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# Multicomponent Evaporation Effects on Particulate Release in a Liquid Fuel Fire


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# Outline

- Motivation
- Experimental Scenario
- Simulation Details
- Results
- Conclusion
- Acknowledgements

# Motivation

- Update "*Department of Energy, DOE HANDBOOK: Airborne Release Fractions/Rates and Respirable Fractions for Nonreactor Nuclear Facilities, Volume 1 and 2*," DOE-HDBK-3010-94, U.S. Department of Energy, (Reaffirmed 2013).
- Contaminant Dispersal→Inhalation Concern
  - Cancer
  - Local mutation of cells
  - Toxicity
  - Birth Defects

- Liquid fuel fires containing hazardous materials pose challenges
  - Entrainment of fuel droplets w/ contaminants
  - Multi-Component Evaporation
  - Transport, surface deposition of droplets w/ contaminants

# Experimental Scenario

- Experiments: Mishima/Schwendiman (1973)
- Previous computational study (nonevaporating) - Brown et al., “Contaminant Entrainment from a Gasoline Pool Fire,” Fall 2015 Western States Section of the Combustion Institute
- Burning of beaker filled with kerosene and 30% tributyl phosphate (TBP) w/ contaminant materials
- $UO_2$ in our case
- Liquid fuel pre-heated to boiling point, ignited in 50 mL beaker

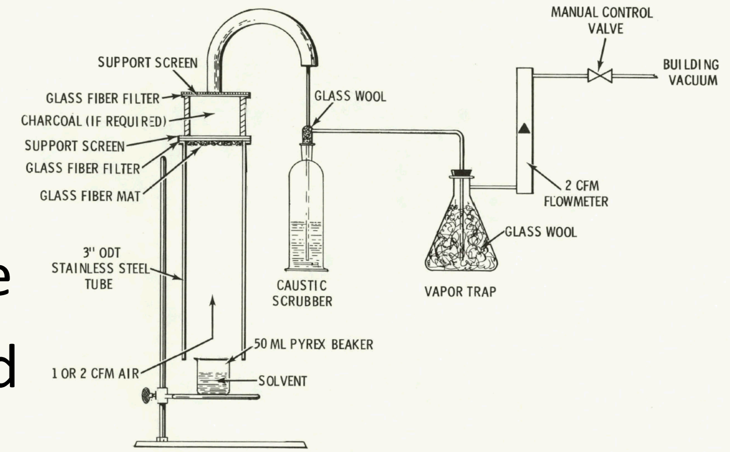
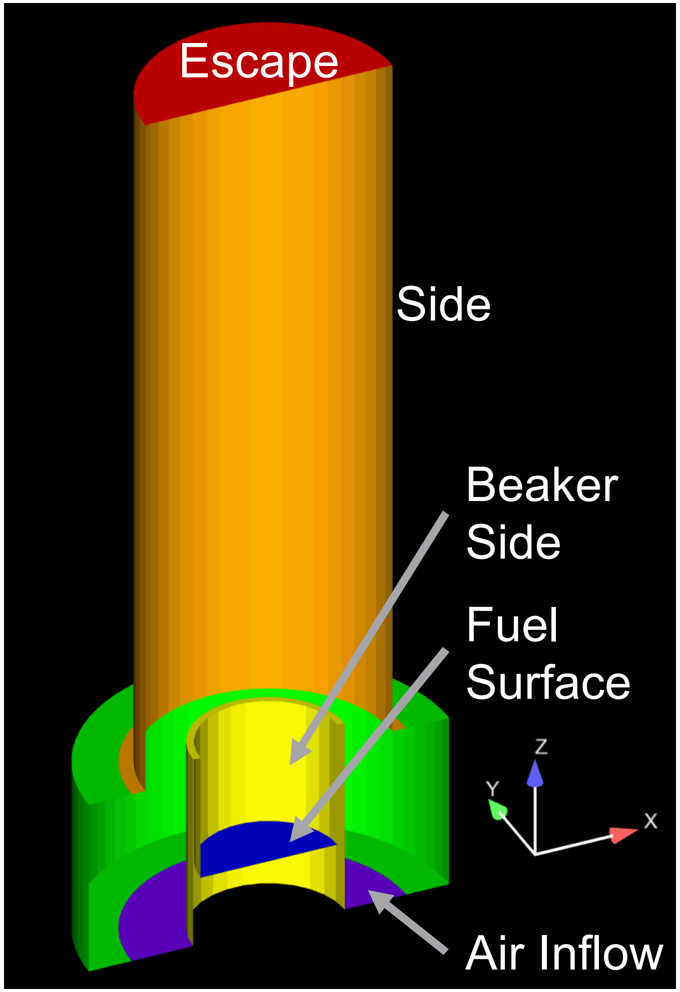


FIGURE 1b
SCHEMATIC DIAGRAM OF EXPERIMENTAL APPARATUS

# Simulation Details

- Fuego – Sierra low Mach module (CFD)
- Fluid
  - CVFEM
  - Combustion (EDC model)
  - Thermal radiation transport (Discrete Ordinates)
- Particles
  - Lagrangian w/ 2 way coupling to fluid
  - Momentum, Heat, Mass, Species
  - Multicomponent
    - Volatile: Kerosene, TBP   Inert: $UO_2$
    - Volatile components enter fluid region, subsequently burn
    - Inert component transports within particle region
- Investigate where $UO_2$ ends up
  - re-absorbed onto fuel surface
  - Deposited on side walls
  - Escaping the upper surface



