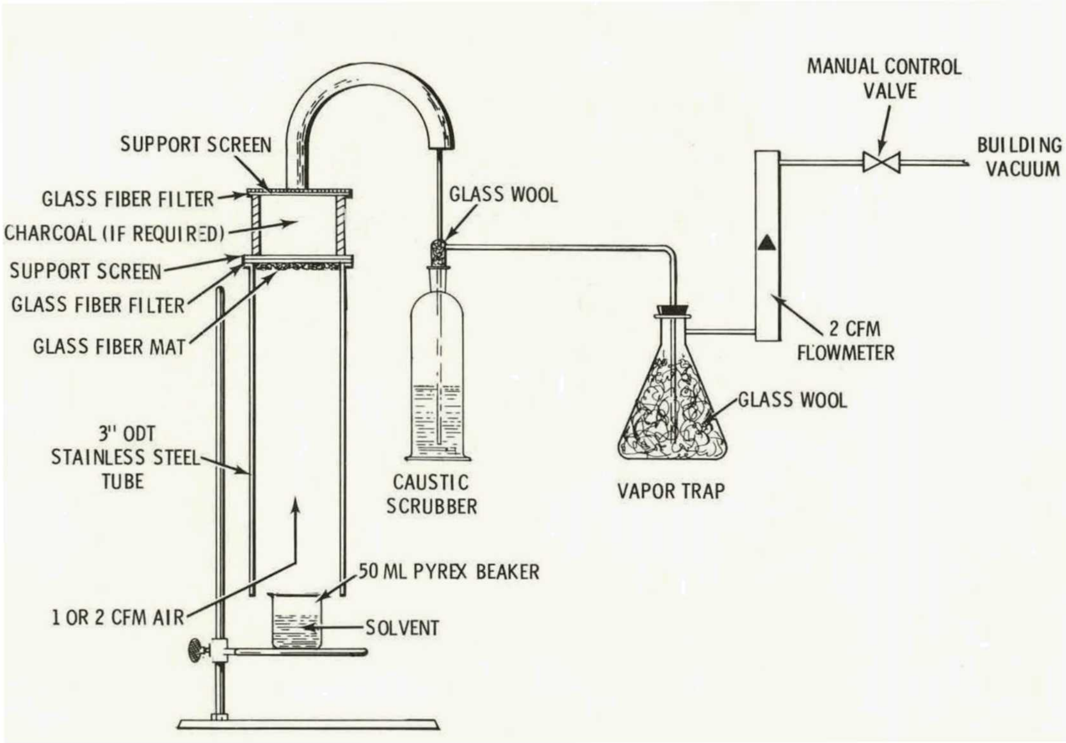
DOE-HDBK-3010-94
December 1994
Reaffirmed 2013

DOE HANDBOOK

AIRBORNE RELEASE FRACTIONS/RATES AND RESPIRABLE FRACTIONS FOR NONREACTOR NUCLEAR FACILITIES

Volume I - Analysis of Experimental Data

Beaker Fire (BNWL-B274)



- Apparatus – 50 ml beaker
- Liquid – kerosene with 30% TBP (25 ml)
- Pre-heated liquid to boiling point then ignited
- Beaker assumed to be 56 mm x 42 mm diameter

FUEGO Simulation:

- Boiling assumed uniformly
- Receded level is not modeled
- Use Kataoka and Ishii boiling model to predict mass flux
- Use Borkowski et al. (1986) for initial drop size distribution
- Simulation Results
    - Much of mass released at the beginning of the fire
    - Wall deposition is significant
    - Turbulence may be important
    - ARF computed are in agreement with the experiment

Entrainment Mechanisms

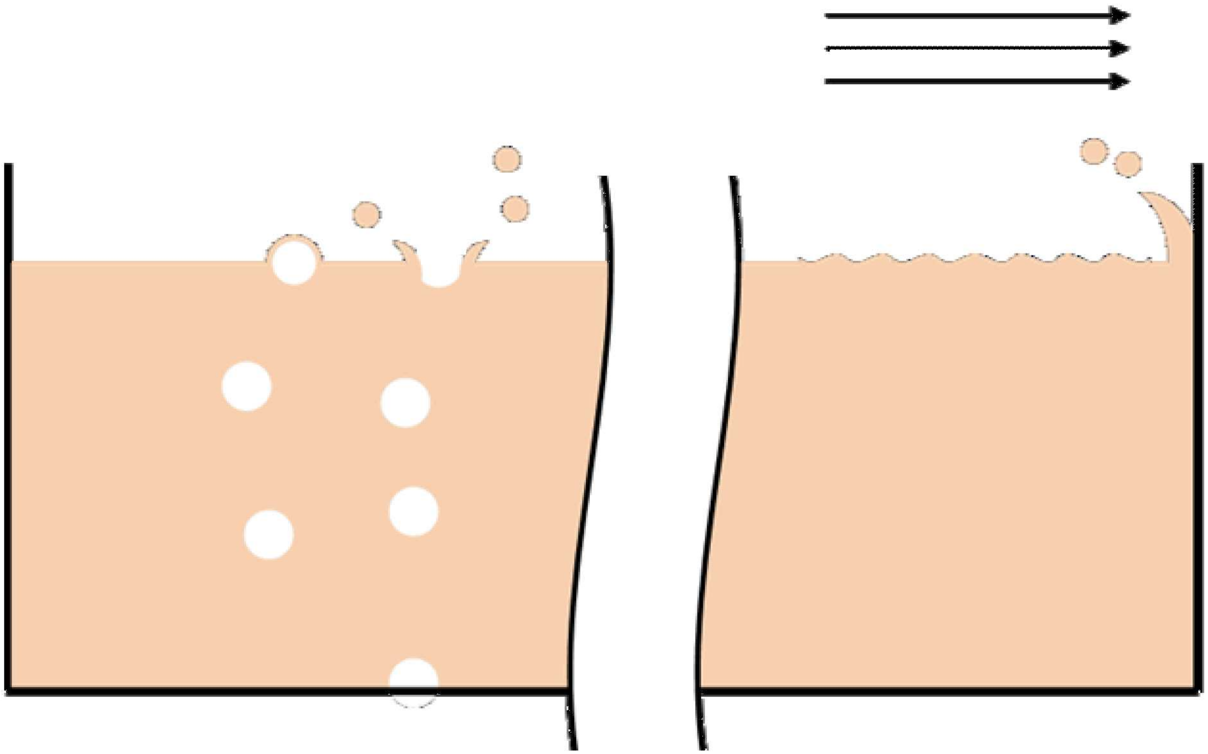
- Four natural mechanisms were identified
  - Evaporation Induced Entrainment [E]
    - Particles ejected from pool by evaporating fluid
  - Surface Agitation by Wind
    - Strong winds create waves which suspend particles upon breaking
  - Surface Agitation by Boiling [B]
    - Droplets become suspended as the gases rupture the liquid surface
  - Residue Entrainment (Resuspension)
    - After liquid has been consumed, remaining solid particles can erode by persisting flow conditions

During Fire

After Fire

- An external mechanism also exists
  - Impact Entrainment
    - Droplets (i.e. rain, water from suppression devices) can impact and disturb the fuel surface

An Illustration of Two Mechanisms

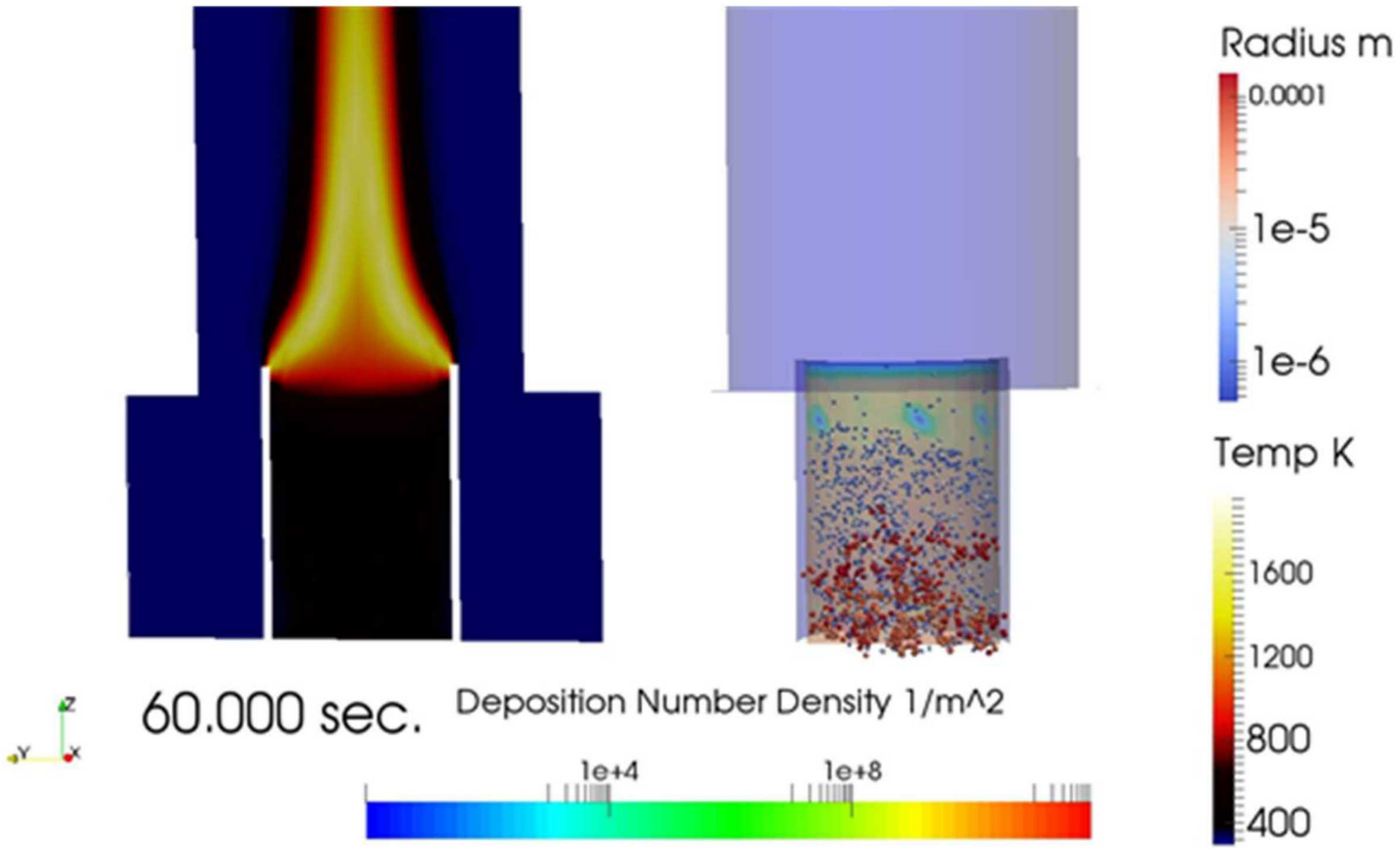


Surface Agitation by Boiling
Involves pinch and rupture of bubbles

Surface Agitation by Wind
Involves waves created by flow

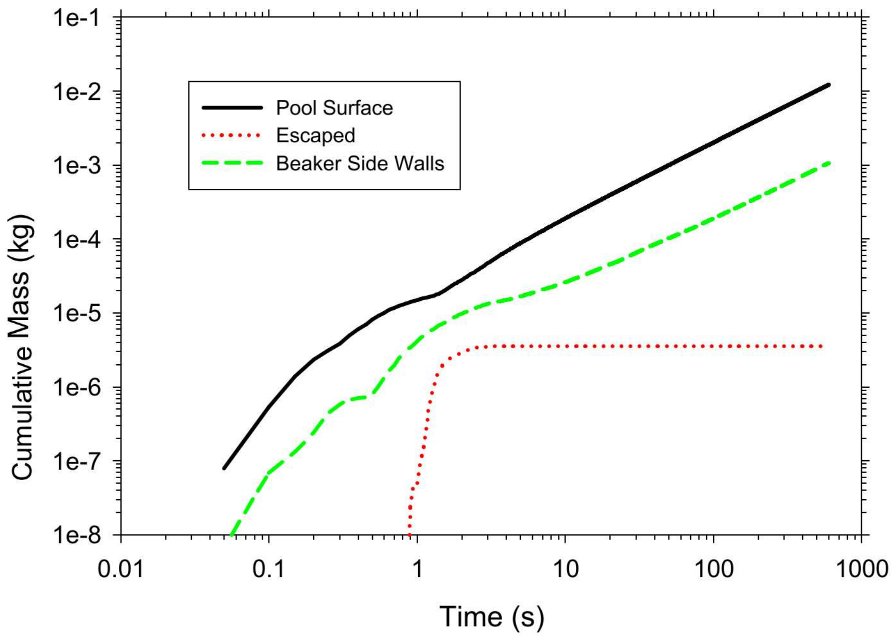
Evaluated Particle Fate

- Below image illustrates typical behavior



Initial Finding (mass)

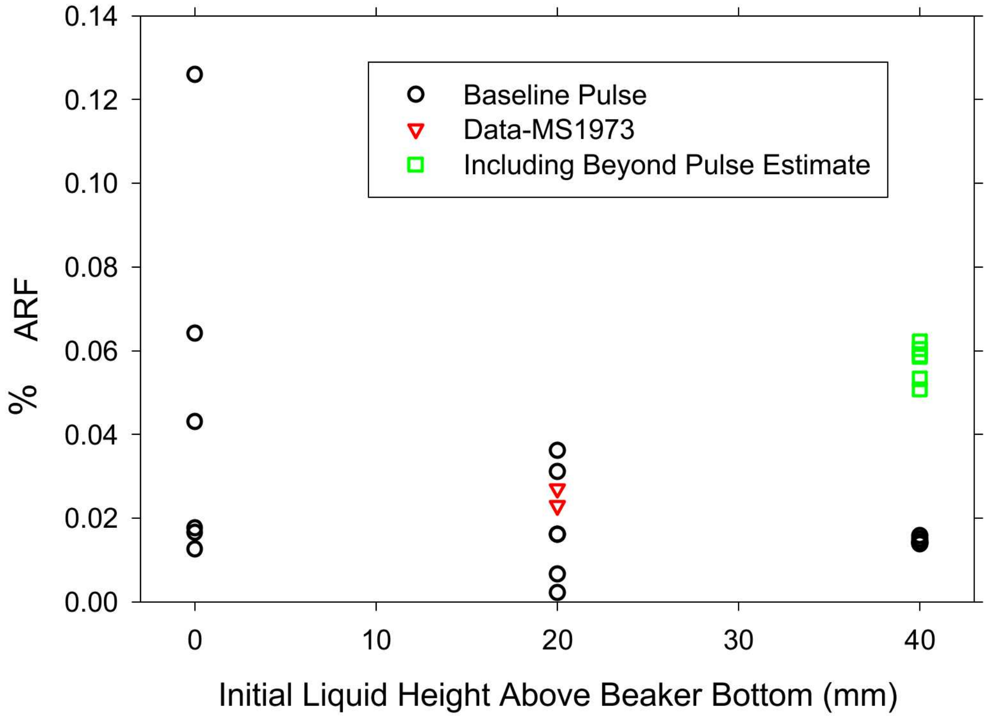
- Mass was almost all released during ignition
- Subsequent was minimal, small particles
- Pool height was varied to capture the effect of the change



