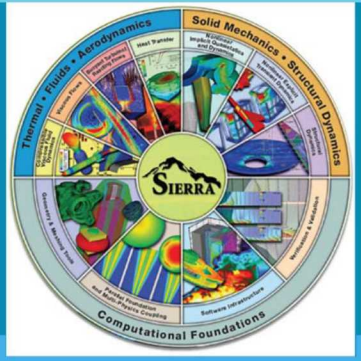
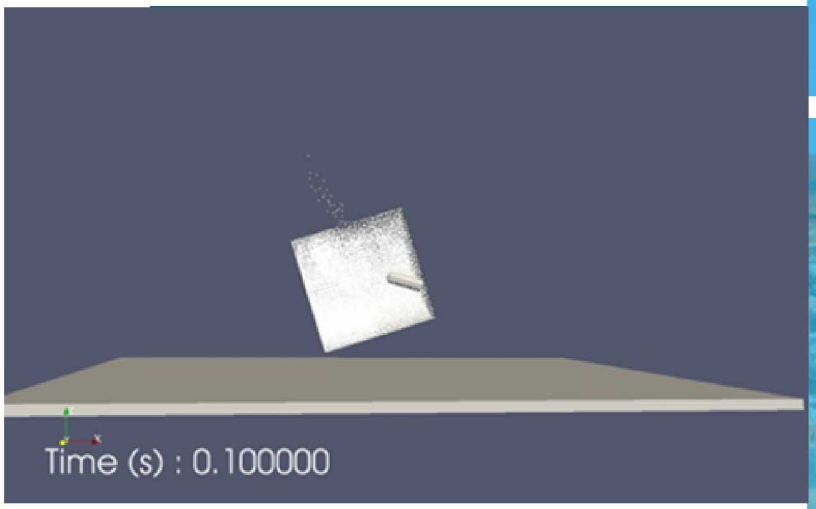
SAND2019-4879C

Sandia National Laboratories

Computational Capability to Study Airborne Release of Solids and Container Breach Due to Mechanical Insults

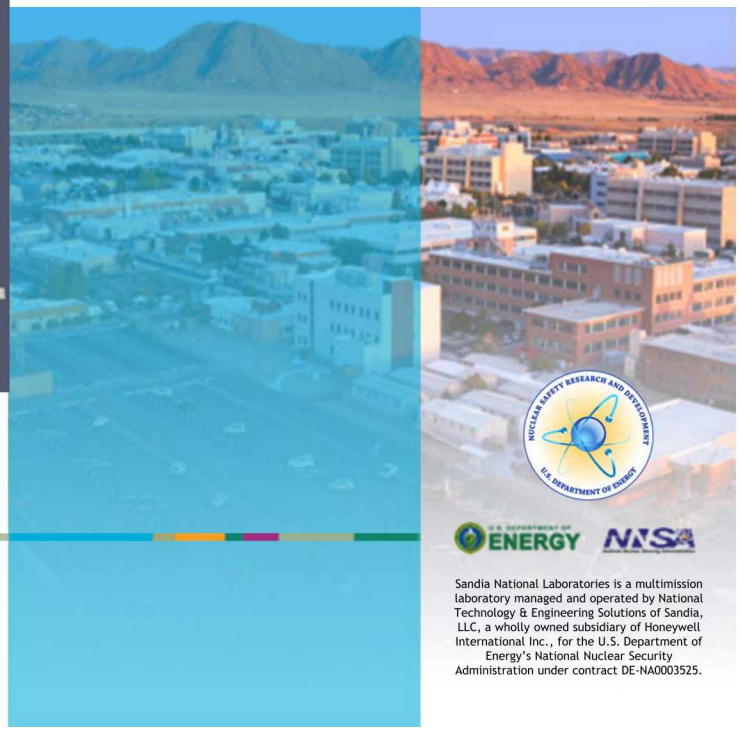




PRESENTED BY

David L.Y. Louie, Ph.D. (dllouie@sandia.gov)

ICONE27-1438, May 19-24, 2019, Ibaraki, Japan



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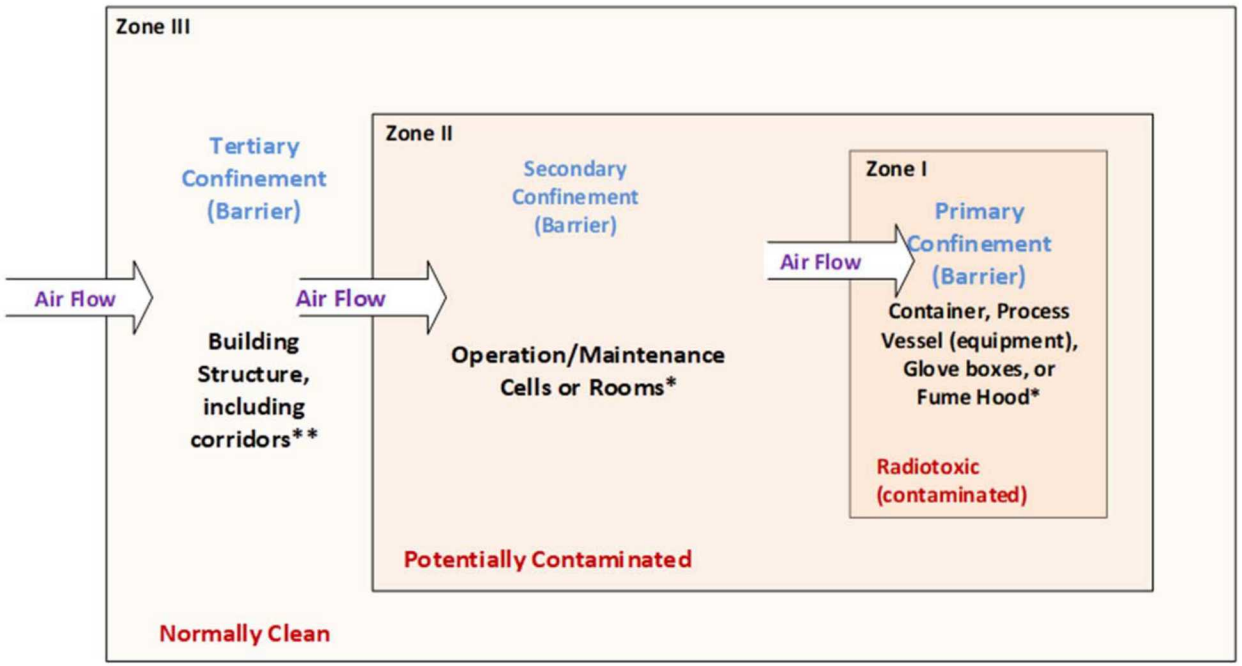
Outline