# Particle Motion

- Drag and Buoyancy

$$\frac{d\mathbf{x}_p}{dt} = \mathbf{v}_{p,current}$$

$$\mathbf{f}_{Drag} = -Cf_D\mathbf{v}_{rel} \qquad C = 6\pi\mu_F r_P$$

$$\mathbf{v}_{rel} = \mathbf{v}_p - \left(\mathbf{v}_{Fluid} + \mathbf{v}_{Fluid,fluctuating}\right)$$

$$f_D = \left(1 + \frac{Re_P^{\frac{1}{3}}}{6}\right) \text{ for } Re_p < 1000 \qquad f_D = \frac{0.424}{24} Re_p \text{ for } Re_p \geq 1000$$

$$\mathbf{f}_{Buoy} = -\Delta M\mathbf{g}$$

$$\Delta M = M_p - \frac{4}{3}\pi\rho_F {r_p}^3$$

$$\frac{d\mathbf{v}_p}{dt} = \frac{\mathbf{f}_{Drag} + \mathbf{f}_{Buoy}}{M_p}$$

# Multicomponent Evaporation

- Each particle component can contribute to evaporation with mass evolved into fluid phase, particle temperature change

$$\mu = \mu_F C_\mu$$

$$C_\mu = \left(\frac{T_\infty + T_p + T_x}{3T_\infty}\right)^{0.7} : T_x = T_{Flame} \text{ (if specified)}, \quad T_x = T_p \text{ (if not)}$$

$$Re_p = \frac{2\rho_F r_p v_{rel}}{\mu_F}$$

$$Nu_p = 1.0 + 0.3 Pr_p^{\frac{1}{3}} \sqrt{Re_p}$$

$$Sh_p = 1.0 + 0.3 Sc_p^{1/3} \sqrt{Re_p}$$

$$h_{vap} = h_{vap,ref} \left(\frac{T_{crit} - T_p}{T_{crit} - T_{vap,ref}}\right)^{0.38} \text{ for } T_p < T_{crit}, \quad 0 \text{ for } T_p \geq T_{crit}$$

$$B_{FO} = \frac{Y_{Ff} - Y_{F,\infty}}{Y_{Fp} - Y_{Ff}}$$

$$B_{TO} = (1 + B_{FO})^{f_{BTO}} - 1$$

$$f_{BTO} = \frac{Pr_p Sh_p}{Sc_p Nu_p}$$

$$P_{Ff} = P_{vap,ref} \exp\left[h_{vap} \frac{MW_f}{R}\left(\frac{1}{T_{vap,ref}} - \frac{1}{T_p}\right)\right] \text{ From the Clausius-Clapeyron relationship}$$

$$X_{Ff} = \frac{P_{Ff}}{P}$$

$$MW_{NF} = MW_G \frac{1 - Y_{F,\infty}}{1 - Y_{F,\infty} \frac{MW_G}{MW_F}}$$

$$Y_{Ff} = \frac{X_{Ff} MW_f}{X_{Ff} MW_f + (1 - X_{Ff}) MW_{NF}}$$

$$\frac{dM_F}{dt} = 4\pi r_p \mu \frac{Sh_p}{Sc_p} \log(1 + B_{FO}) Y_{F,p}$$

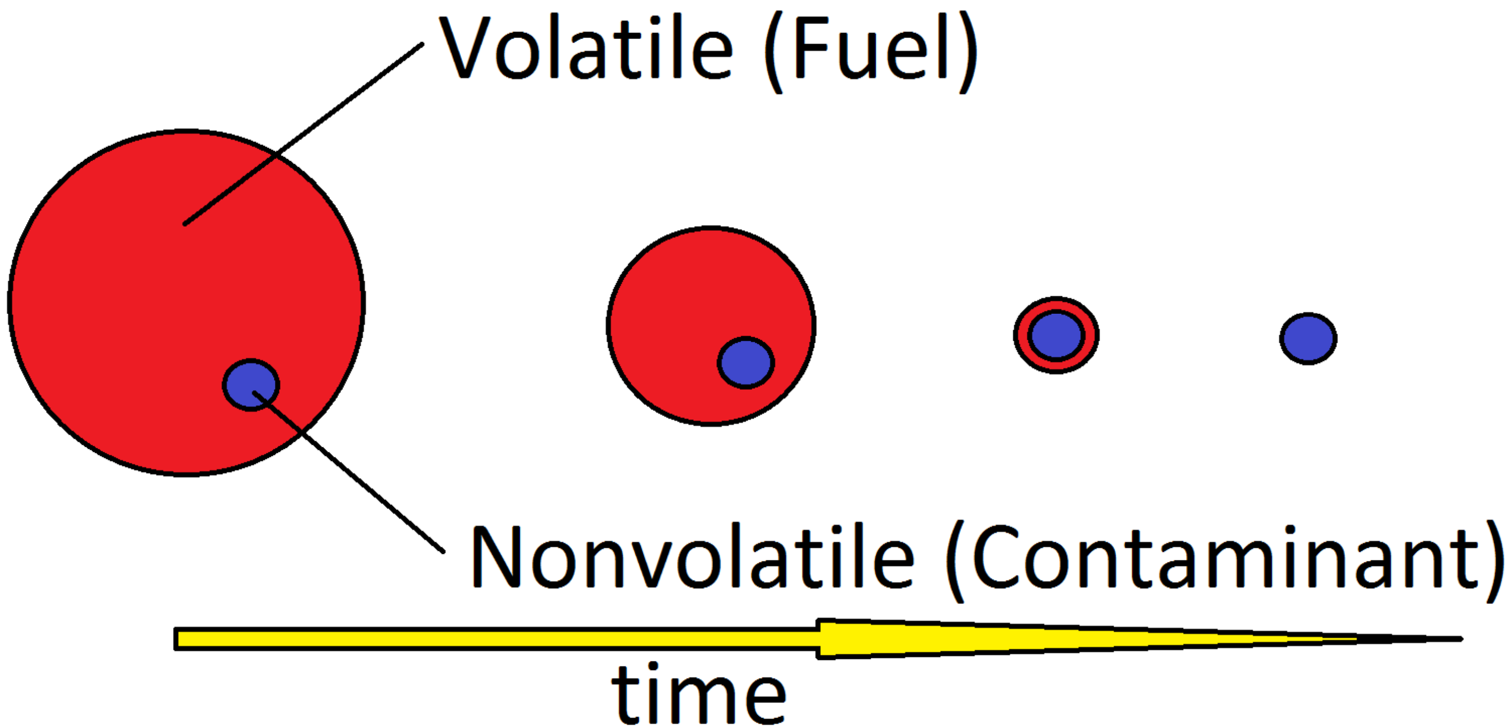
$$H_{sensible} = H_{T_\infty} - H_{T_p}$$