20 mm initial height

Initial fuel height significant

- Simulation work allows exploration of larger parameter space
- Differences observed – experimental result not the most conservative
  - Different mechanisms dependent on initial condition
- Sensitivity to other parameters also explored



Selected findings (summary)

- Major findings:
  - The release was mostly during start-up in the simulation
  - Initial liquid level was a significant parameter, non-conservative
  - Historical experiments were incomplete
    - No temporal resolution
    - Variation of initial fluid height
    - No turbulence data
    - Description of ignition methods
    - No data on distillation
    - Minimal observations on liquid behavior
- 2018 NSRD project filling experimental data gaps

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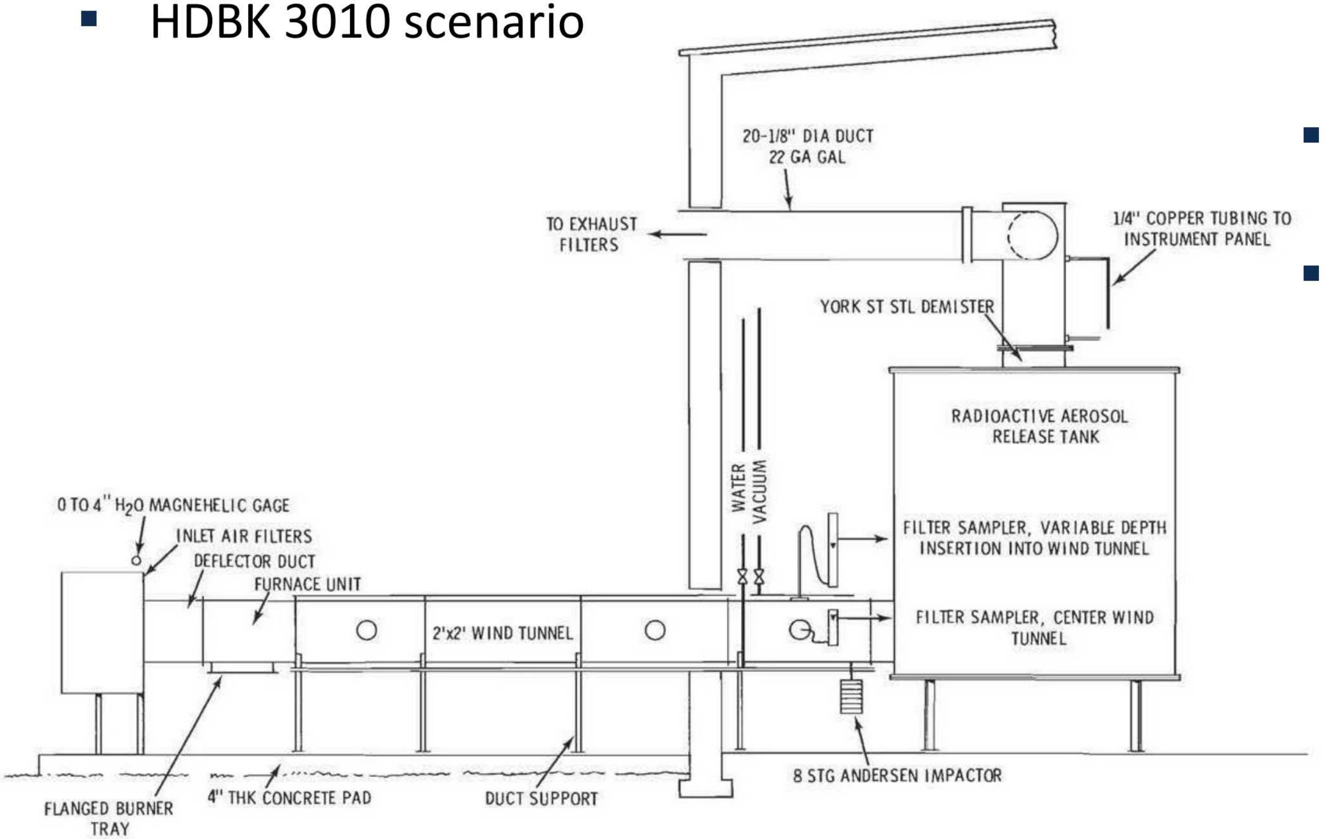
Gasoline Pool Fire (BNWL-1732)

- 1 gallon gasoline onto pan surface
- UO_2 powder, 50 g poured before gasoline
- Pan size 15-inch diameter tray used
- HDBK 3010 scenario



- FUEGO Simulation
  - Reproducing the test environment as closely as possible
- Simulation Results
  - Base case -20 s run
- Sensitivity Study – particle generation
  - Gasoline vaporization
  - Boiling surface rupture
  - Residue re-suspension

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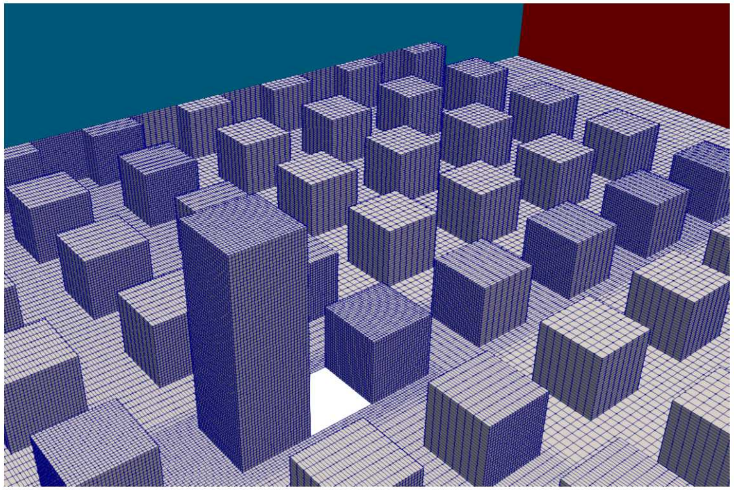
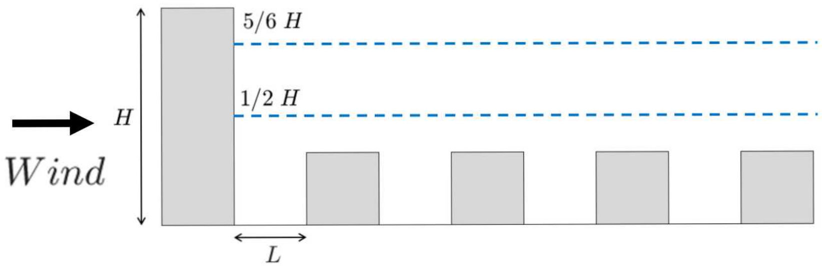
Why Can We Trust the Models?

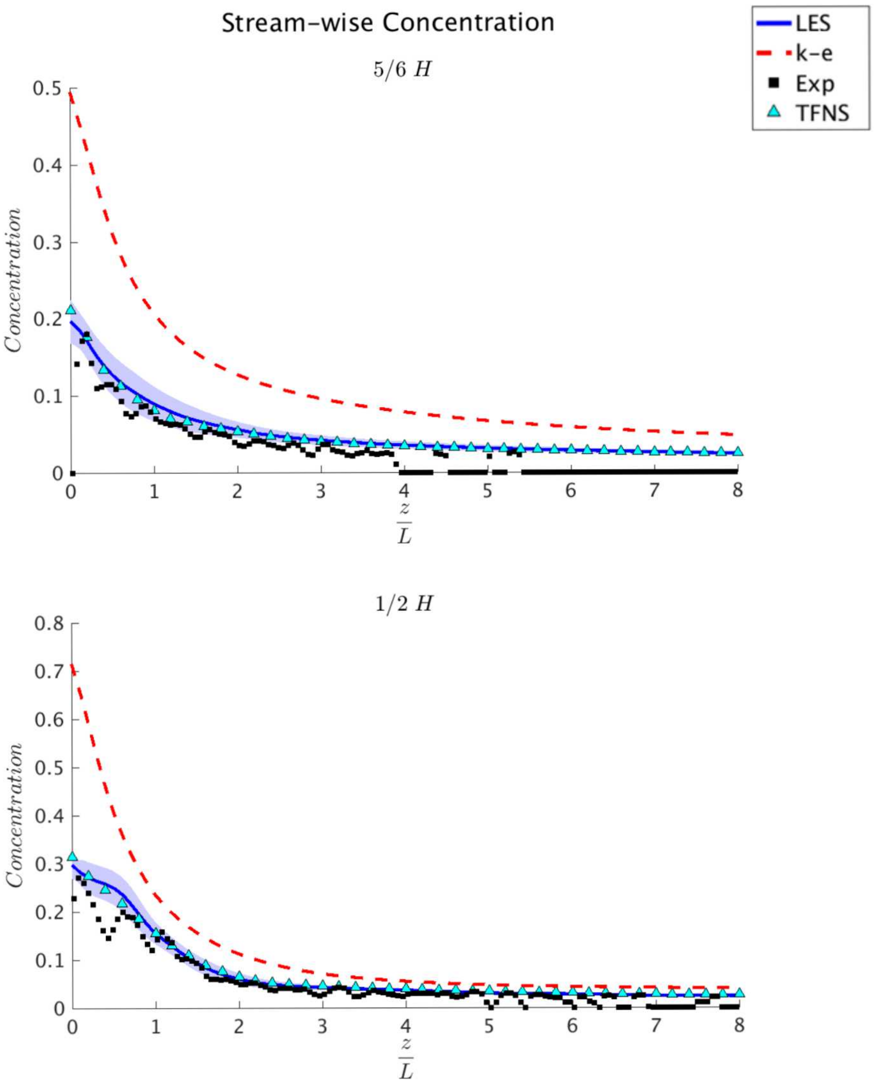
- Verification and Validation
- Representative datasets for the physics
- 3D print and tomography used to create high-fidelity scenario for MRI



Downwind Concentration

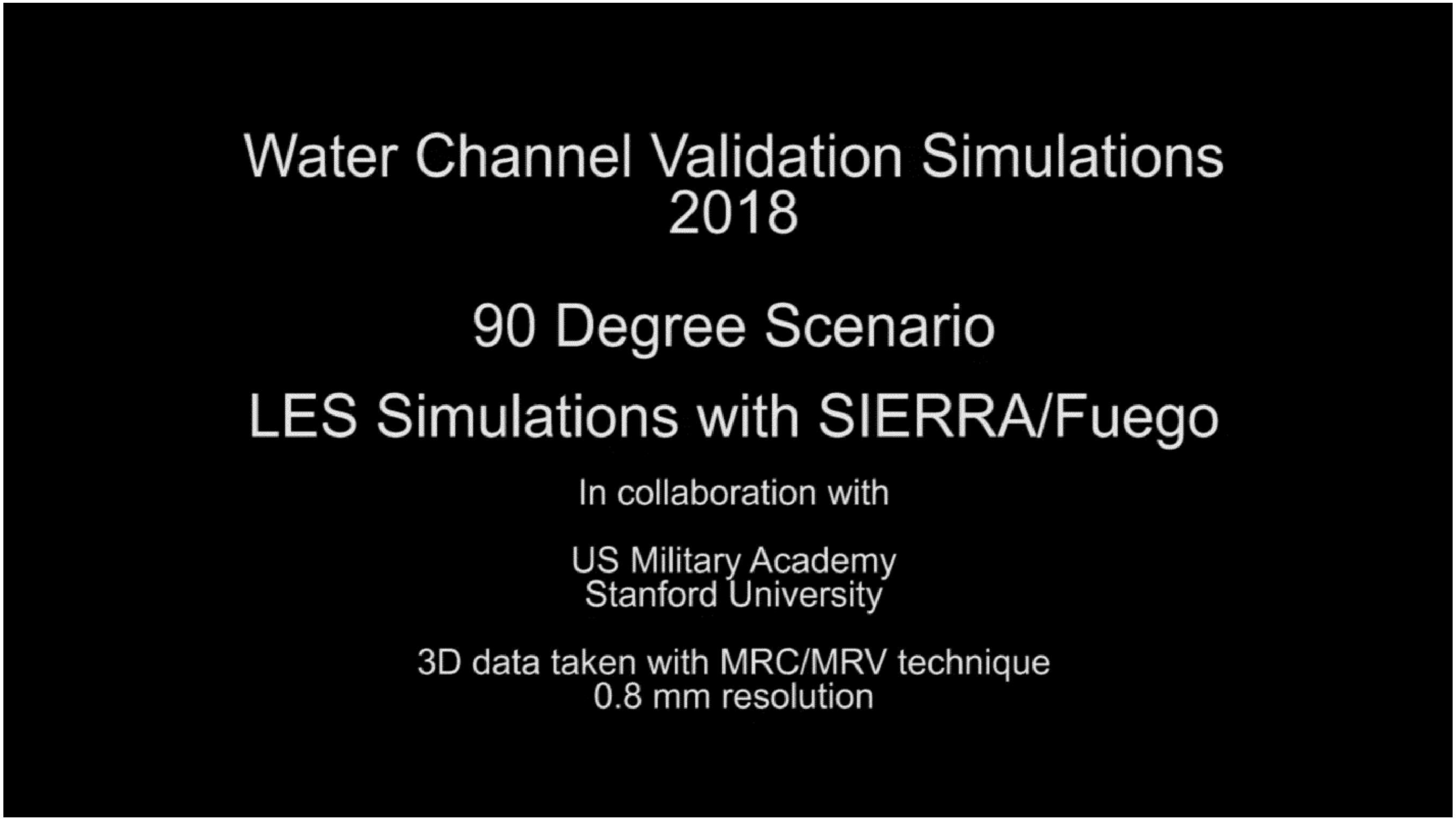
- LES models experimental concentration well throughout domain
- k-ε approaches observed results further downstream