- What is Five Factor Formula?
- What is SIERRA Engineered Tool developed at Sandia National Laboratories (SNL)?
- Damage ratio simulations on breaching of waste containers used in U.S.
- Airborne release simulations on fragmentation of brittle/ceramic solids
- Conclusions

Five-Factor Formula

$$ST = MAR \cdot DR \cdot ARF \cdot RF \cdot LPF$$

ST – source term, MAR - material at risk, DR – damage ratio, ARF – airborne release fraction, RF – respirable fraction and LPF – leak path factor



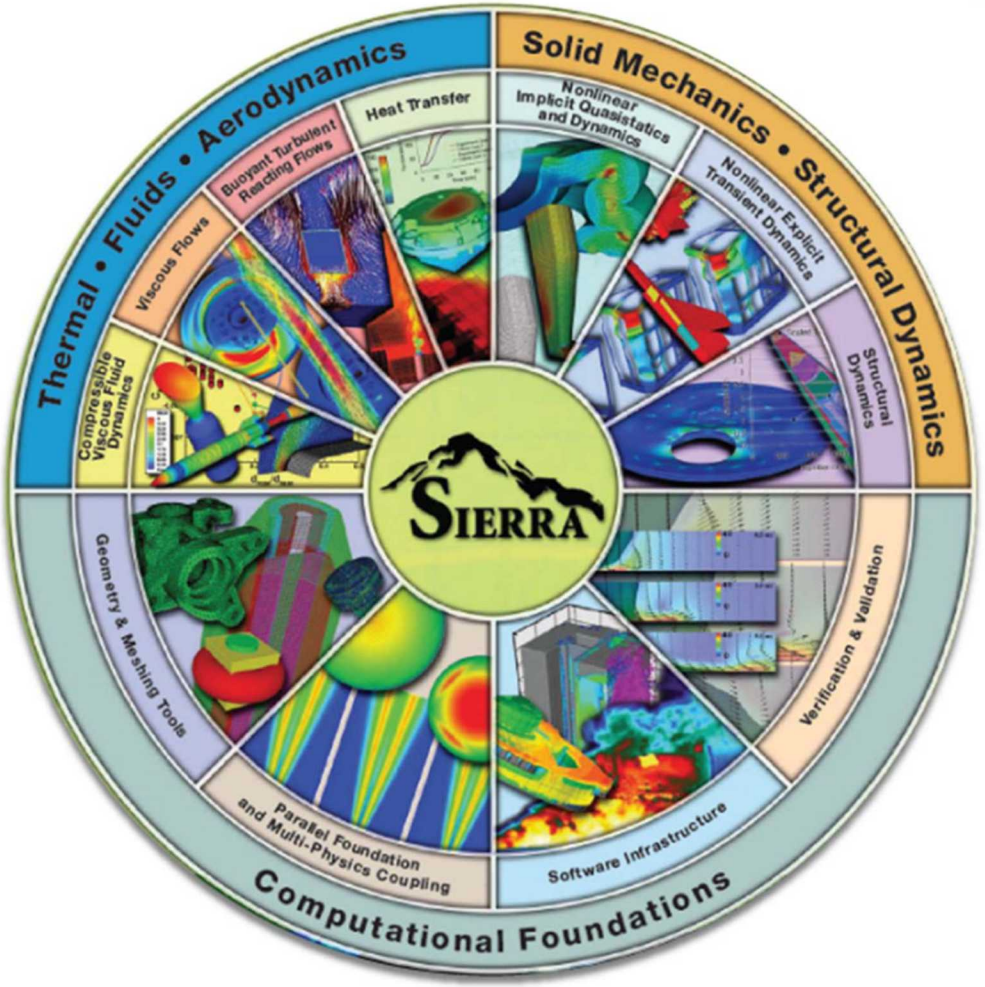
Sandia's SIERRA High Fidelity Code Suites

SIERRA Framework

- Cubit – Mesh generator
- Paraview, EnSight – Post processing

Solid Mechanics

- Adagio –Quasi-static (implicit)
- Presto – Transient (explicit), can handle explosions (ITAR)
- Both codes have smoothed particle hydrodynamics (SPH) to model particles



Damage Ratio (DR) Study on Container Breach

Develop a test matrix for the DR study

- Utilize the waste stream data from Los Alamos National Laboratory
  - Identify the waste form, container types and quantities
- Containers chosen: 7A (55-gal) drum, and standard waste box (SWB)

Develop 7A drum DR for free fall and puncture cases

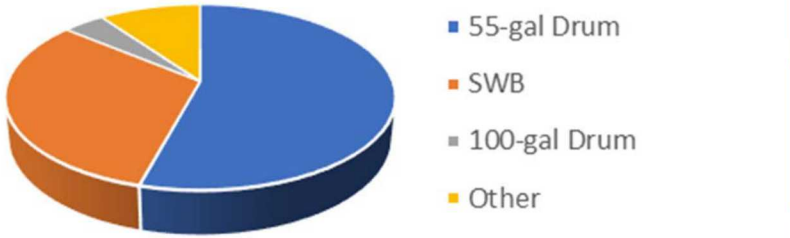
- Using existing 7A drum model from previous work
- Run simulations according to the test matrix

Develop a second container model to be simulated the same cases as in 7A.