$$R_{mdot,BTO} = \frac{\frac{dM_F}{dt}}{B_{TO}} \text{ if } (B_{TO} > tol), = 4\pi r_p \mu \frac{Nu_p}{Pr_p} Y_{F,p} \text{ if } (B_{TO} < tol)$$

$$\frac{dT_p}{dt} = \frac{1}{M_p C_p}\left(-\frac{dM_F}{dt} h_{vap} - Q_{rad} + R_{mdot,BTO} H_{sensible}\right) Y_{F,p}$$

# Multicomponent Evaporation (cont.)

Heat Applied ⟹ Droplet Evaporation



# Simulation Parameters Varied

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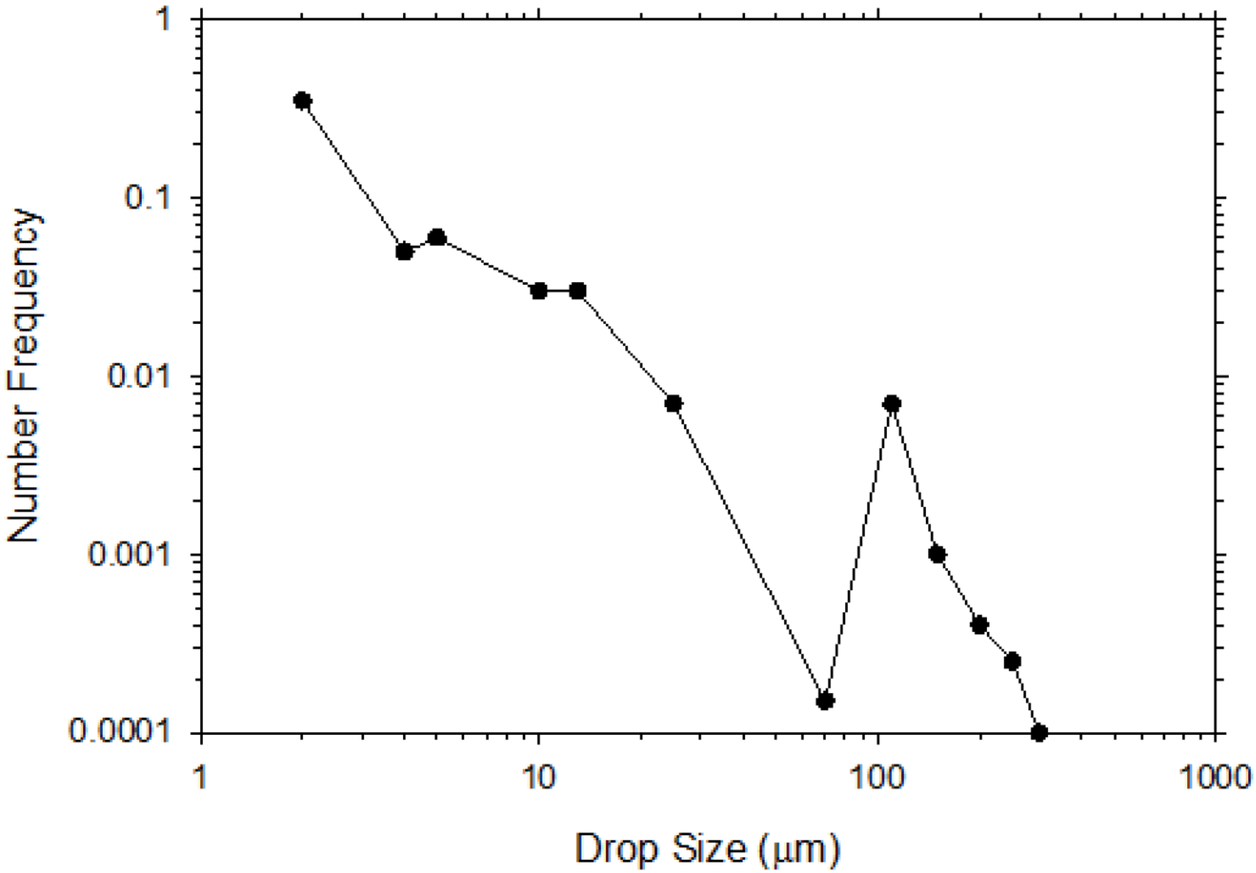
| *Simulation* | *duration (sec)* | *particle file* | *turbulent KE* | *turbulent dissipation* | *pool height(mm)* |
|---|---|---|---|---|---|
| **EARLY** | | | | | |
| Early Base 1 | 160 | short1a_1.txt | 1.1130E-06 | 1.1230E-06 | 40 |
| Early Base 2 | 160 | short1a_2.txt | 1.1130E-06 | 1.1230E-06 | 40 |
| Early Base 3 | 160 | short1a_3.txt | 1.1130E-06 | 1.1230E-06 | 40 |
| Early Base 4 | 160 | short1a_4.txt | 1.1130E-06 | 1.1230E-06 | 40 |
| Early Base 5 | 160 | short1a_5.txt | 1.1130E-06 | 1.1230E-06 | 40 |
| Early Base 6 | 160 | short1a_6.txt | 1.1130E-06 | 1.1230E-06 | 40 |
| **MID** | | | | | |
| Base 1 | 6 | start6s1.txt | 1.1130E-06 | 1.1230E-06 | 20 |
| Base 2 | 6 | start6s2.txt | 1.1130E-06 | 1.1230E-06 | 20 |
| Base 3 | 6 | start6s3.txt | 1.1130E-06 | 1.1230E-06 | 20 |
| Base 4 | 6 | start6s4.txt | 1.1130E-06 | 1.1230E-06 | 20 |
| Base 5 | 6 | start6s5.txt | 1.1130E-06 | 1.1230E-06 | 20 |
| TurbMod7A | 60 | short_input.txt | 5.9480E-05 | 1.5300E-04 | 20 |
| TurbMod7B | 60 | short_input.txt | 5.9480E-05 | 1.9200E-06 | 20 |
| TurbMod7C | 60 | short_input.txt | 5.9480E-03 | 1.5300E-01 | 20 |
| TurbMod7D | 60 | short_input.txt | 5.9480E-03 | 1.9200E-03 | 20 |
| TurbMod8A | 60 | short_input1.txt | 5.9480E-05 | 1.5300E-04 | 20 |
| TurbMod8B | 60 | short_input1.txt | 5.9480E-05 | 1.9200E-06 | 20 |
| TurbMod8C | 60 | short_input1.txt | 5.9480E-03 | 1.5300E-01 | 20 |
| TurbMod8D | 60 | short_input1.txt | 5.9480E-03 | 1.9200E-03 | 20 |
| **LATE** | | | | | |
| Late Base 1 | 200 | end_200s1.txt | 1.1130E-06 | 1.1230E-06 | 0 |
| Late Base 2 | 200 | end_200s2.txt | 1.1130E-06 | 1.1230E-06 | 0 |
| Late Base 3 | 200 | end_200s3.txt | 1.1130E-06 | 1.1230E-06 | 0 |
| Late Base 4 | 200 | end_200s4.txt | 1.1130E-06 | 1.1230E-06 | 0 |
| Late Base 5 | 200 | end_200s5.txt | 1.1130E-06 | 1.1230E-06 | 0 |
| Late Base 6 | 200 | end_200s6.txt | 1.1130E-06 | 1.1230E-06 | 0 |