Video of Instantaneous Results

- LES baseline case



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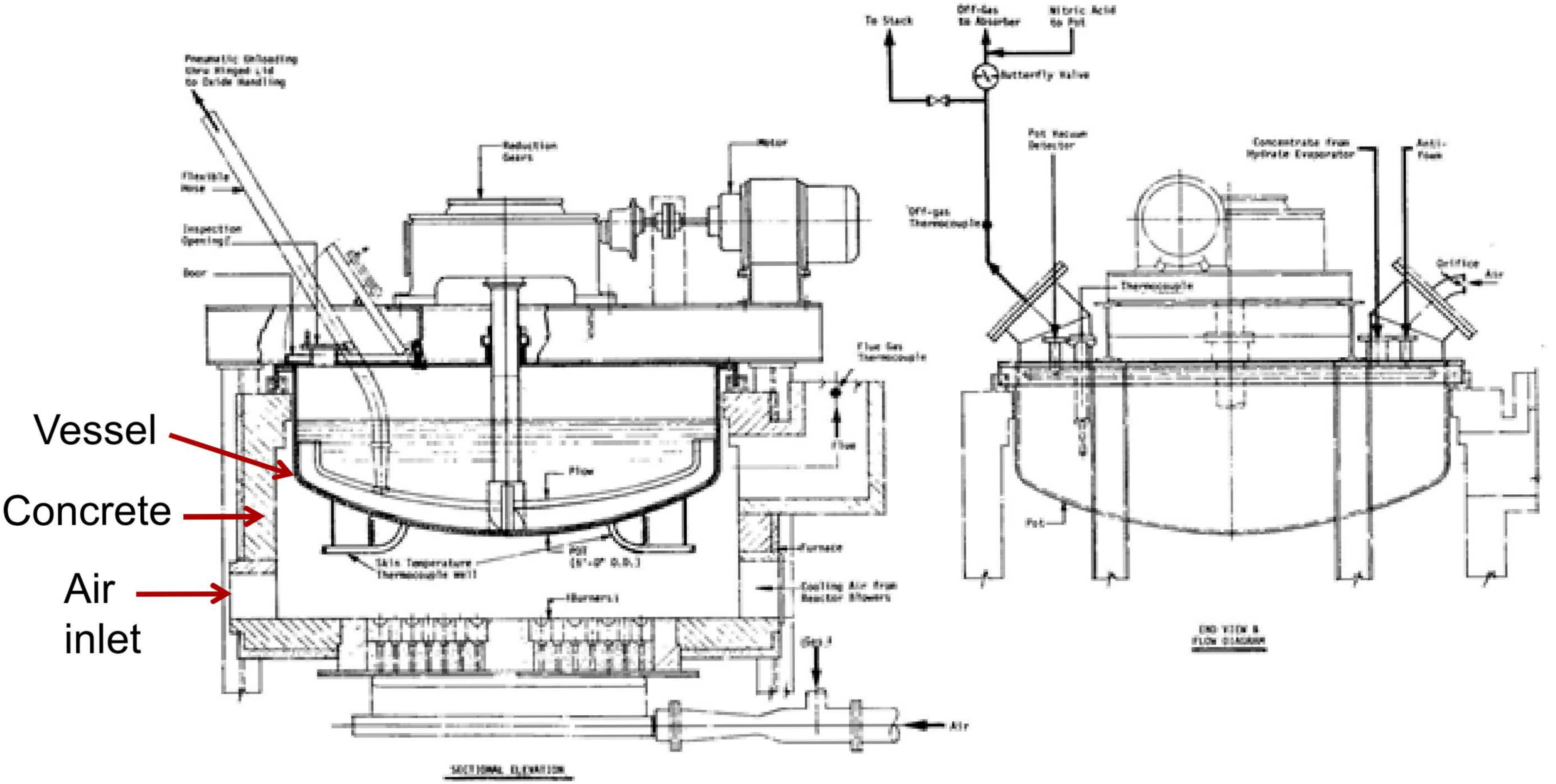
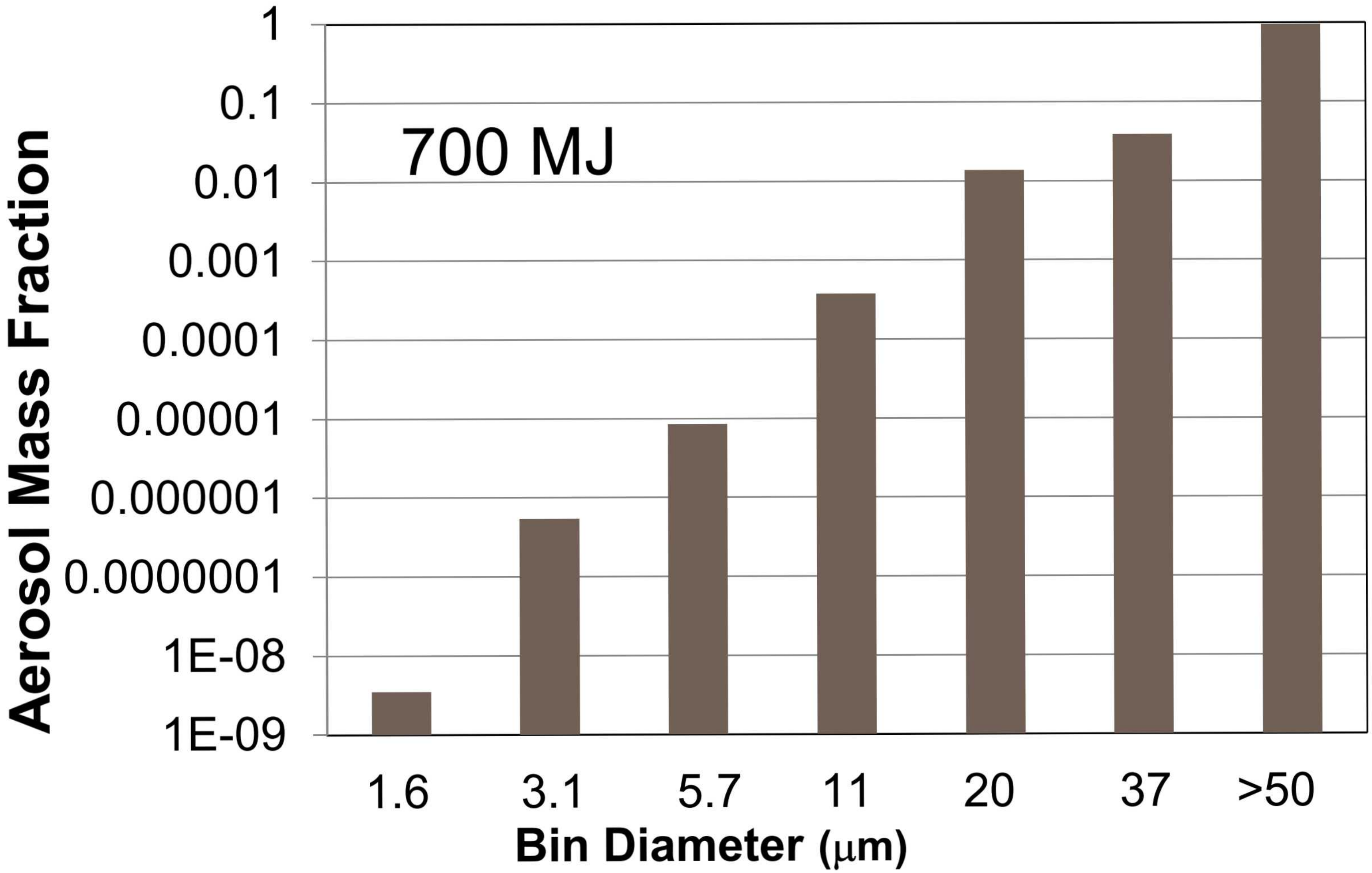
Denitrator Explosion Scenario

- ARF/RFs are obtained through look-up tables in Handbook 3010
  - Release data may be of marginal relevance to specific scenarios
- Spent nuclear fuel refining accident
- Replicated the accident to assess release potential
  - Varied explosive intensity because it was not well known
  - Used the TAB model for particle break-up and sizing

Schematic of Denitrator
(J. M. McKibben, 1976)



Preliminary Estimate of Aerosol Distribution 10^{-5}% Respirable (~<20 Micrometer Diameter)



Demonstration Calculation

- Final ARF/RF significantly below handbook estimates
- Technique requires validation, but huge gap exists between model and expectation

Comparison to DOE Handbook 3010

- DOE Handbook: “Airborne Release Fractions/Rates and Respirable Fractions for Nonreactor Nuclear Facilities: Volume I”
  - ARF x RF = 0.2 : 0.1 : 0.07 (upper bound : median : lower bound)
- 50 MJ explosion: 10^{-9} respirable fraction (preliminary)
- 700 MJ explosion: 10^{-7} respirable fraction (preliminary)

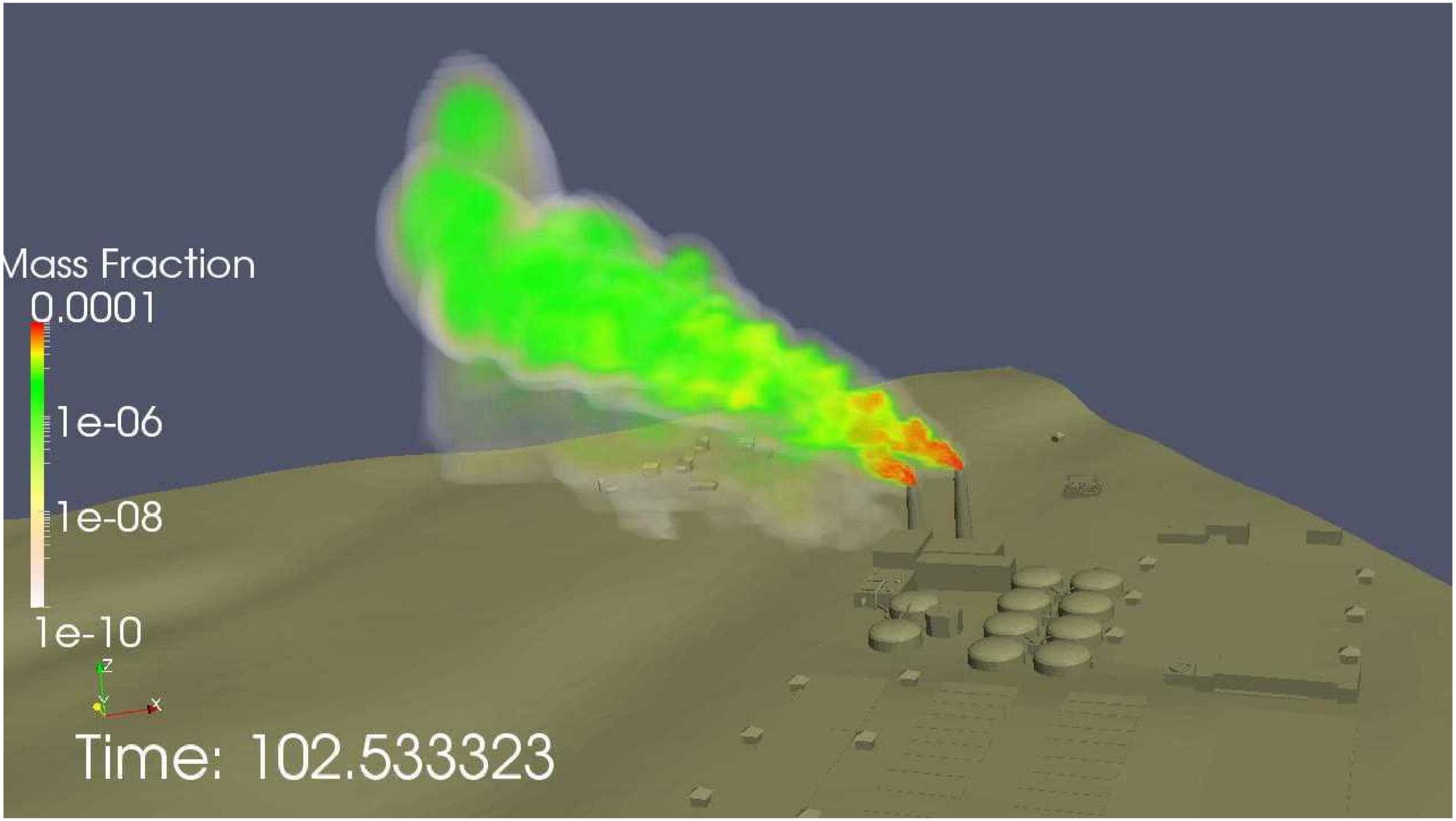
Summary

- SIERRA/Fuego is Sandia/DOE's low-Mach tool for reacting flows
  - Can add value to safety assessment activities
- Meets high QA standards, compliant to DOE orders
  - Designed primarily for abnormal thermal analysis of DOE systems
- Safety assessments suffer from inaccurate ARF approximations
  - Recommended ARF is not necessarily conservative
  - Operational ARFs may be severely conservative and drive substantial costs

Acknowledgements

- Sandia National Laboratories is a multimission laboratory operated by National Technology and Engineering Solutions of Sandia, LLC, a wholly owned subsidiary of Honeywell International, Inc. for the United States Department of Energy's National Nuclear Security Administration under Contract No. DE-NE0003525.
- The SIERRA development, department 1541
- Many others who made contributions to the various efforts shown in this presentation (Erik Benavidez, Michael Clemenson, Stefan Domino, Lindsay Gilkey, John Hewson, Hector Mendoza, Flint Pierce, Jon Rogers, Sheldon Tieszen, Tyler Voskuilen, Ethan Zepper, David Louie)

Questions?



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Why Want to Substantiate Handbook?