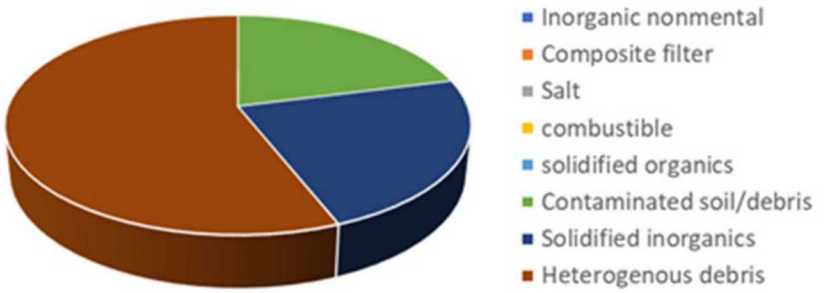
- Develop a SWB model
- Run simulations according to the test matrix

Document the models and correlation, including the development of DRxARFxRF relationship examples

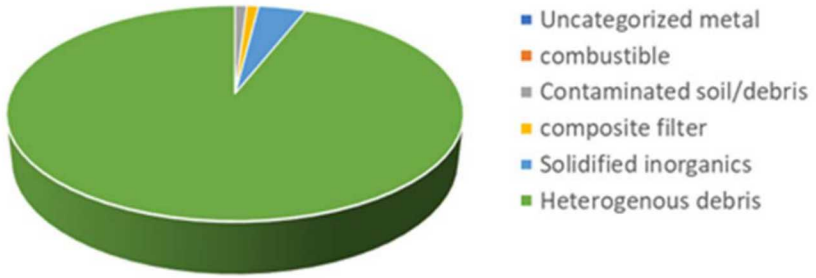
- Develop a SWB model
- Run simulations according to the test matrix



Fraction of Waste Volume Container Type



Fraction of 7A Content Types



Fraction of SWB Content Types

Free-Fall Impact –Analysis Combinations

55-GAL DRUM

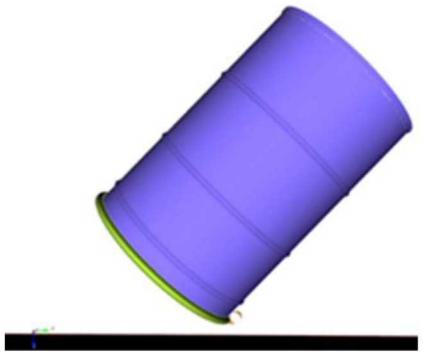
CONTENT TYPE (3)
- HETEROGENOUS DEBRIS WASTE
- SOLIDIFIED INORGANICS
- CONTAMINATED SOIL/DEBRIS WASTE

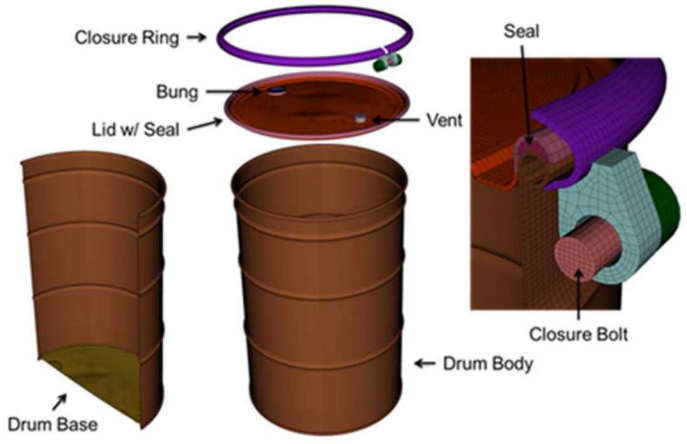
DROP HEIGHT (4)
- 2.5, 5.0, 10.0, 20.0 M

CONTENT MASS/WEIGHT (1)
- MAX OR LIMIT

ORIENTATION (5)
- PITCH RANGE: 0 TO 180 DEGREES
- INCREMENT: 45.0 DEGREES

TOTAL # OF ANALYSES:
- 3 X 4 X 1 X 5 = 60





SWB

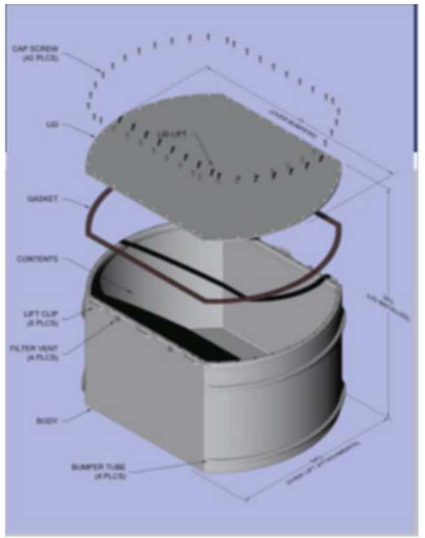
CONTENT TYPE (1)
- HETEROGENOUS DEBRIS WASTE

DROP HEIGHT (4)
- 2.5, 5.0, 10.0, 20.0 M

CONTENT MASS/WEIGHT (1)
- MAX OR LIMIT

ORIENTATION (5 X 1 = 5)
- PITCH RANGE: 0 TO 180 DEGREES
- PITCH INCREMENT: 45.0 DEGREES
- ROLL RANGE: 0

TOTAL # OF ANALYSES:
- 1 X 5 X 1 X 4 = 20



Puncture –Analysis Combinations

55-gal Drum

Content Type (3)
- Heterogenous Debris Waste
- Solidified Inorganics
- Contaminated Soil/Debris Waste

Content Mass/Weight (1)
- Max or Limit

Impactor Mass/Weight (1)
- Fork Lift

Constraint (2)
- Free to Move
- Constrained From Motion (Backed)

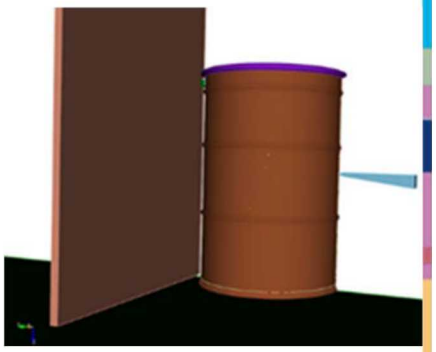
Impact Location (3)
- Lid-Center, Side-Lid, Side-Middle

Impactor Shape (1)
- Fork Lift Tine

Impactor Speed (3)
- 0.5, 2.5, 5.0 m/s

Total # of Analyses
- 3 x 1 x 1 x 2 x 3 x 1 x 3 = 54

SWB



Content Type (1)
- Heterogenous Debris Waste

Content Mass/Weight (1)
- Max or Limit

Impactor Mass/Weight (1)
- Fork Lift

Constraint (2)
- Free to Move
- Constrained From Motion (Backed)