**Table 1** The simulation matrix showing all parameters varied in these simulations, including duration, particle data file used, turbulence parameters at the pool surface, and pool height.

# Evaporating Particle Distribution

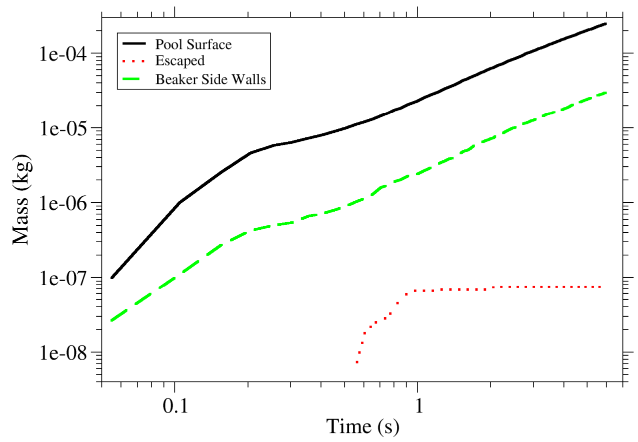
- Each particle component can contribute to evaporation with mass evolved into fluid phase, temperature change of particle

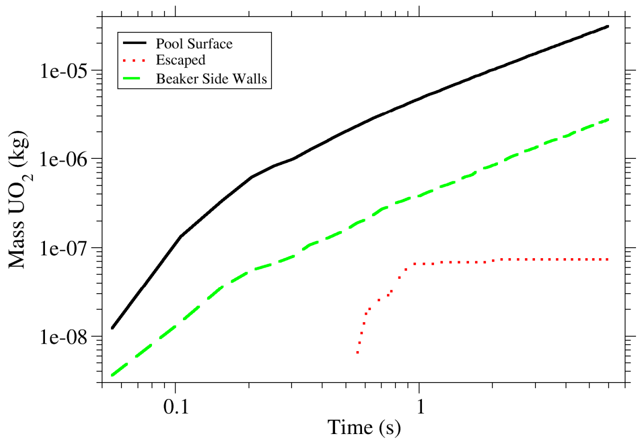