- Safety analysts at DOE complex rely heavily on the data provided in this Handbook to determine the source term (ST)
- Five Factor Formula
  - $ST = MAR \cdot DR \cdot ARF \cdot RF \cdot LPF$
    - MAR - material at risk, DR – damage ratio, ARF – airborne release fraction, RF – respirable fraction & LPF – leak path factor
- More often, analysts simply take the bounding values to perform ST calculations to avoid regulatory critique
- Derived data (i.e., ARF & RF) from Handbook:
  - Very limited table-top and bench/laboratory experiments
  - Engineering judgement which may not have adequate bases
  - Actual situation may not be represented

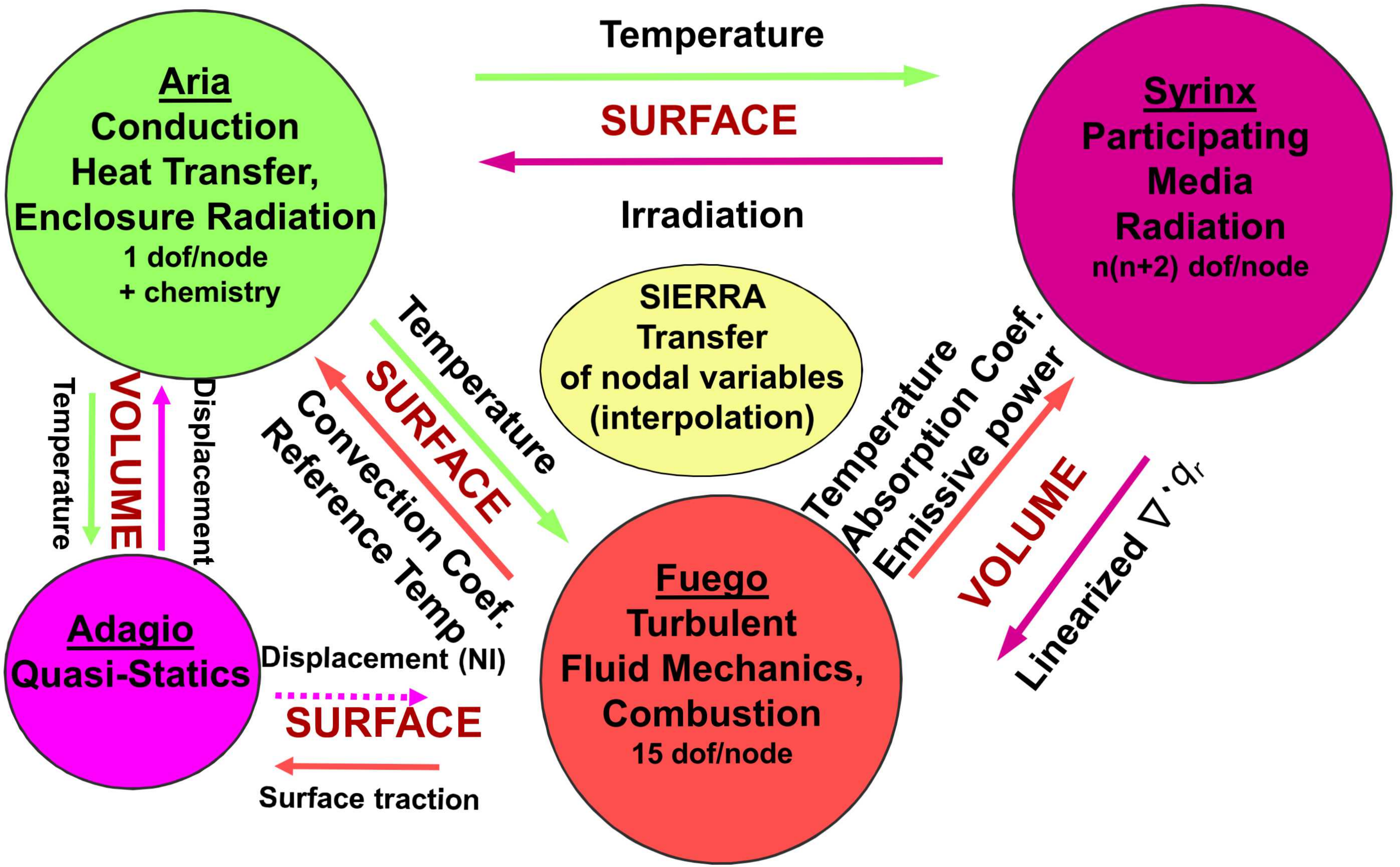
HPC Platforms

- As of April 2018, 237,978 processors are available within Sandia network across 10 machine platforms
  - Provides more than 2B CPU hours per year
  - High-end computing capacity: 2.1-2.7GHz with 3.5-4GB per processor
  - Ample storage: more than 50PB with high-speed access from computational processors
  - Only 2.5 years old in average; 5 of them are launched in 2017 or later
  - Not included are jointly funded machines that are located outside Sandia (ex> Trinity)

Sierra : Thermal/Fluid

- DOE O 414.1D
  - Code is maintained to order standards
  - Regularly audited
- SAND 2008-5517, Software Quality Plan for ASC codes
- SIERRA tools are used for safety case relating to stockpile performance
  - Abnormal environment (fires)
  - Normal environment (day-to-day operations)

SIERRA Enables Coupling (example)

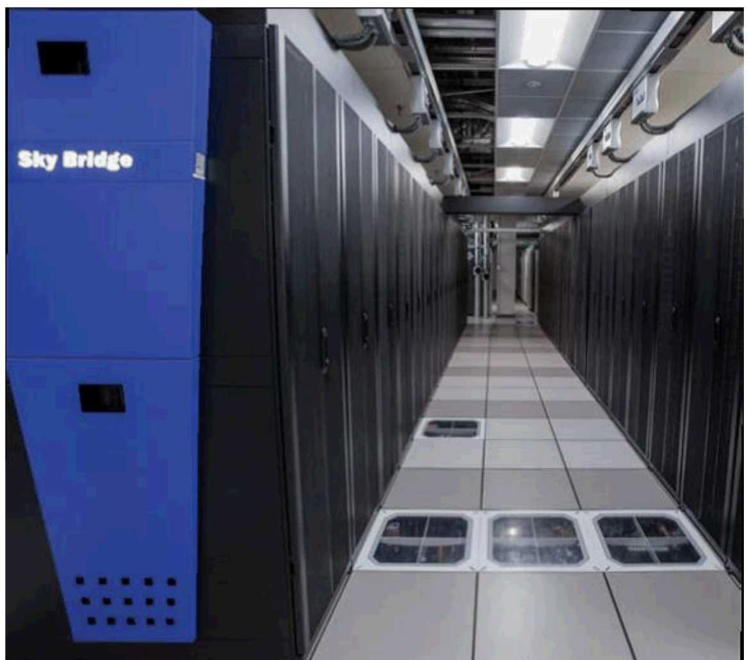


HPC at Sandia

- Sandia is a leader in HPC technology
  - Advanced hardware configurations and performance
  - Large lab, large resource
  - Thousands of teraFLOPS
  - Resources on red networks as well

System	Status	Notes
* ACES Trinitite @LANL	●	DST 4/18 completed 15:34 MDT
* CEE SCN TeamForge	●	SCN TeamForge returned to service 2:08 pm, 4/17
* CEE SRN Apps	●	SRN cee-apps.sandia.gov accepting logins, but the apps are still down. No ETA 9:00 4/9
* CEE SRN Resources	●	4/6/18 9am CEE Resources that are still unavailable are after power outage; ceerws2907a,b,c,d,e,f No ETR
*CEE SCN Apps	●	Citrix XenApps https://ceescn-apps is out of service. Currently no ETA 2/12 2:30pm
*SMSS - SCN	●	RTS 4/18 4:40PM
ACES Mutrino @SNL	●	
ACES Trinity @LANL	●	
Cayenne SCN	●	
Chama	●	
Eclipse	●	
Ghost	●	
gitlab	●	
IHPC	●	
Jemez SCN	●	
Lynx	●	
Lynx-s SCN	●	
Pecos SCN	●	
Sequoia @ LLNL	●	
Serrano	●	
Skybridge	●	
SMSS-ECN/SRN	●	
Solo ECN	●	
Uno	●	

Skybridge has 1,848 compute nodes, 29,568 cores

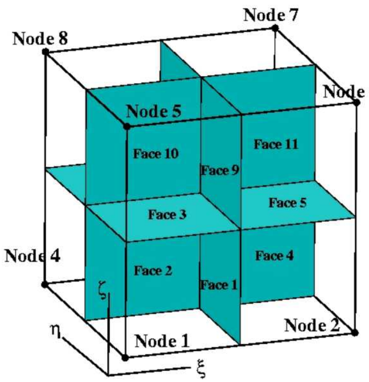


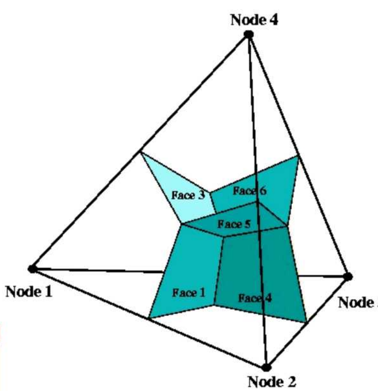
SIERRA/Fuego/Syrinx/Aria Methodology and Framework

Sandia National Laboratories

- Common application framework
  - Shared data structure, parser, file I/O, parallel communication, solvers, etc.
- Data exchange for application coupling

- SIERRA/Fuego: Low-Mach turbulent fire
  - Hybrid control volume finite element method (CVFEM)
- SIERRA/Syrinx: Participating media radiation (PMR)
  - Streamwise-upwind Petrov-Galerkin FEM
- SIERRA/Aria: Heat conduction, enclosure radiation, viscous multi-phase flow
  - Galerkin FEM



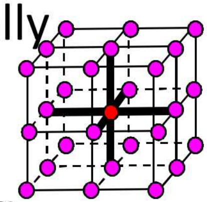


Each code has completed a detailed verification suite!

Numerics and Math Models

Sandia National Laboratories

- Segregated, backward Euler or Crank-Nicholson time solution
  - Equal-order interpolation CVFEM technique for low-Mach or acoustically compressible mechanics
  - Approximate pressure projection method for continuity/momentum
  - Convection operators: Central, pure upwind, skew upwind, MUSCL w/flux limiters (Van Leer, Superbee, etc.)



- Basic Favre-filtered equation set (integral form):

Turbulence closure models required

Continuity: $$\int \frac{\partial \bar{\rho}}{\partial t}\mathrm{d}V + \int \bar{\rho}\,\tilde{u}_j n_j dS = 0$$

Momentum: $$\int \frac{\partial \bar{\rho}\tilde{u}_i}{\partial t}\mathrm{d}V + \int \left(\bar{\rho}\,\tilde{u}_i\tilde{u}_j n_j + \bar{p} n_j \delta_{ij}\right) dS = \int \left(\bar{\tau}_{ij} - \tau_{u_i u_j}\right) n_j dS + \int \left(\bar{\rho} - \rho_o\right) g_i \mathrm{d}V$$

Enthalpy: $$\int \frac{\partial \bar{\rho}\tilde{h}}{\partial t}\mathrm{d}V + \int \bar{\rho}\,\tilde{h}\tilde{u}_j n_j dS = -\int \left(\bar{q}_j + \tau_{hu_j}\right) n_j dS - \int \frac{\partial \bar{q}_i^{\,r}}{\partial x_i}\mathrm{d}V + \int \left(\frac{\partial P}{\partial t} + \tilde{u}_j \frac{\partial P}{\partial x_j}\right) dV + \int \overline{\tau_{ij}\frac{\partial u_i}{\partial x_j}}\, dV$$

Species: $$\int \frac{\partial \bar{\rho}\tilde{Y}_k}{\partial t}\mathrm{d}V + \int \bar{\rho}\tilde{Y}_k \tilde{u}_j n_j dS = \int \left(\overline{\rho \mathrm{Y}_\mathrm{k} \hat{u}_{j,k}} - \tau_{Y_k u_j}\right) n_j dS + \int \overline{\dot{\omega}}_\mathrm{k} \mathrm{d}V$$

- Additional equations for turbulence closures, soot transport

Large Eddy Simulations

- LES is a turbulent flow model that solves larger scales directly and models smaller scales

Turbulence closure models required

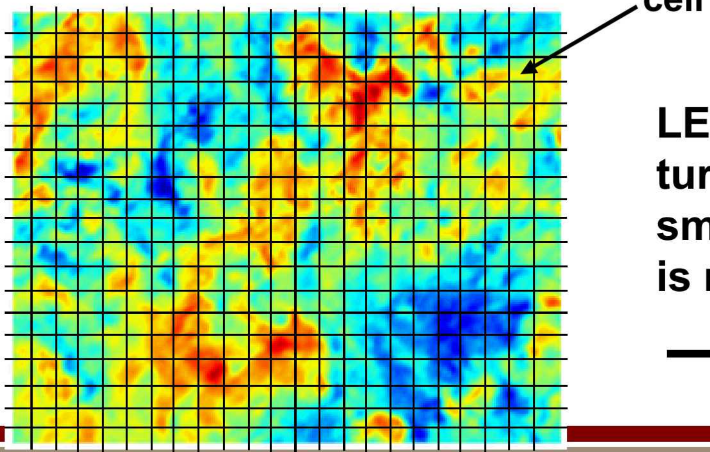
Momentum: $$\int \frac{\partial \bar{\rho}\tilde{u}_i}{\partial t} \mathrm{d}V + \int \left(\bar{\rho}\,\tilde{u}_i\tilde{u}_j n_j + \bar{p} n_j \delta_{ij}\right) dS = \int \left(\bar{\tau}_{ij} - \tau_{u_i u_j}\right) n_j dS + \int \left(\bar{\rho} - \rho_o\right) g_i \mathrm{d}V$$

$$\tau_{u_i u_j} = \frac{\mu_t}{\mu}\tau_{ij}$$

  - KSGS one-eq. model: μ_t is modeled using sub-grid kinetic energy

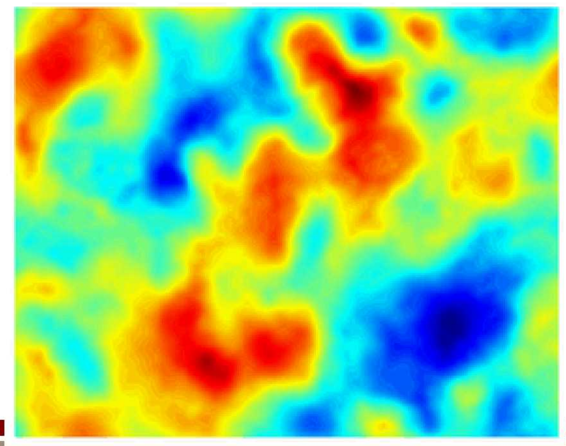
$$\mu_t = C_{\mu_\epsilon} \Delta k^{\mathrm{sgs}\,\frac{1}{2}}$$

A real turbulent flow



LES solves cell-averaged turbulence. Any physics smaller than the cell size is modeled using μ_t