Impact Location (3)
- Lid-Center, Side-Lid, Side-Middle

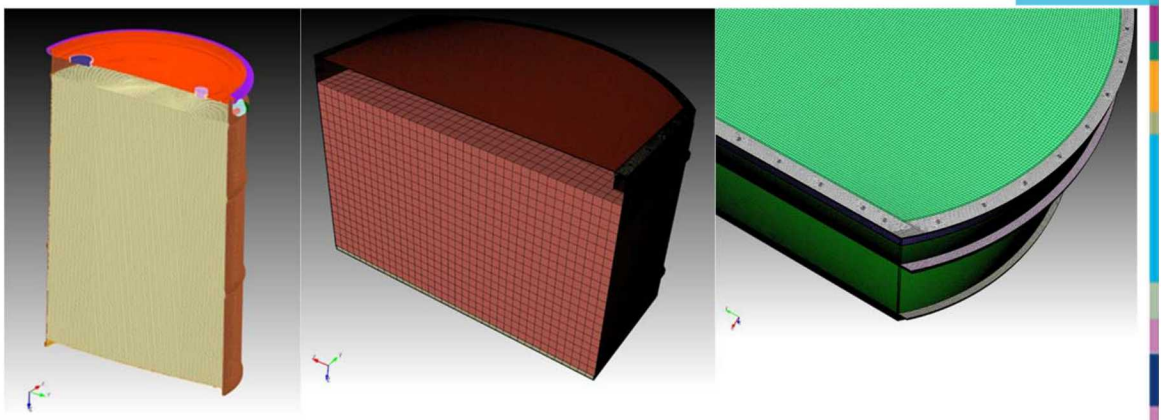
Impactor Shape (1)
- Fork Lift Tine

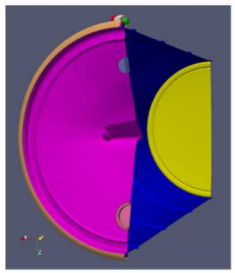
Impactor Speed (3)
- 0.5, 2.5, 5.0 m/s

Total # of Analyses
- 1 x 1 x 1 x 2 x 3 x 1 x 3 = 18

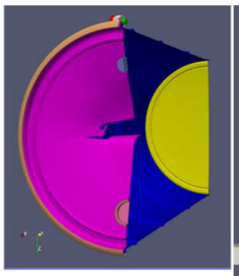
Model Development, Validation and Result Determination

- Employ half-symmetry models for all simulations
  - Punctured by tine of Forklift
  - Free-fall drop angle
- Validation of 7A model only
  - Simulated a 1 m drop
  - Resulted similar findings in experiments
- Simulations and results:
  - Extensive running time required
  - Breach area determines graphically
  - DR values extrapolated and extended from DOE-STD-5506 [DOE 2007]