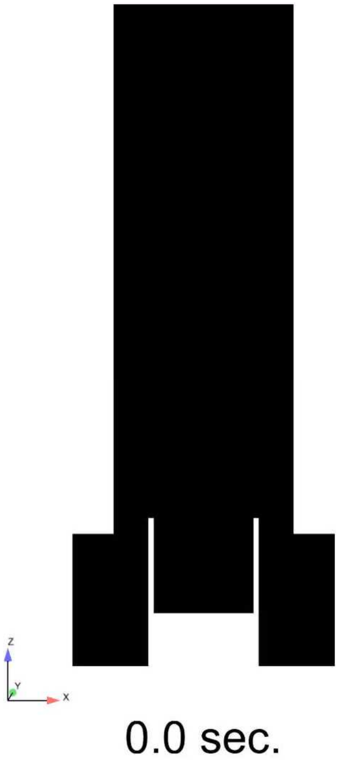
# Results

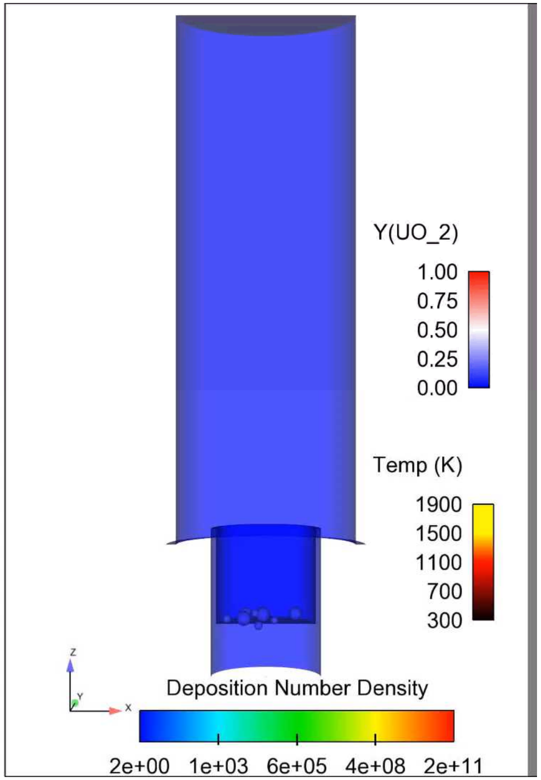
# Base 1

- 20 mm Height
- Baseline parameters



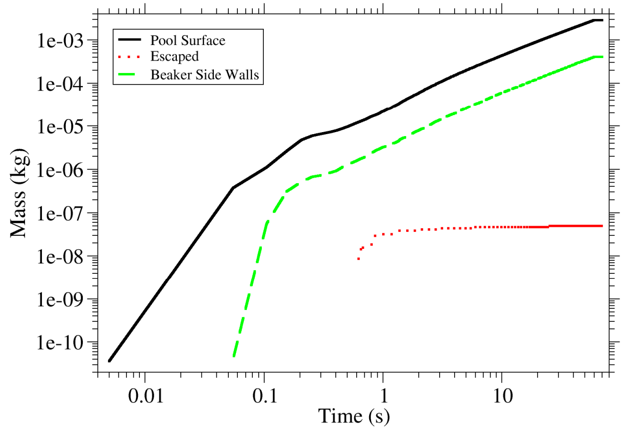



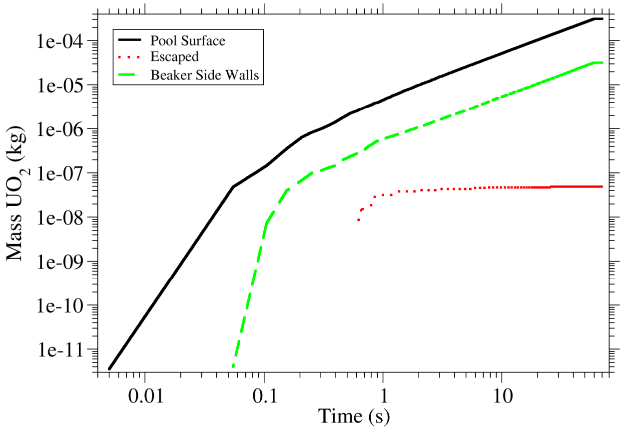



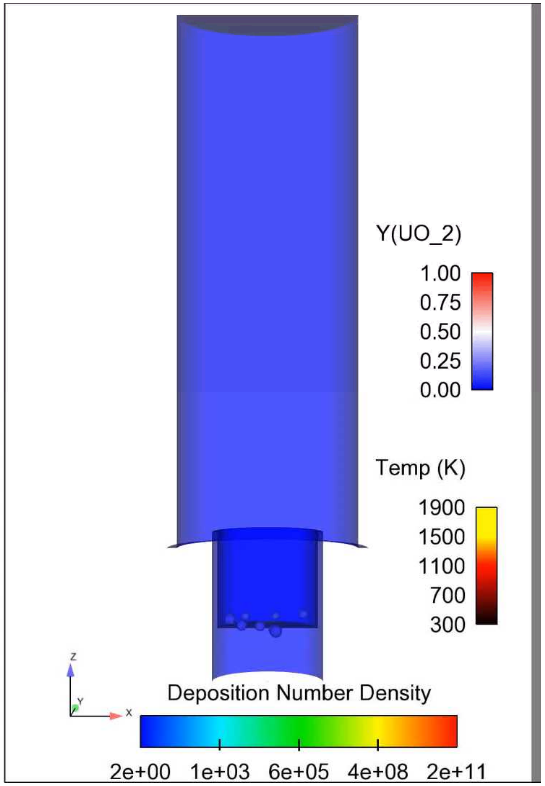
# TurbMod 7A

- 20mm Height
- Higher Turbulent KE, dissipation



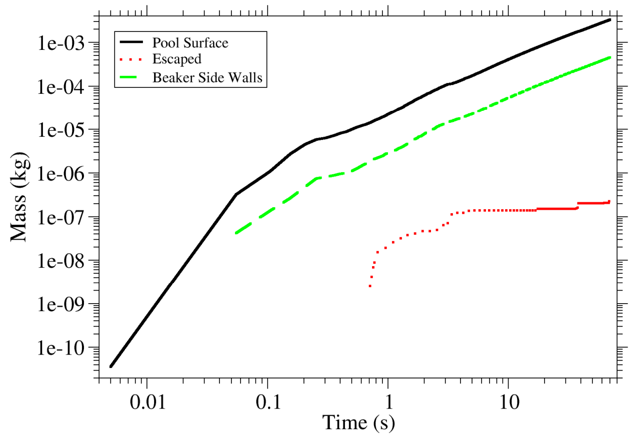



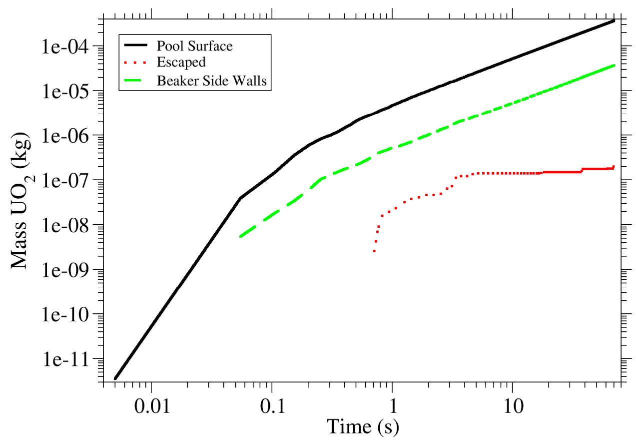


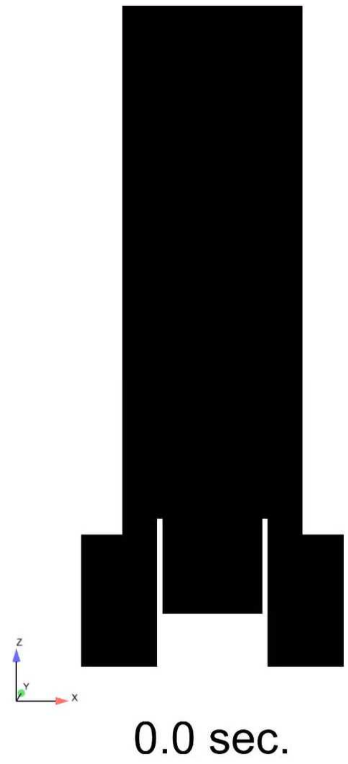