LES field



Entrainment Theory

- Kataoka and Ishii (1983) suggest entrainment can be described:

$$E_{fg} = 4.84 \times 10^{-3} \left(\frac{\rho_g}{\Delta\rho}\right)^{-1.0}$$

$$E_{fg} = \frac{\rho_f j_{fe}}{\rho_g j_g}$$

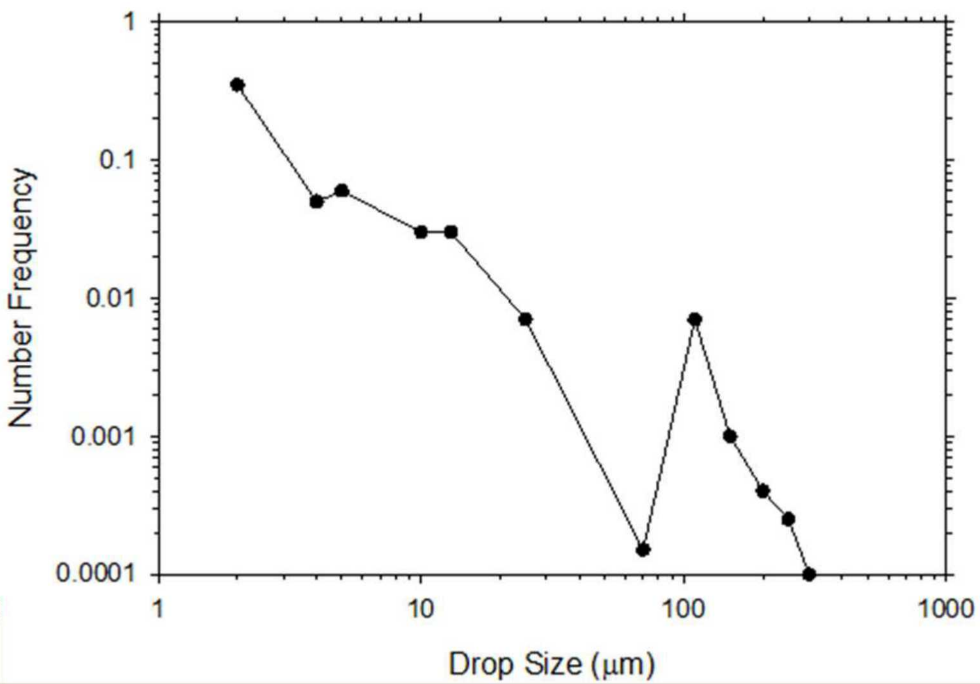
Valid for: $0 \le h^* \le 1.038 \times 10^3 j_g^* N_{\mu g}^{0.5} D_H^{*0.42} \left(\frac{\rho_g}{\Delta\rho}\right)^{0.23}$

$$j_g^* = \frac{j_g}{\left(\sigma g \Delta\rho/\rho_g^2\right)^{1/4}} \qquad h^* = \frac{h}{(\sigma/g\Delta\rho)^{1/2}} \qquad N_{\mu g} = \frac{\mu_g}{\left[\rho_g \sigma (\sigma/g\Delta\rho)^{1/2}\right]^{1/2}}$$

$$D_H^* = \frac{D_H}{(\sigma/g\Delta\rho)^{1/2}}$$

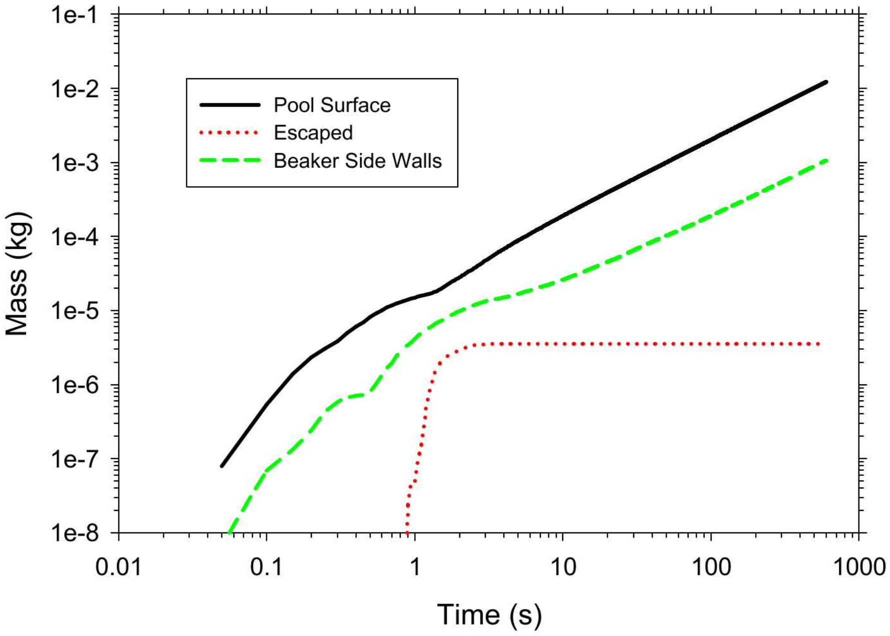
- Borkowski et al. (1986) measured the particle distribution from a boiling scenario:

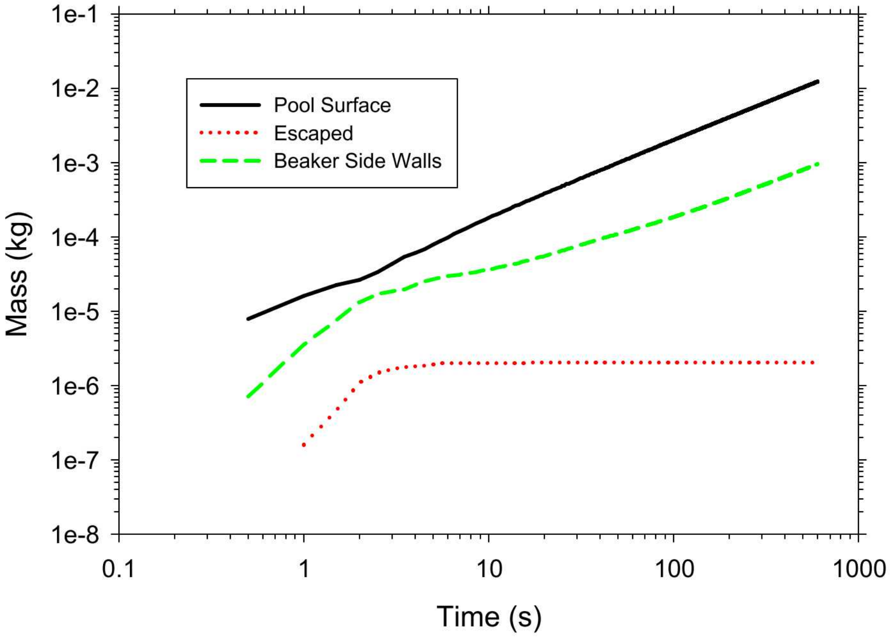
- Primary entrainment includes all drops formed by surface boiling, but most drops fall back to the surface



Initial Finding (mass)

- Mass was almost all released during ignition
- Subsequent was minimal, small particles
- Pool height was varied to capture the effect of the change





20 mm initial height

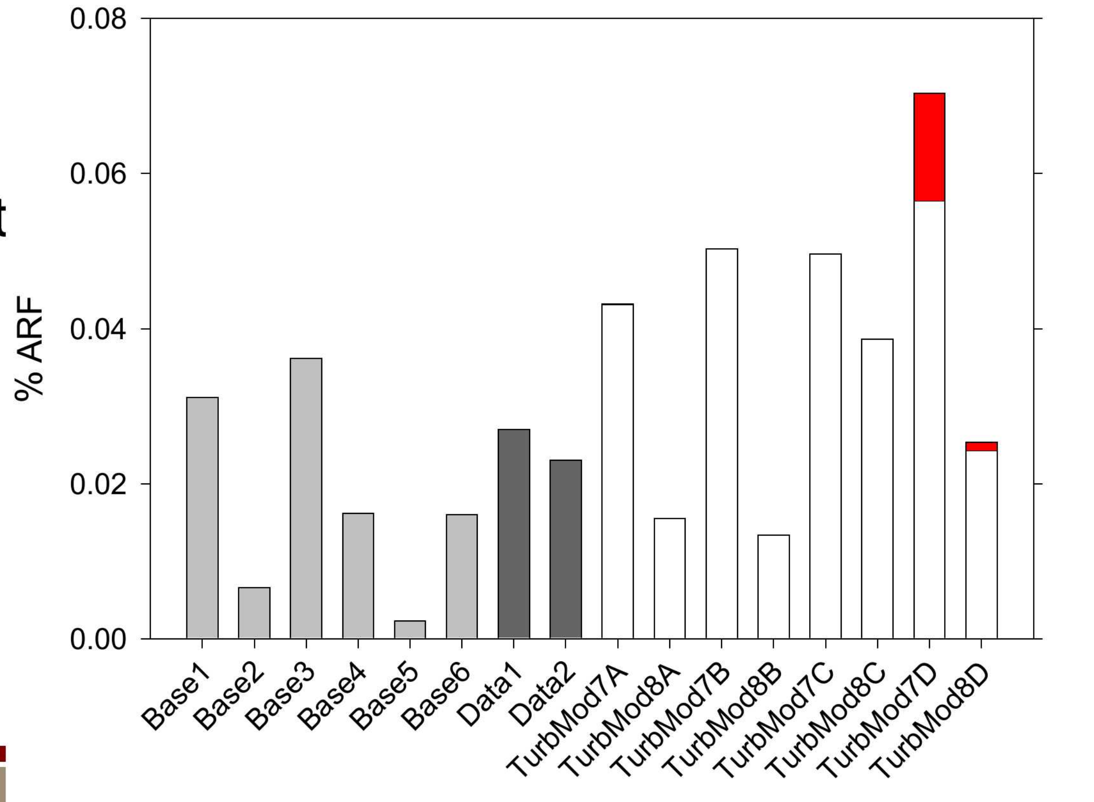
0 mm initial height

Effect of turbulence (20 mm height)

- Including turbulence effects results in minor ARF increase

Runs	k [m²/s²]	epsilon [m²/s³]	Corresponding length scale [m]	Corresponding turbulence intensity [%]
Baseline	5.95e-7	4.56e-7	1.7×10^{-4}	100
A variation	5.95e-5	1.53e-4	5×10^{-4}	1000
B variation	5.95e-5	1.92e-6	4×10^{-2}	1000
C variation	5.95e-3	1.53e-1	5×10^{-4}	10000
D variation	5.95e-3	1.92e-3	4×10^{-2}	10000

- Varied particle input file distribution
- Red is after pulse contribution



Entrainment Mechanisms

- Four natural mechanisms were identified
  - Evaporation Induced Entrainment [E]
    - Particles ejected from pool by evaporating fluid
  - Surface Agitation by Wind
    - Strong winds create waves which suspend particles upon breaking
  - Surface Agitation by Boiling [B]
    - Droplets become suspended as the gases rupture the liquid surface
  - Residue Entrainment (Resuspension)
    - After liquid has been consumed, remaining solid particles can erode by persisting flow conditions
- An external mechanism also exists
  - Impact Entrainment
    - Droplets (i.e. rain, water from suppression devices) can impact and disturb the fuel surface

During Fire

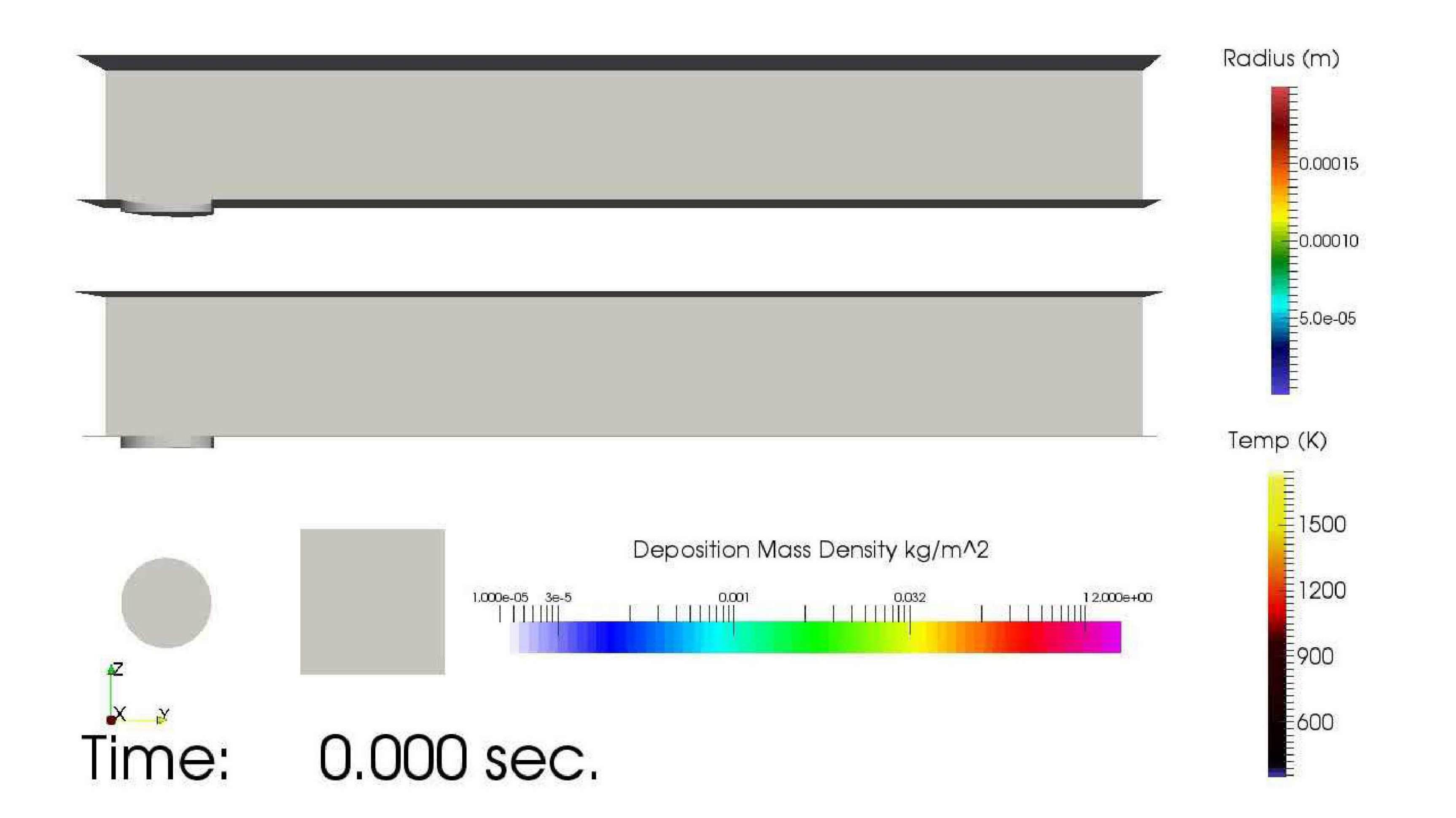
After Fire

Simulation Scenarios

Run	Sim. Time (s)	Duration† (s)	Fuel Height (m)	Injected Mass (kg/s) [wt% UO_2]	Particle Size (um)	Turbulence	Injection Height (mm)
1E*	20	540	3.3E-2	1.64E-13 [100%]	0.2	Normal	10
2E*	20	540	3.3E-2	1.64E-13 [100%]	0.7	Normal	10
3E*	20	540	3.3E-2	1.64E-13 [100%]	2	Normal	10
4E*	20	98	6.0E-3	1.64E-13 [100%]	0.2	Normal	10
5E*	60	540	3.3E-2	1.64E-13 [100%]	0.2	Normal	10
6E*	20	540	3.3E-2	1.64E-13 [100%]	0.2	High	10
7E*	20	540	3.3E-2	1.64E-13 [100%]	0.2	Normal	5
1B**	20	20	0.002	8.3E-3 [25%]	Distribution	Normal	10
2B**	30	30	0.002	8.3E-3 [25%]	Distribution	Normal	10
3B**	20	20	0.002	8.3E-3 [25%]	Distribution	High	10
4B**	20	20	0.001	4.15E-3 [25%]	Distribution	Normal	10
5B**	20	20	0.003	1.25E-2 [25%]	Distribution	Normal	10
6B**	20	20	0.002	8.3E-3 [25%]	Distribution	Normal	5

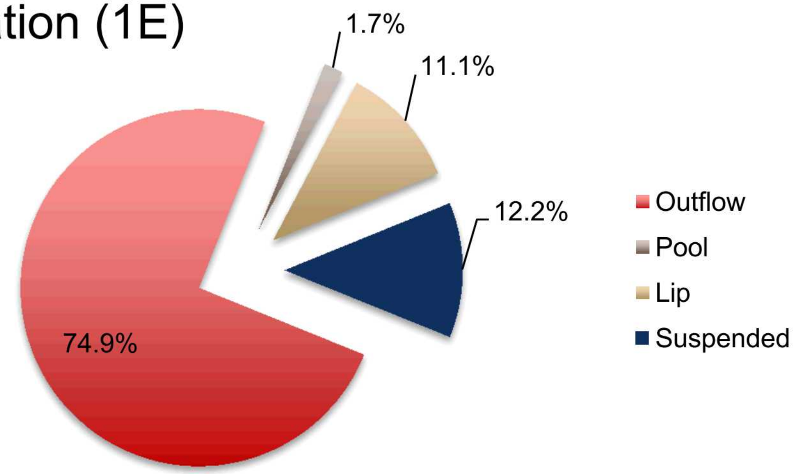
* = Solid Contaminant
** = Combined Fuel & Contaminant
†= Note: Duration for Evaporation [E] denotes the entire burn, while duration for Boiling [B] denotes the portion of the burn when the fuel was assumed to be boiling.