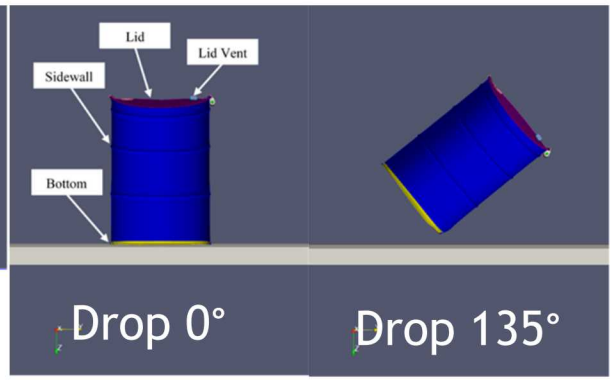




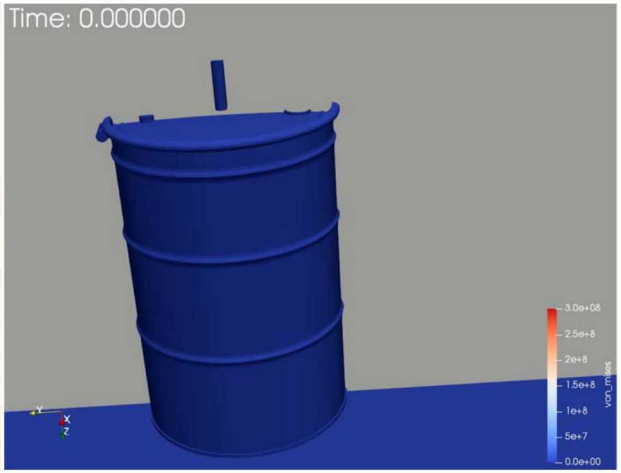
Before filtering

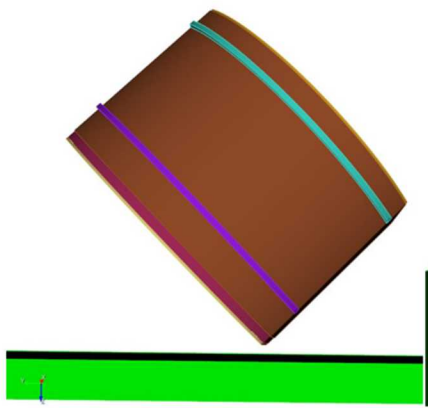


After filtering

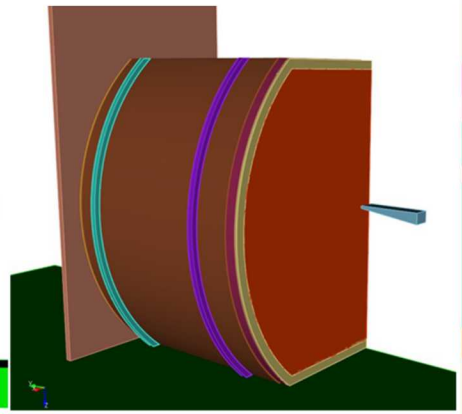


Skolnik 2009





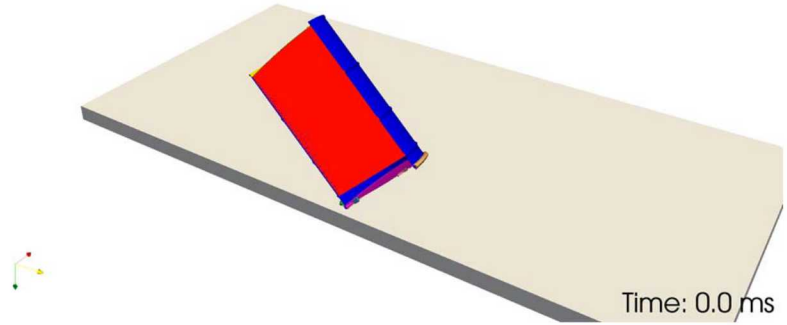
Drop 135°



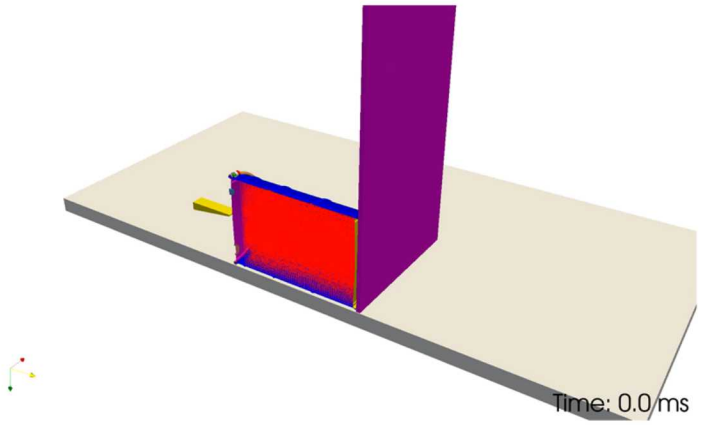
Forklift tine at center surface

7A Simulations

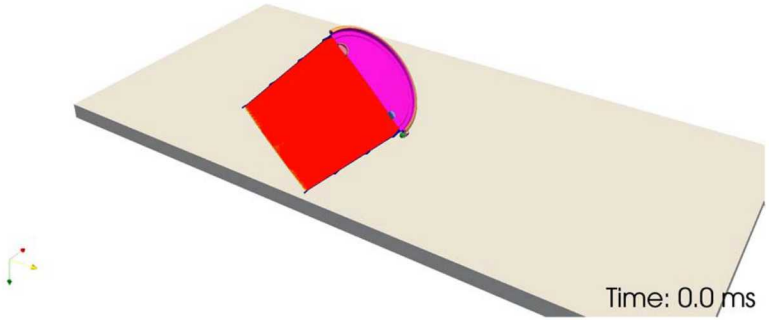
135 deg 20 m drop CS



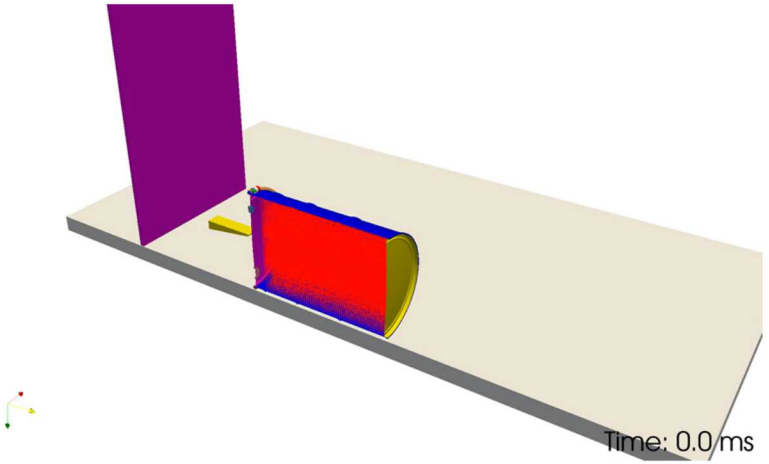
Fixed 5 m/s side lid



45 deg 20 m drop CS



Free 5 m/w side lid



Estimate of Damage Ratio from Drum Puncture Simulations

Content Type	Constraint, Impact Location, Impactor Speed*	Total Breach Area (10^{-3} m^2)	Damage Ratio	Mode of Failure	
				Puncture	Lid, Sidewall Separation
HD	C(Fi), IL(LC), IS (2.5)	5.28	0.1	✓	
HD	C(Fi), IL(LC), IS (5)	11.54	0.2	✓	
HD	C(Fi), IL(SL), IS (2.5)	3.71	0.01+		✓
HD	C(Fi), IL(SL), IS (5)	28.54	0.02+	✓	✓
HD	C(Fi), IL(BC), IS (2.5)	3.37	0.1	✓	
HD	C(Fi), IL(BC), IS (5)	8.14	0.2	✓	
SI	C(Fi), IL(LC), IS (2.5)	16.25	0.1	✓	
SI	C(Fi), IL(LC), IS (5)	13.74	0.2	✓	
SI	C(Fi), IL(SL), IS (2.5)	4.52	0.01+		✓
SI	C(Fi), IL(SL), IS (5)	98.31	0.02+		✓
SI	C(Fi), IL(SM), IS (5)	8.63	0.2	✓	
SI	C(Fi), IL(BC), IS (2.5)	5.58	0.1	✓	
SI	C(Fi), IL(BC), IS (5)	6.45	0.2	✓	
SI	C(Fr), IL(LC), IS (5)	9.13	0.2	✓	
SI	C(Fr), IL(BC), IS (2.5)	0.53	0.1	✓	
SI	C(Fr), IL(BC), IS (5)	4.97	0.2	✓	
CS	C(Fi), IL(LC), IS (2.5)	5.44	0.5**	✓	
CS	C(Fi), IL(LC), IS (5)	8.92	0.5**	✓	
CS	C(Fi), IL(SL), IS (2.5)	94.49	0.01+		✓
CS	C(Fi), IL(SL), IS (5)	165.90	0.02+		✓
CS	C(Fi), IL(BC), IS (2.5)	3.91	0.5**	✓	
CS	C(Fi), IL(BC), IS (5)	8.01	0.5**	✓	

* For constraint type: Fi=fixed, Fr=free; impact location type: LC=Lid-center, SL=Side near lid, BC=Bottom center, SM=Side middle; impact speed type in meter/second: 2.5 or 5.

+ For the impact location at SL, it is assumed a small release.