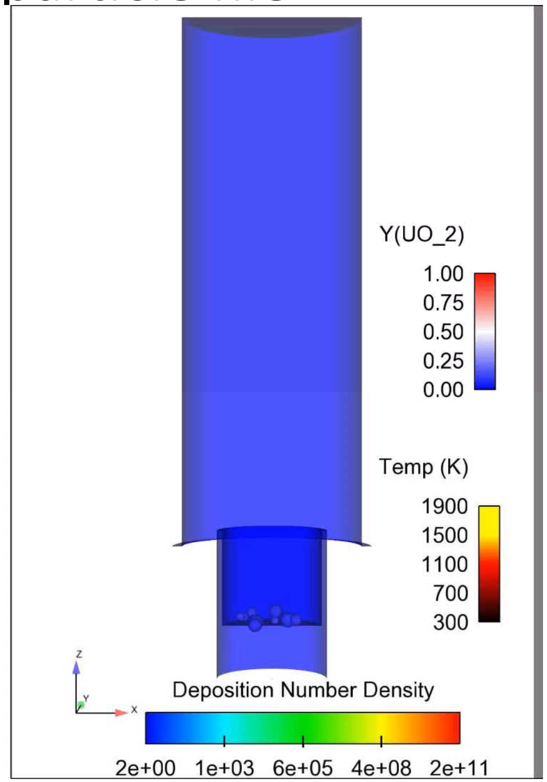
# TurbMod 8A

- 20mm Height
- Same as TurbMod 7A but different particle file



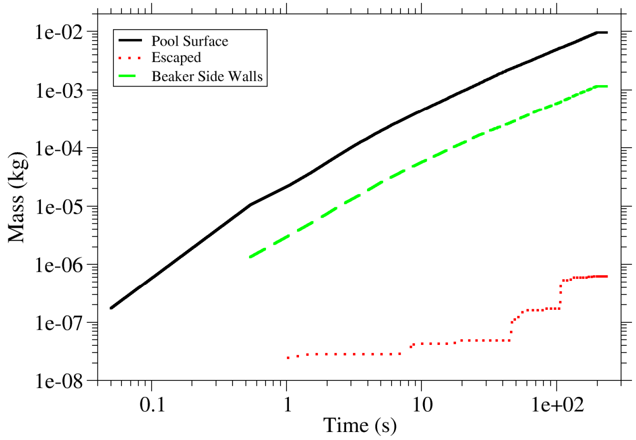



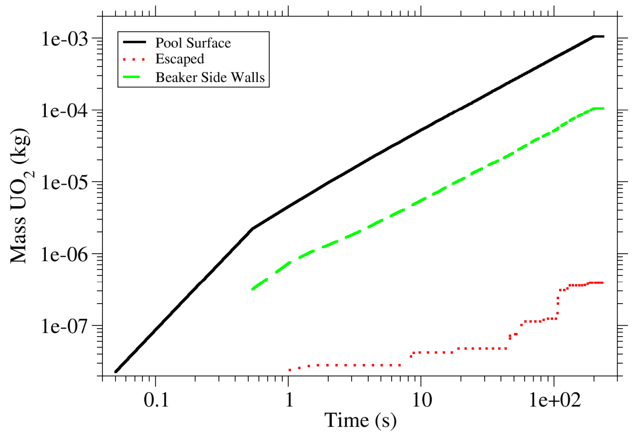



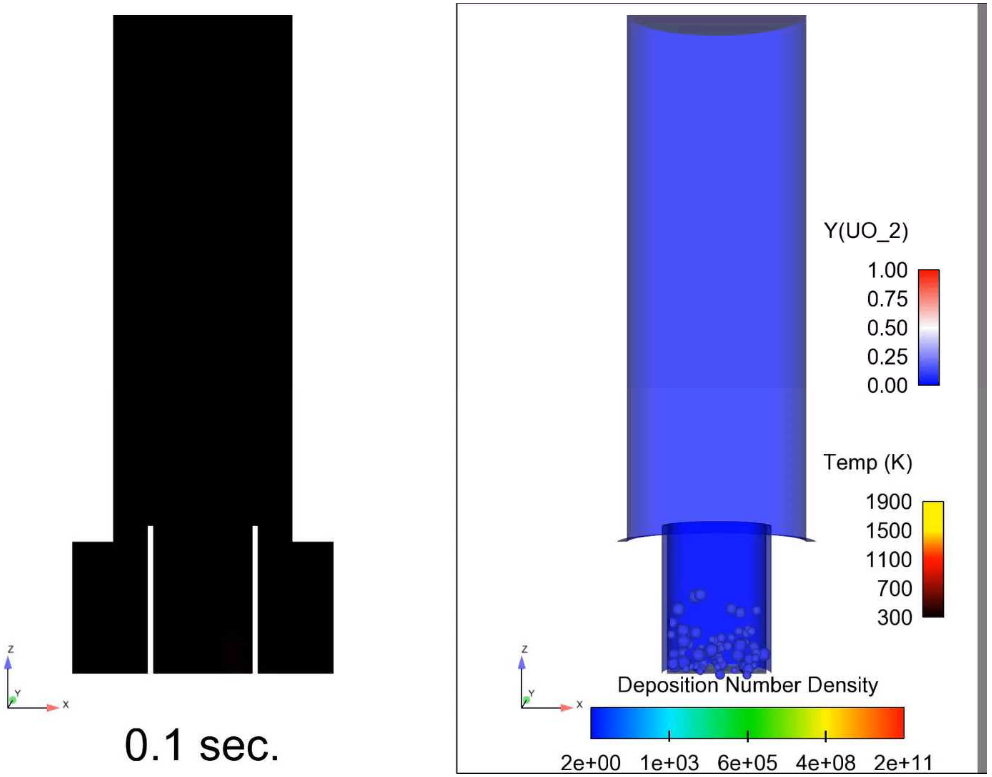



# Late Base 1

- 0mm Height

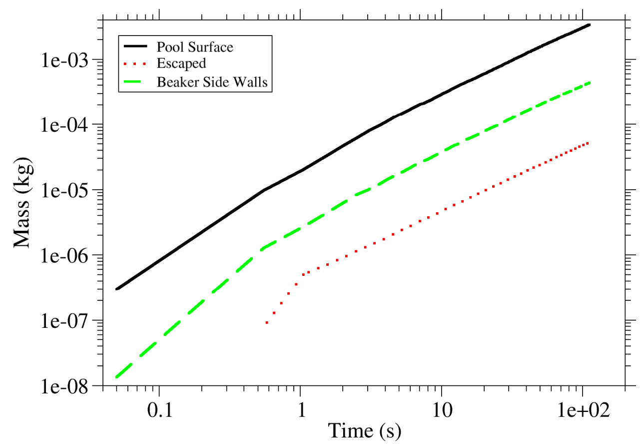


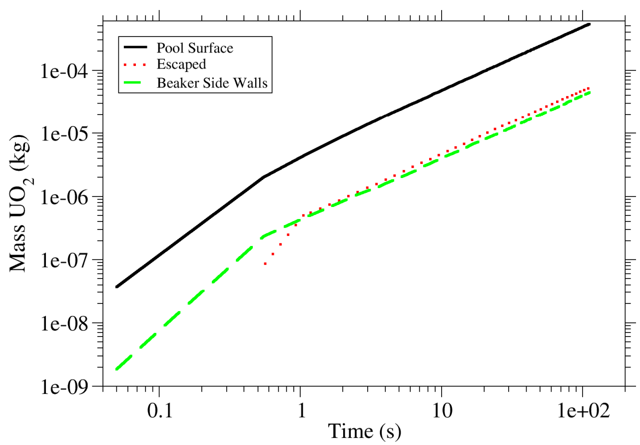



# Early Base 1

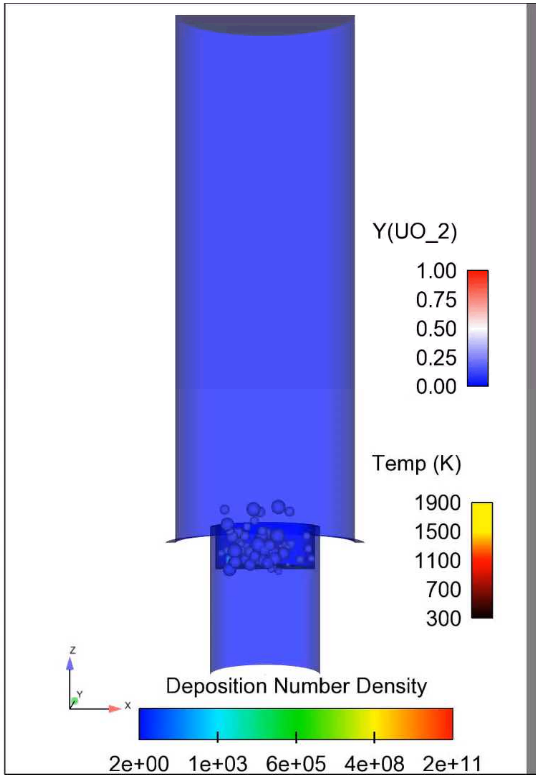
- 40mm Height