Simulation Visualization: Boiling (1B)

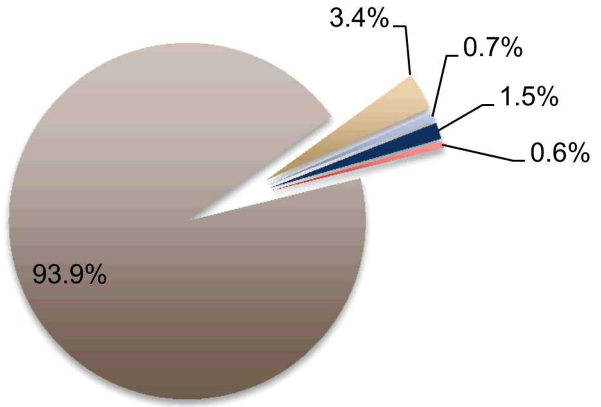


Baseline Case Final Mass

- Evaporation (1E)

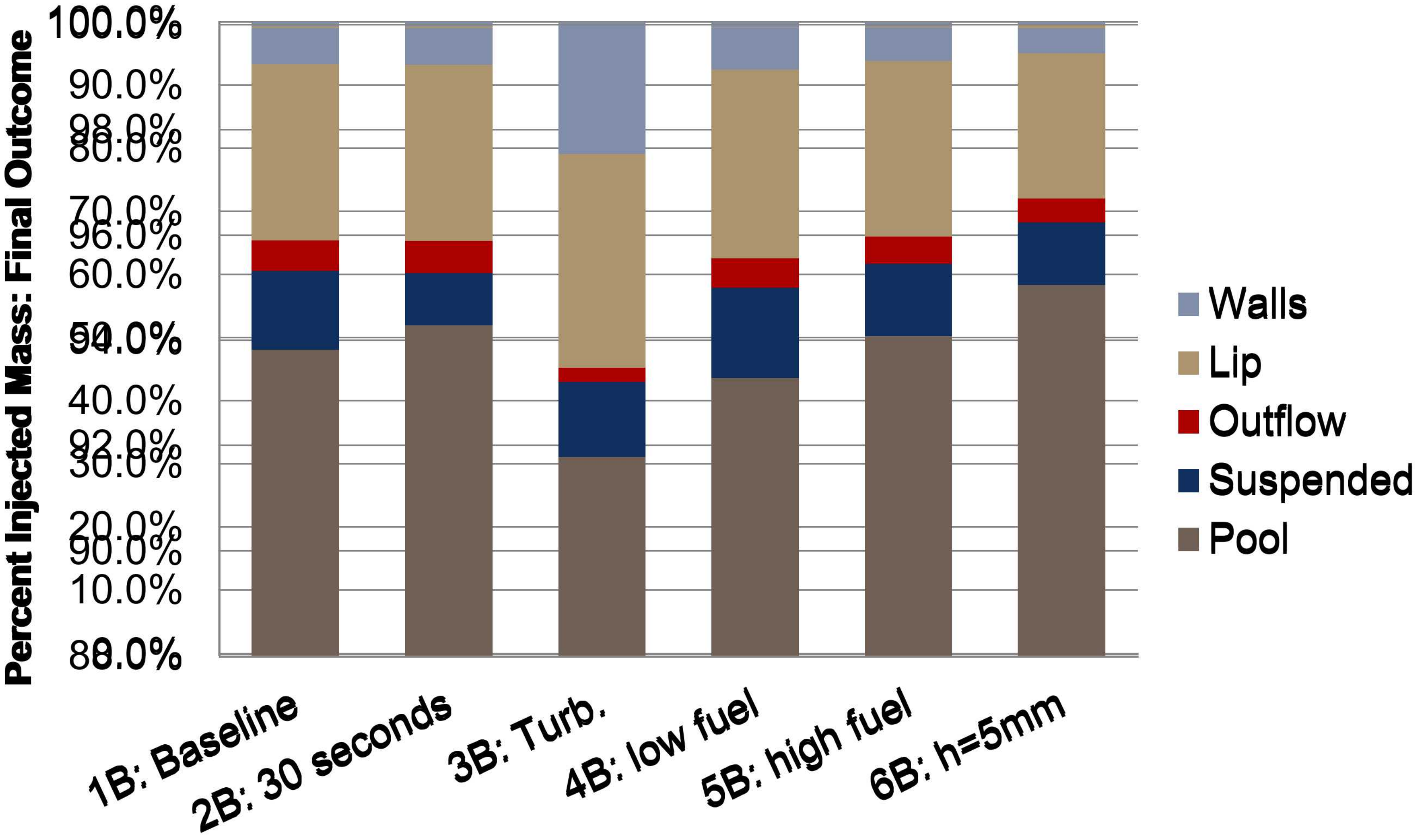


- Boiling (1B)



- “Suspended” mass would be omitted in longer simulation runs
- Evaporation: Most entrained particles reach the outflow
- Boiling: Most entrained particles fall back into the pool

Boiling Final Deposition



ARF - Significant Parameters

- Turbulence
  - Varying the turbulence changed the deposition location and ARF for both entrainment mechanisms.
- Boiling Duration
  - The predicted ARF is most dependent on the boiling mechanism, yet the precise duration is unknown
- Original Empirical Datasets in 3010 just use ARF
  - No credit for importance of either of these parameters
  - Value could be overly conservative or non-conservative

Selected findings (summary)

- Code development needs to better simulate this problem:
  - Resuspension, multi-component particle evaporation, volumetric flow BC, film deposit flow and evaporation, improved reaction model, regressing liquid surface, multi-component pool model
- Issues with experiments:
  - No temporal resolution, no indication of ignition methods, no variation of initial fluid height and liquid level below lip, no turbulence data, no data on distillation, no observations on liquid behavior
- Major findings:
  - The release was mostly during start-up in the simulation
  - Sensitivity to turbulence parameters was slight
  - Initial liquid level was a significant parameter, non-conservative
- We have a current project to collect new data

Future Work

- Suspension distribution of particles in gasoline pool will affect the ARF
  - Presumed to be homogeneous; lacking a more accurate model.
  - Large difference in particle and fuel density, 10970 and 679.5 kg/m^3
    - Suggests settling would occur
    - Alters the ARF.
- Resuspension mechanism is important for understanding what happens after the fire
- Multi-component particles will enhance the predictive capability of the simulations
- Surface agitation by wind

Rubble Fire Test Arrangement

Composite Rubble Fire Test

Assembly Time Lapse

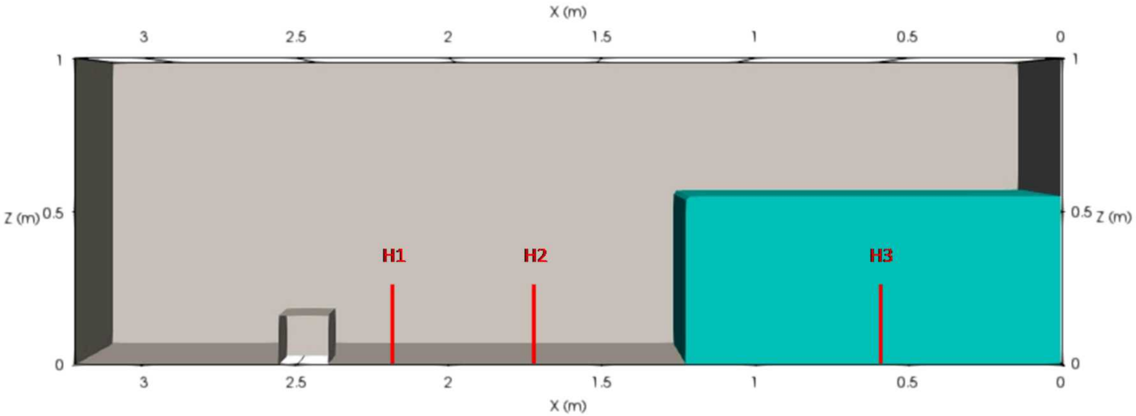
9/4/14

Rubble Fire Test Video

Validation Scenario (VOF)

- Dam burst scenario was created experimentally
- Provides a good test of the advection and surface models
- References:

- K. Kleefsman, G. Fekken, A. Veldman, B. Iwanowski, and B. Buchner. A volume-of-fluid based simulation method for wave impact problems. Journal of Computational Physics, 206(1):363-393, JUN 2005.
- C. Crespo, J. M. Dominguez, A. Barreiro, M. Gomez-Gesteira, and B. D. Rogers. GPUs, a new tool of acceleration in CFD: Efficiency and reliability on smoothed particle hydrodynamics methods. PLOS ONE, 6(6), JUN 2011.



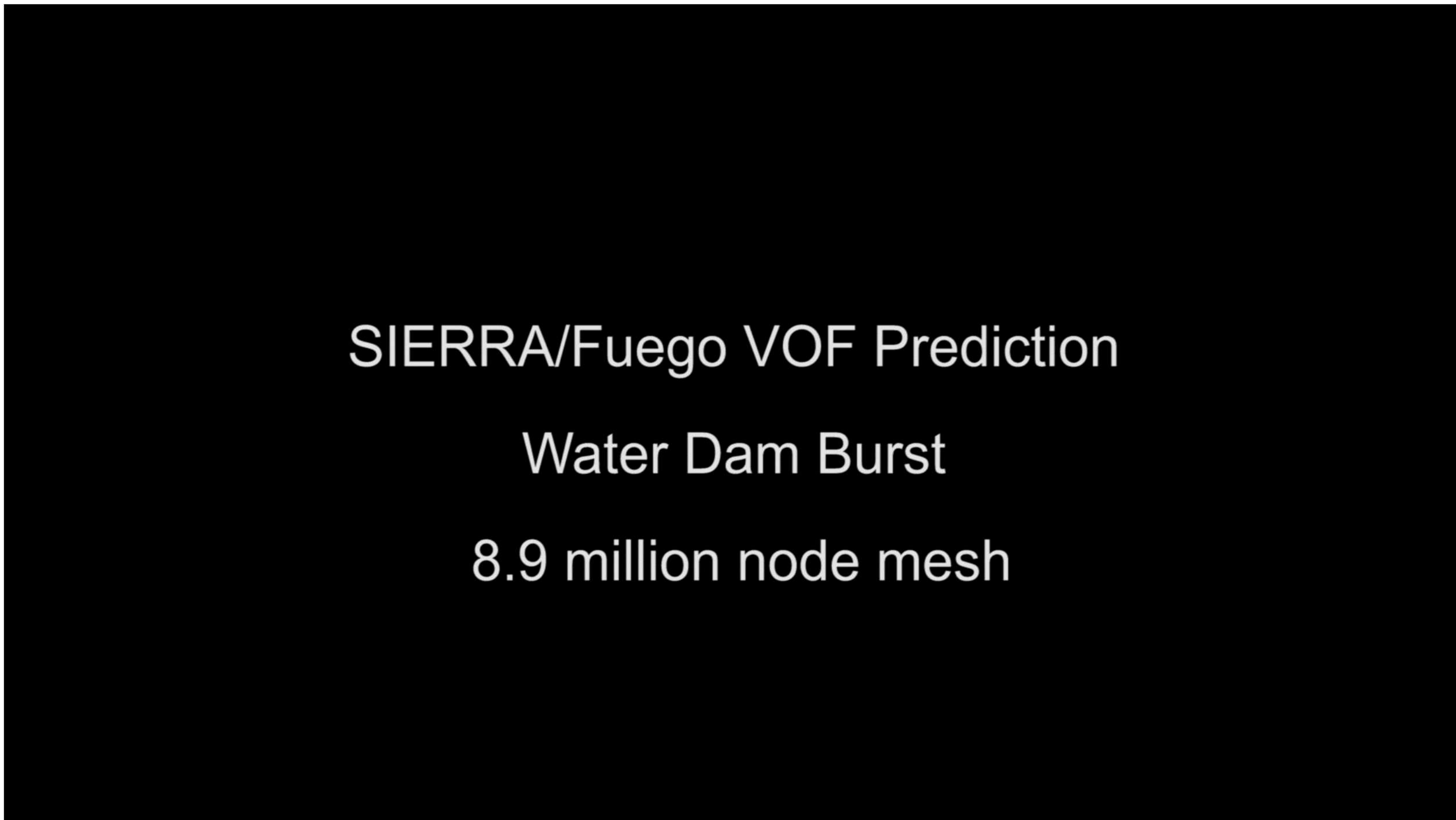
Dam burst scenario (initial configuration above)
Blocking obstacle
Three measurement points where data were extracted

#	Mesh	Nodes	Nominal Mesh Spacing	Time Step (s)
1	coarse	28,600	0.05000 m	0.00250
2	med	216,400	0.02500 m	0.00125
3	fine	716,500	0.01667 m	0.00100
4	xfine	1,682,000	0.01250 m	0.00100
5	xxfine	3,266,300	0.01000 m	0.00050
6	xxxfine	5,622,400	0.00833 m	0.00050
7	xxxxfine	8,903,500	0.00714 m	0.00050