**It is assumed to be 50%, because the impact location is mid-point, regardless the extent of the opening.

Estimate of Damage Ratio from Drum Drop Simulations

Content Type	Drop Height (m), Orientation (°)	Breach Area (10^{-3} m^2)	Damage Ratio	Mode of Failure			
				Lid, Sidewall Separation	Complete Lid Failure	Lid Vent Failure	Bottom Failure
HD	20, 135	9.21	0.04[A]	✓			
HD	20, 180	1.49	0.01[C]			✓	
SI	5, 180	1.62	0.01 [C]			✓	
SI	10, 135	254.30	0.5[B]		✓		
SI	10, 180	1.58	0.02 [C]			✓	
SI	20, 45	8.78	0.04 [C]				✓
SI	20, 135	250.00	0.5[B]		✓		
SI	20, 180	1.63	0.04 [C]			✓	
CS	10, 45	10.93	0.01 [C]				✓
CS	10, 135	251.40	1.0[B]		✓		
CS	20, 45	173.60	1.0[B]				✓
CS	20, 135	248.90	1.0[B]		✓		
CS	20, 180	1.59	0.02 [C]			✓	

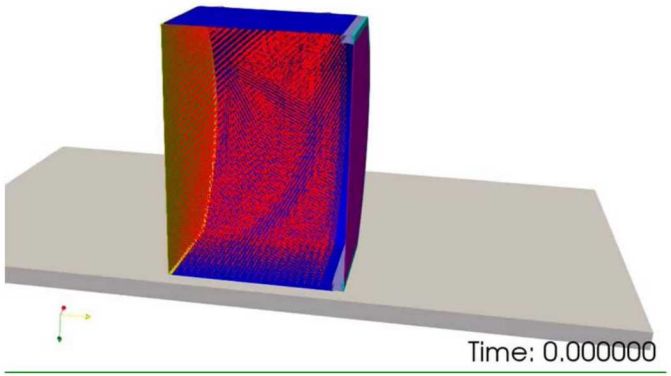
[A] Even though there is clear separation, but because the opening is small, it is assumed only very small release

[B] Complete lid failure or bottom failure with a very large breach area calculated. Assumed that sufficient kinetic energy remains to push majority of the materials out for CS type content. For both HD and SI, it is assumed only 50% material release, due to solids and large debris, which unlike sands/soils can easily flows out.

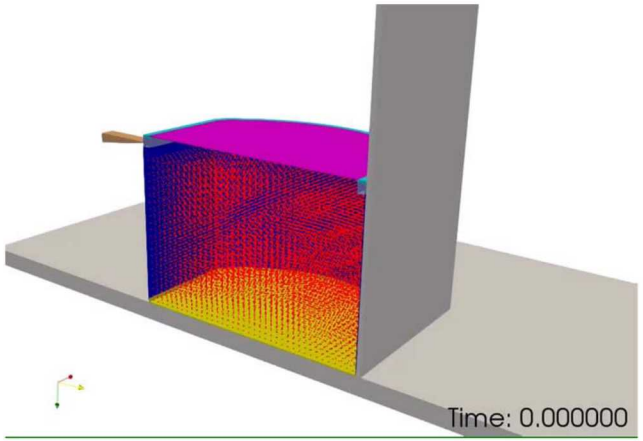
[C] Small breach area, such as lid vent failure and minor bottom separation from sidewall of the container. It is assumed at DR of 0.01, then progress doubling if the kinetic energy is also doubled.

SWB CS Simulations

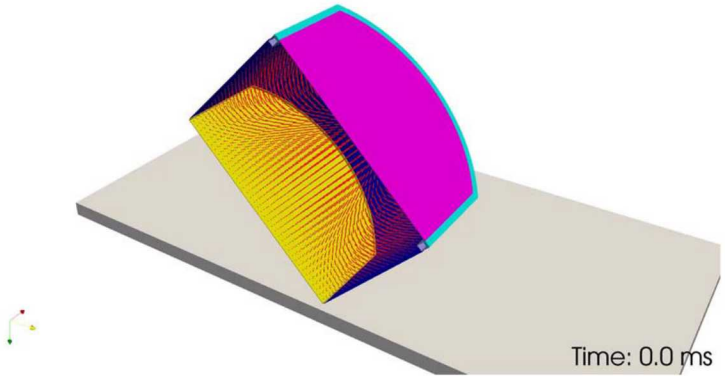
20 m drop 90 degree

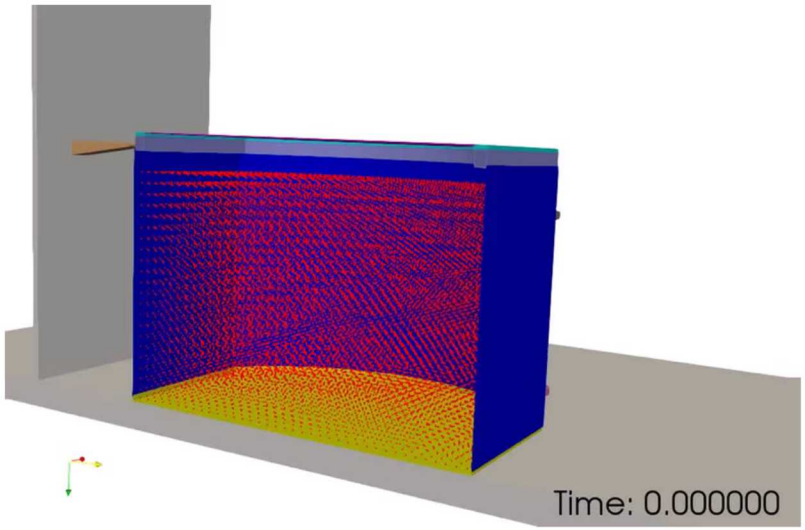


Fixed 5 m/s near lid



10 m drop 45 degree





Estimate of Damage Ratio from SWB Puncture Simulations

Content Type	Constraint, Impact Location, Impactor Speed (m/s)	Total Breach Area (10^{-3} m^2)	Damage Ratio	Mode of Failure	
				Puncture	Lid, Sidewall Separation
CS	Fixed, Side-Near Lid, 2.5	65.599728	0.05		✓
CS	Fixed, Side-Near Lid, 5.0	106.448776	0.1		✓
CS	Free, Side-Near Lid, 2.5	10.625484	0.05		✓
CS	Free, Side-Near Lid, 5.0	135.583108	0.1		✓
CS	Fixed, Side-Middle, 5.0	5.945719	0.5	✓	
CS	Fixed, Lid-Center, 5.0	6.581837	0.5	✓	