- Steady particle flux escaping at late times



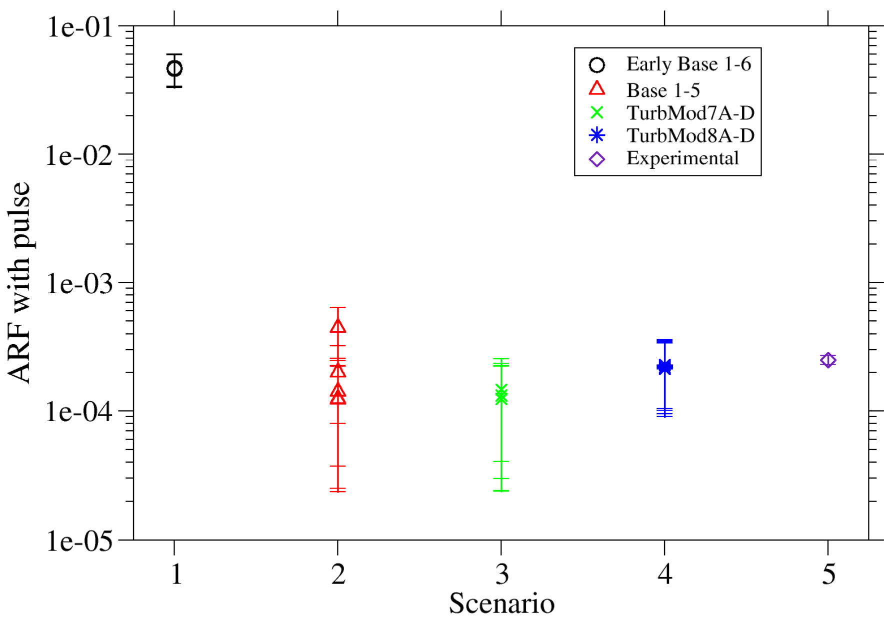


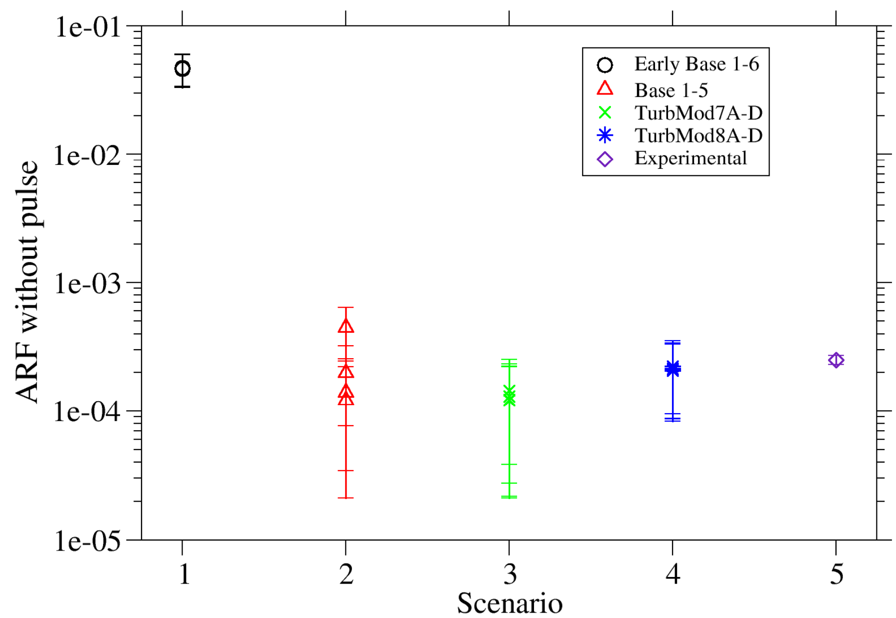
0.1 sec.



# Airborne Release Fraction (ARF)

- Ignition causes some release of particles from upper surface but over the course of the simulation, is not a significant contributor



# Conclusions

- ARF results are in good agreement with experimental results
- Statistical differences in particle introduction are important
- Past initial transient, particle deposition rate on fuel surface and side surfaces is nearly constant
- Ignition event at beginning results in transport of contaminated particles to upper surface
- Flare ups can occur (especially in late scenarios) and may result in significant particles transported to escape surface – not observed in original experiment

# Acknowledgements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