Study consisted of mostly mesh refinement variations

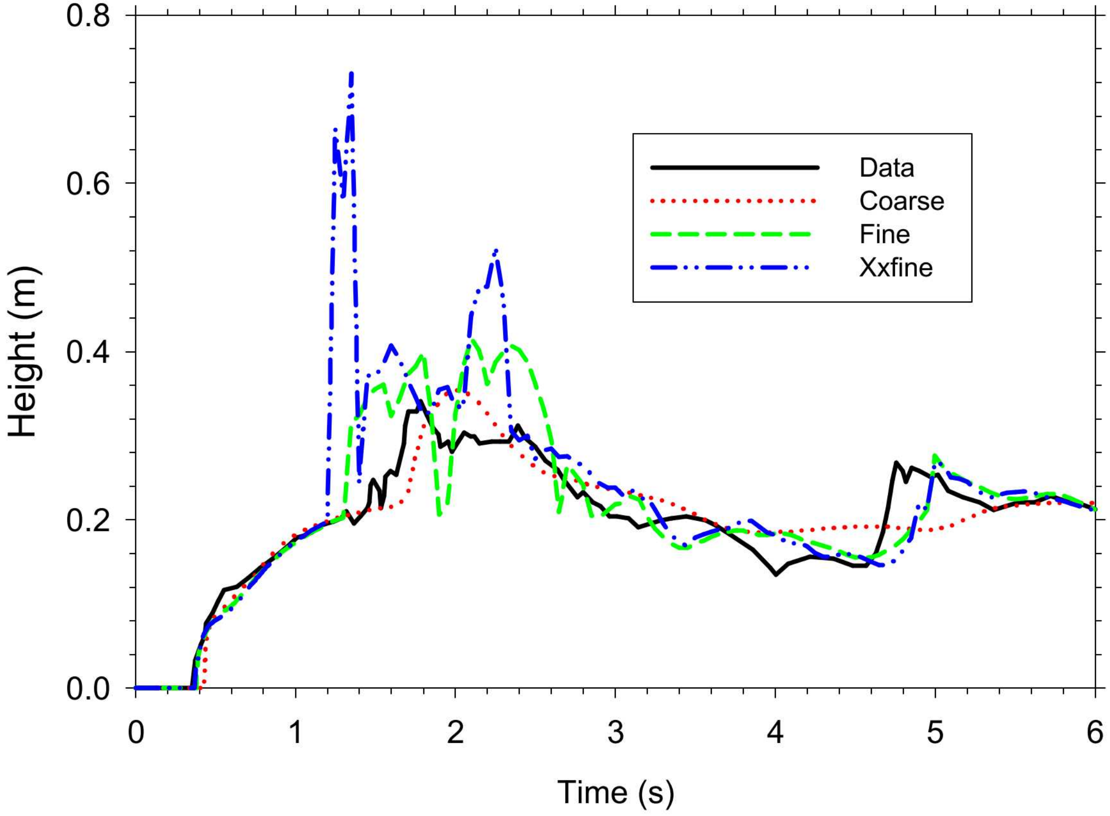
Highest Resolution Video

- The highest resolution case results in a very complex surface flow



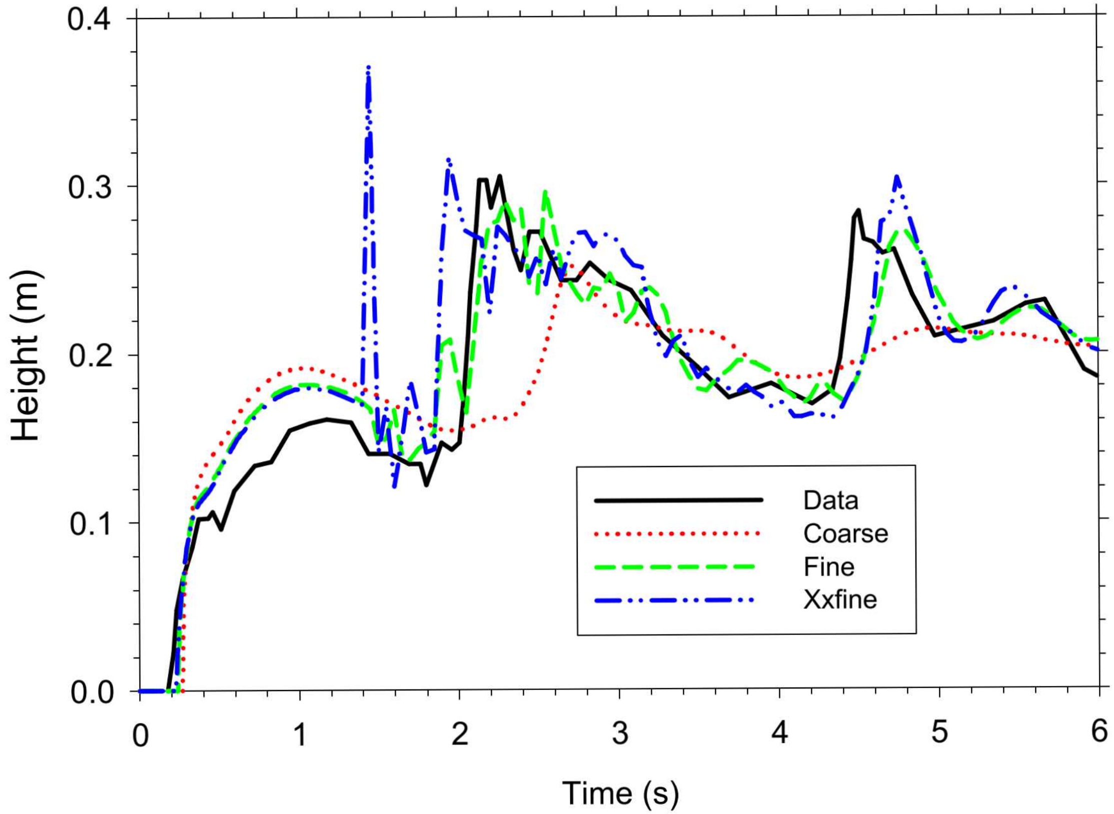
Fluid Height at H1

- Increased resolution generally matches the data peak heights better



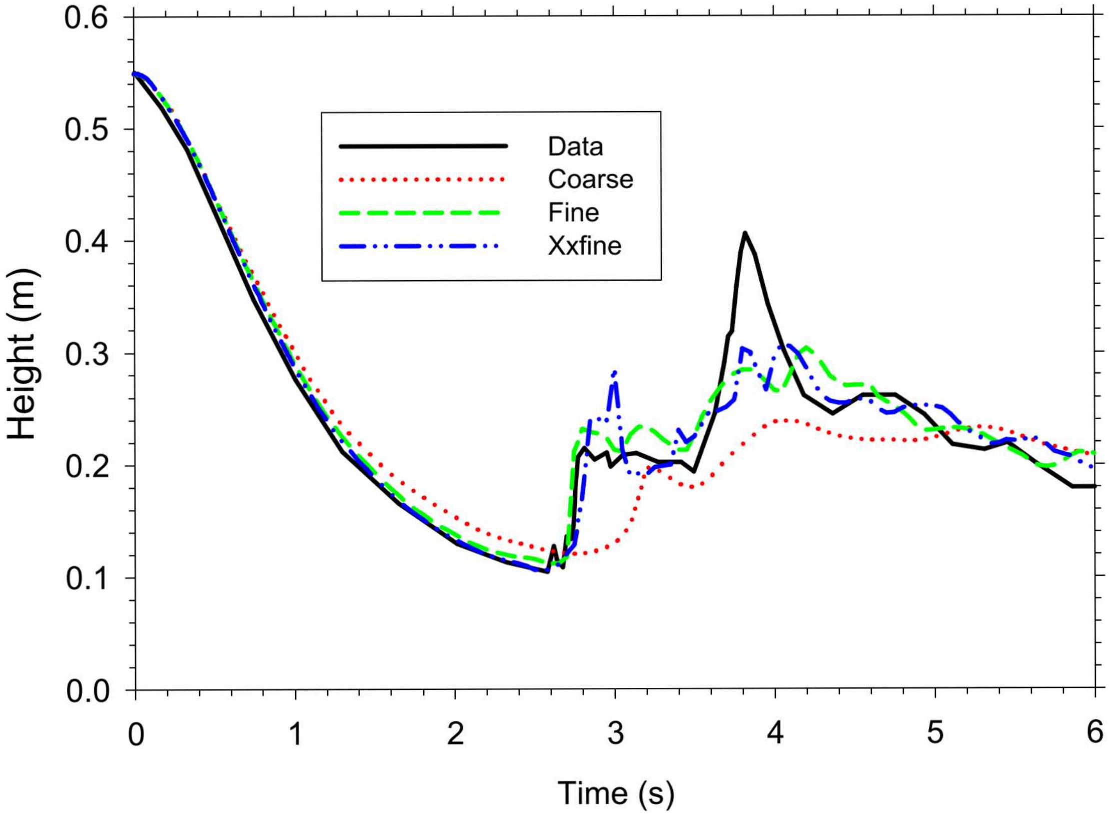
Fluid Height at H2

- Coarse calculation is appreciably worse than the fine and xxfine



Fluid Height at H3

- Very good temporal predictions for higher resolution models, moderate difference in peak magnitudes

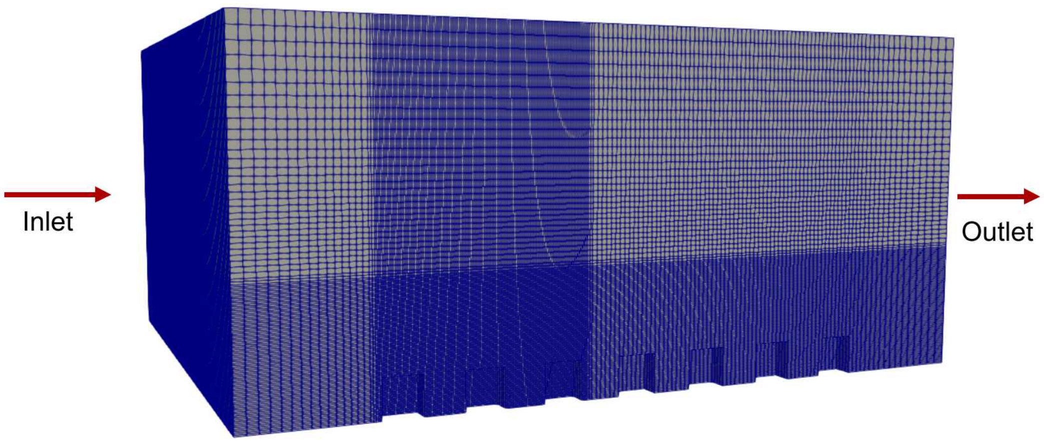


Show latest model results

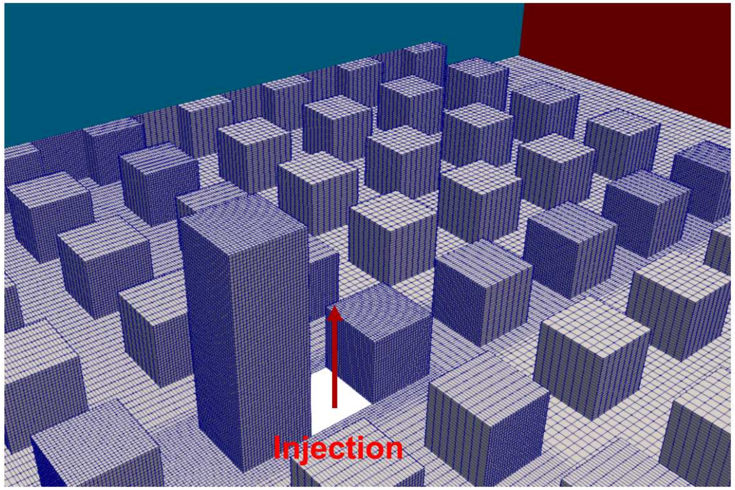
- Here we show the first multiphase burn modeling results

Numerical Configuration

- 196 x 110 x 239mm computational domain
- Localized mesh refinement utilized
  - Highest resolution (0.5mm) closest to target building
- ~ 3.55 million elements, 350 processors requiring 16 hrs runtime