Estimate of Damage Ratio from SWB Drop Simulations

Content Type	Drop Height (m)	Orientation (°)	Damage Ratio	Mode of Failure
				Complete Lid Failure
CS	2.5	135	1.0	✓
CS	5	45	1.0	✓
CS	5	135	1.0	✓
CS	10	45	1.0	✓
CS	10	135	1.0	✓
CS	20	45	1.0	✓
CS	20	90	1.0	✓
CS	20	135	1.0	✓

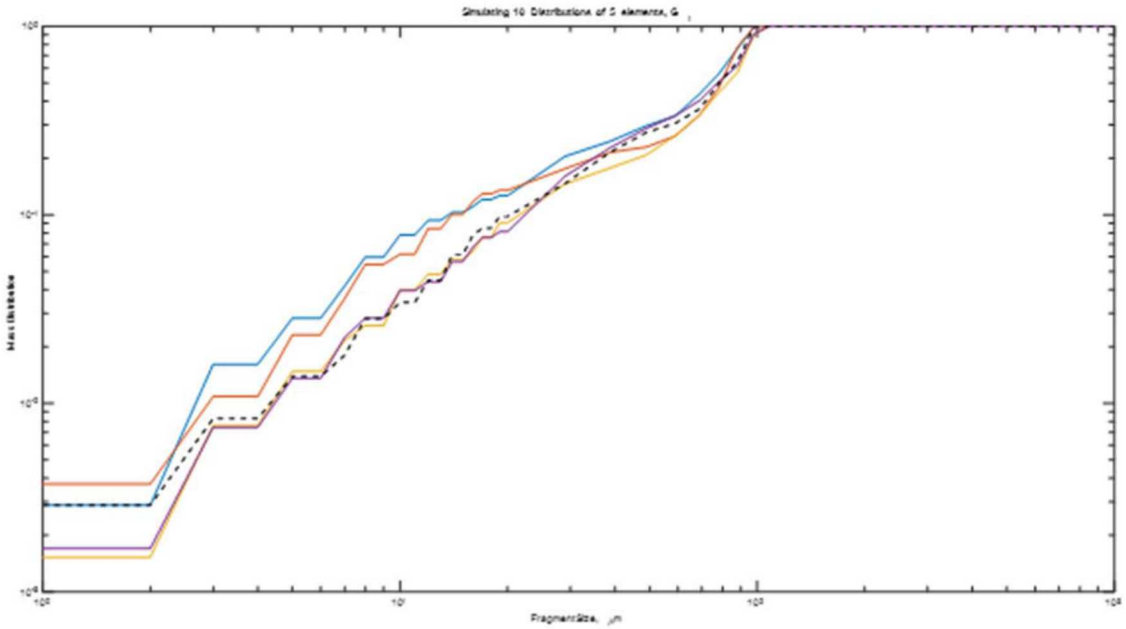
Fragmentation of Brittle and Ceramic Solids

SIERRA/SM is used to model the fragmentation of these solids:

- Due to length scale, two fragmentation model approach was used: macro- and micro-fragmentation models adapted
- Macro-fragmentation using the hierarchical gradient damage explicit (HGDE) model exists
- Micro-fragmentation is developed to be implemented in SIERRA/SM

Distributions of microscale parameters (Gi, sigmaci, thetai) have been implemented in microscale model. Parameters at microscale determine macroscale Fracture Energy and Critical Stress values (1D bar at microscale is assumed to break at weakest node, which should be also reflected by the macroscale parameters).

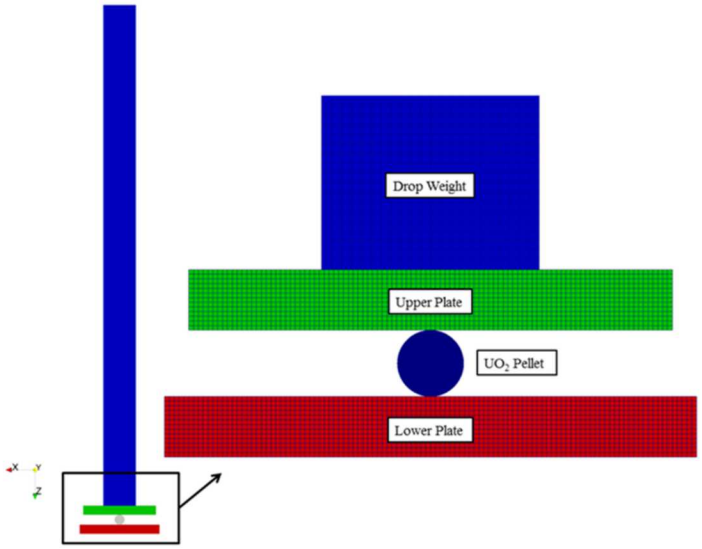
Changing Gi has a small effect on the distribution of mass at the microscale.