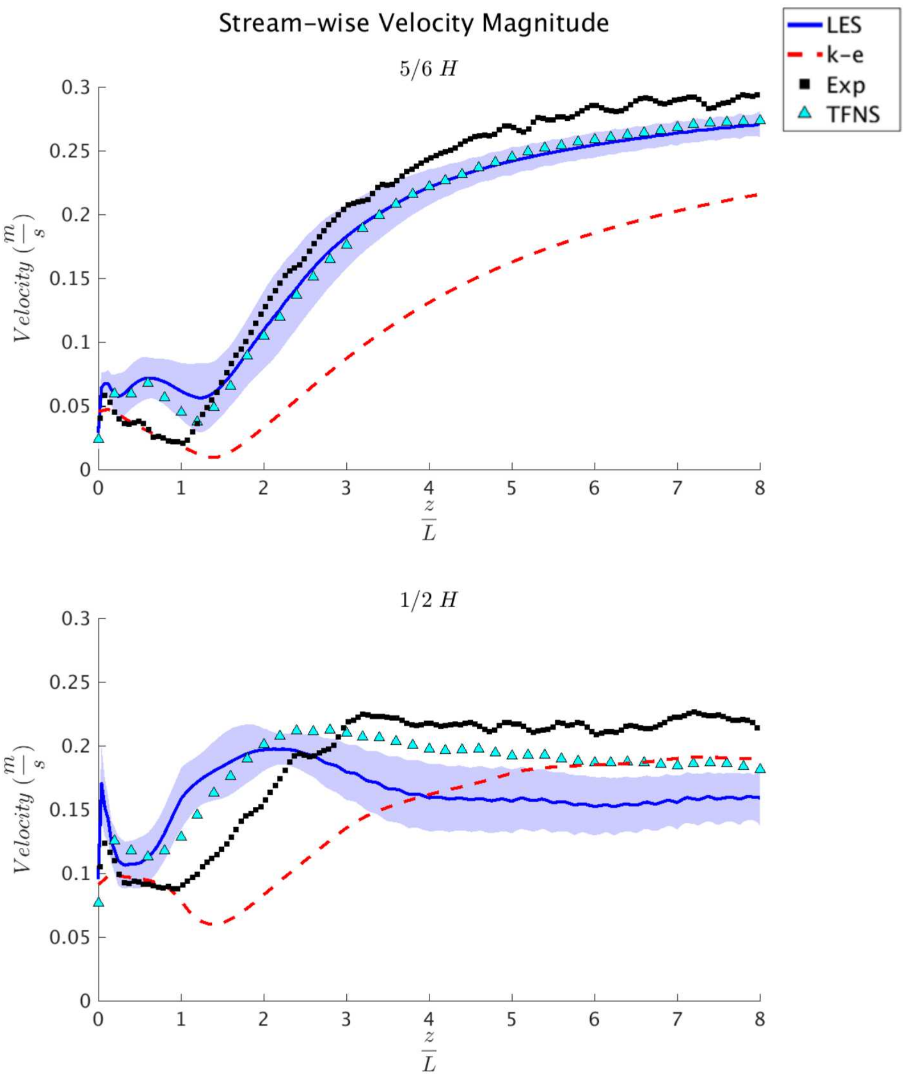
Domain

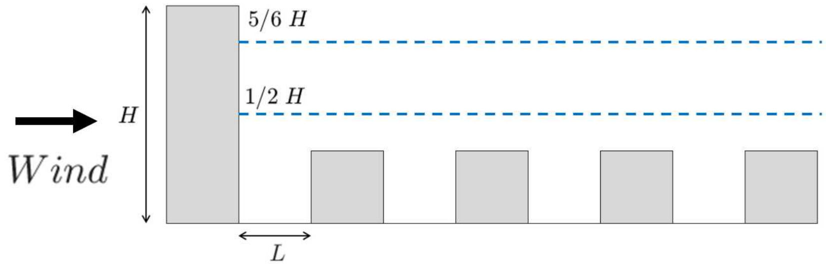


"Medium" Mesh & Boundaries

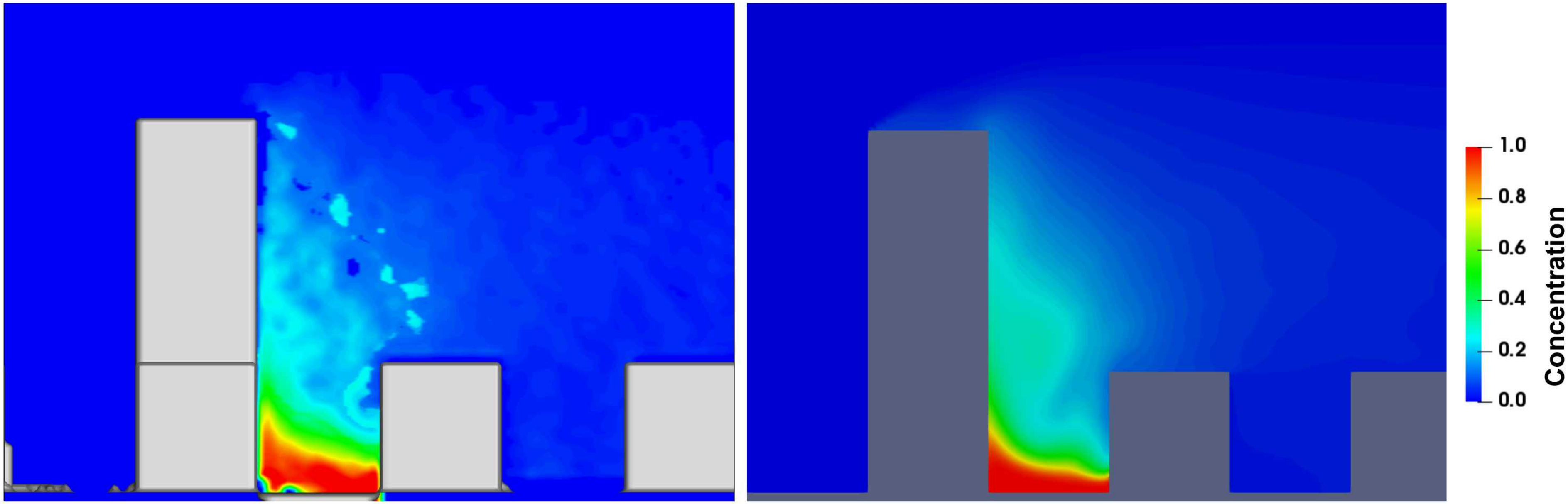
Downwind Velocity

- Velocity magnitude comparisons extended beyond target street canyon
- LES overestimates velocity near target building
  - 5/6H - Displays behavior matching experiment further upstream
  - 1/2H – larger stagnation zones near small buildings cause decrease in velocity





Center Plane Concentration



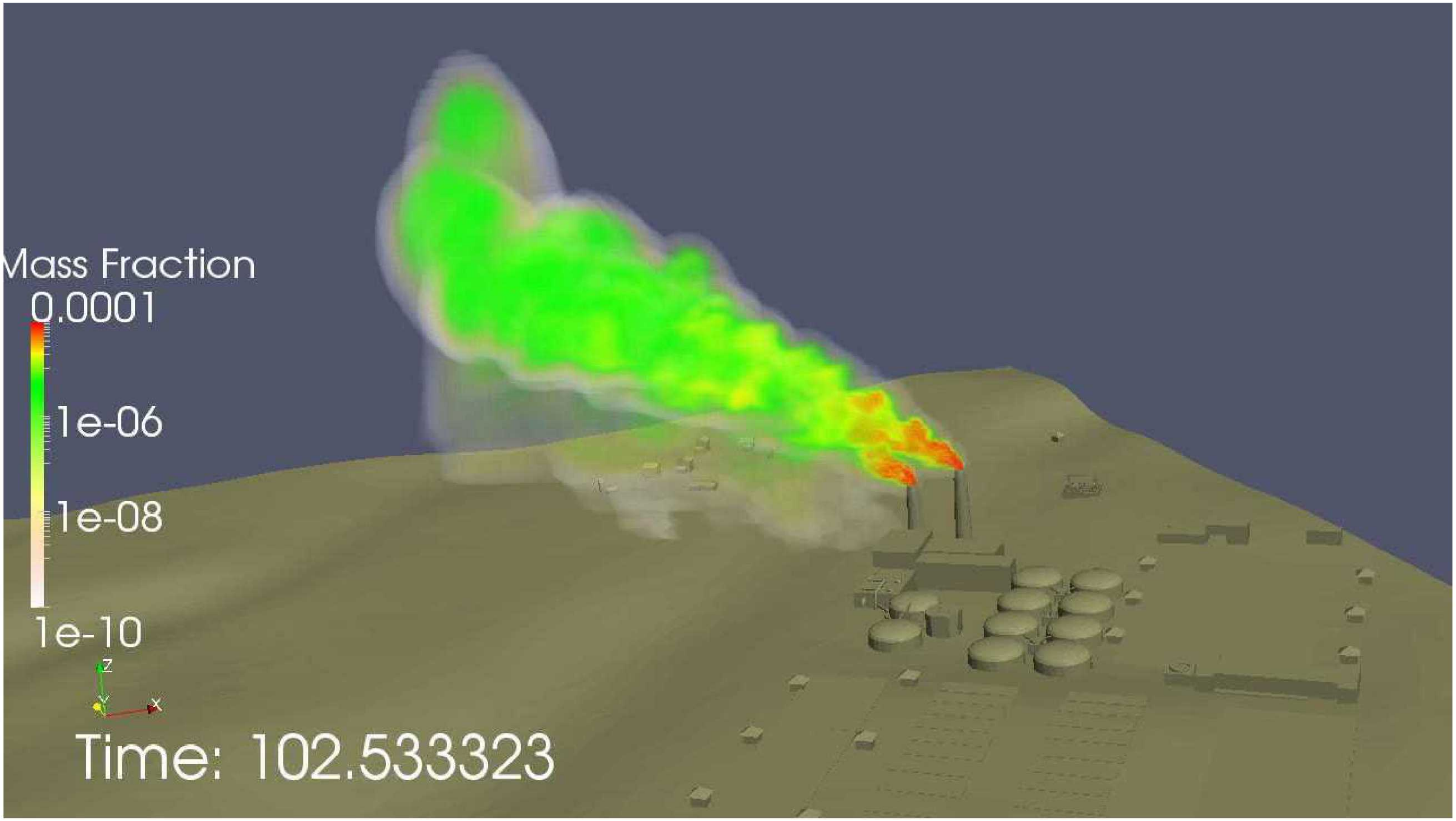
Experimental

Baseline LES

- Concentration contour plots and iso-surface comparisons exhibit good qualitative match

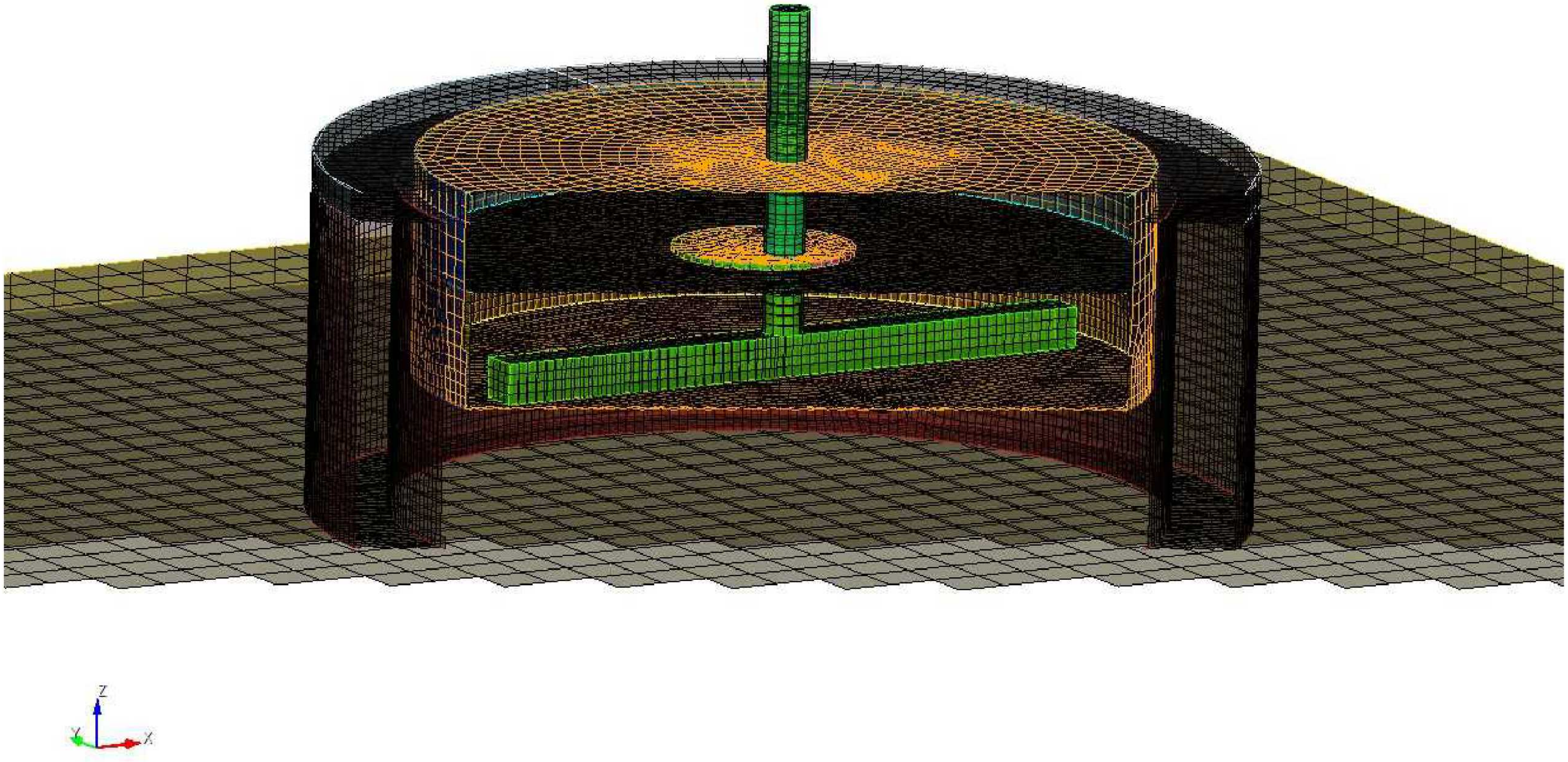
Legacy SIERRA/Fuego predictions

- Generic NH_3 facility plume in cross-wind
  - 5.4 m/s stack velocity, 2 m/s cross-wind
- Plume volume grows spatially in turbulent flow



Discretized Model of Denitrator

Created with CUBIT Software

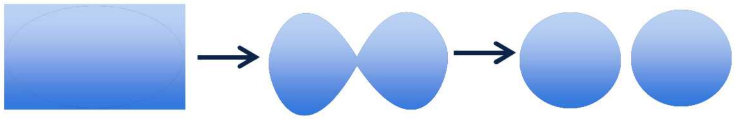


Taylor Analogy Break-up (TAB) Model

- Originally by O'Rourke and Amsden (1987)
- Approximates the drop as a damped oscillator, formulated as a second-order differential equation, with y as a deformation parameter:

$$m_d \frac{d^2 y}{dt^2} = \underbrace{m_d \frac{C_F}{C_b}\frac{\rho_g}{\rho_l}\frac{|u_d - u_g|^2}{r^2}}_{\text{Aerodynamic Forcing}} - \underbrace{m_d \frac{C_k \sigma}{\rho_l r^3} y}_{\text{Surface Energy Damping}} - \underbrace{m_d \frac{C_d \mu_l}{\rho_l r^2}\frac{dy}{dt}}_{\text{Viscous Damping}}$$

Simplified Schematic



- Discretized solution for y is:

$$y(t+\Delta t) = \frac{We}{C} + \left\{ \left(y(t) - \frac{We}{C} \right)\cos(\omega \Delta t) + \frac{1}{\omega}\left(\dot{y}(t) + \frac{y(t) - We/C}{\tau_b} \right)\sin(\omega \Delta t) \right\}\exp(-\Delta t/\tau_b)$$

$$\dot{y}(t+\Delta t) = \frac{\frac{We}{C} - y(t)}{\tau_b} + \left\{ \frac{1}{\omega}\left(\dot{y}(t) - \frac{y(t) - We/C}{\tau_b} \right)\cos(\omega \Delta t) - \left(y(t) - We/C \right)\sin(\omega \Delta t) \right\}\omega \exp(-\Delta t/\tau_b)$$

$$\omega = \sqrt{\frac{8 C_k \mu}{\rho_l d_p^3} - \frac{1}{\tau_b^2}}$$ Oscillation Frequency

$$\tau_b = \frac{1}{2}\frac{\rho_l d_p^2}{C_d \mu_l}$$ Viscous Damping Time

$$We = \frac{\rho_l d_p (u_p - u_g)^2}{\sigma}$$ Weber Number

- New drop diameters can be calculated:

$$d(t+\Delta t) = d(t) / \left[1 + \frac{C_k K}{20} + \frac{\rho_l d_p(t)^3}{8\sigma}\frac{6K-5}{120}\dot{y}(t)^2 \right]$$

- We modified the algorithm to limit break-up for new particles

Next Steps-Denitrator

- Incorporate appropriate chemical explosive energy and density for reprocessing vessels.
- Incorporate actual solution physical properties: density, viscosity, and surface tension.
- Refine vessel geometry and materials model based on vessel design and room floor plan.
- Refine liquid model: increase number of particles from 100,000 to about 500,000.
- Compare calculation results with limited observations from reported accidents.
- Perform large-scale experimental tests to validate model.