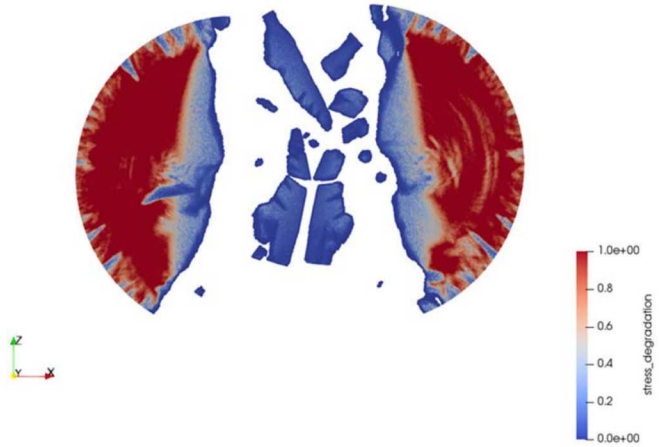


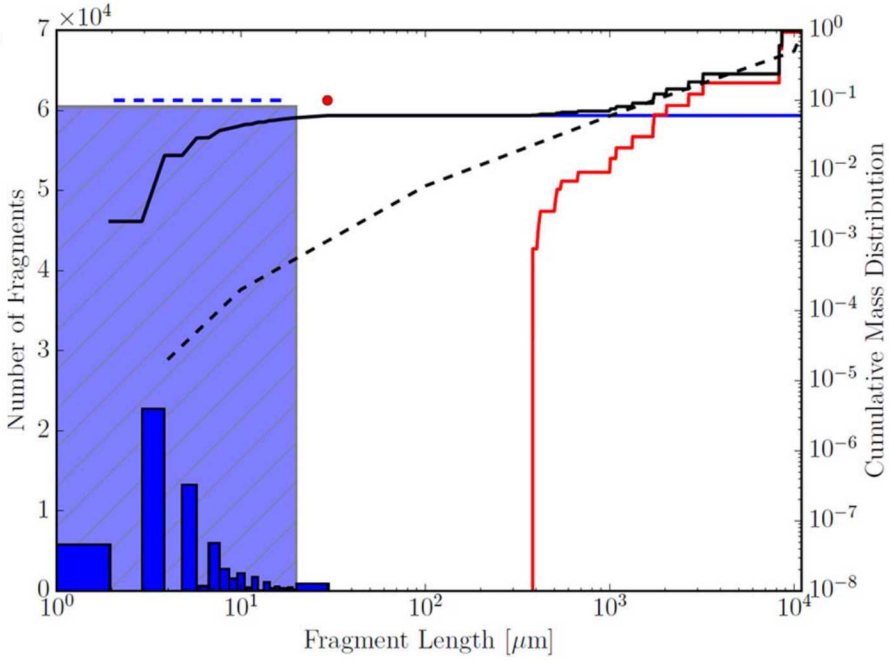
Concurrent-Coupled Fragmentation Model

It consists two models (macro and micro):

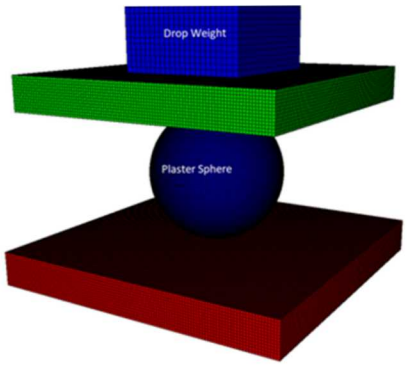
- Micro-fragmentation model implemented as a 1-D model to estimate the fragmentation in micron range.
- Coupling micro- to macro-fragmentation models remains challenging.
- Model is matching at the macroscale more closely now than previously, however too many small fragments are being produced as a result of an increased number of elements reaching the degradation criterion.
- Using Jardine 1982 experiment to benchmark the models





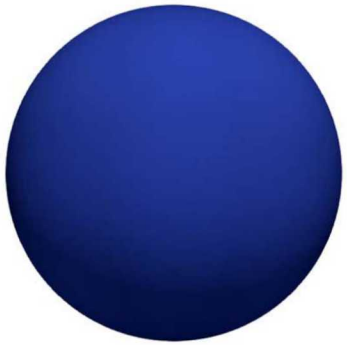


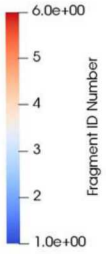
Validation of Macro-Fragmentation Model Benchmarked by Wu 2004 Experiment



Colored by fragment

23.6% of elements dead at this time, T = 4 ms

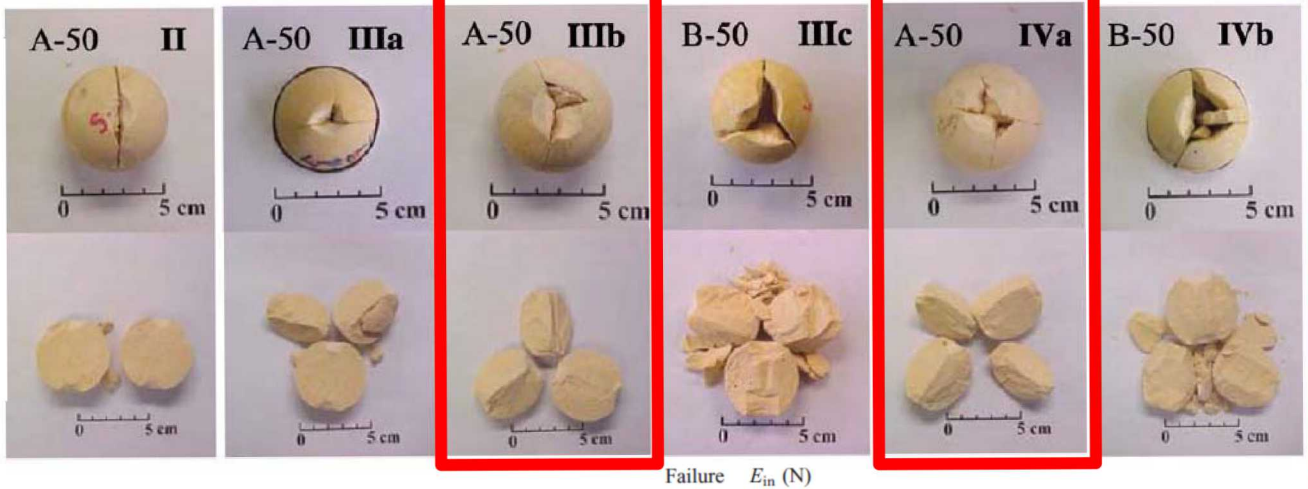




This is also close in terms of KE, 5 slices seen

35.7 J

39.9 J



Failure mode	E_{in} (N) $D = 50$ mm	
	Material A	Material B
II	5.0 (2)	4.6 (1)
IIIa	5.6 (4)	5.8 (3)
IIIb	11.2 (4)	7.2 (2)
IIIc	–	–
Iva	12.5 (5)	8.6 (5)
Ivb	–	23.8 (1)
Ivc	36.3 (2)	42.4 (3)
Va	11.1 (1)	5.2 (1)
Vb	48.3 (1)	37.8 (2)
Vc	–	–
VI	39.7 (1)	43.2 (1)
X	72.6 (7)	69.4 (8)

KE for the cases isn't too different actually

Conclusions

- The use of SIERRA/SM developed at SNL demonstrates the predictability of waste container failures (i.e., 7A and SWB) in various configurations and conditions of mechanical insults beyond those conditions described DOE-STD-5506
  - Using the visual examinations of the simulations can estimate the breach area reasonably
  - DR interpolated and extended from using existing DOE-SRD-5506, DOE Standard Preparation of Safety Basis Documents for Transuranic (TRU) Waste Facilities, can provide reasonably bounding DR values
- SIERRA/SM can be used to model fragmentation of brittle and ceramic type of solids. Model improvement is needed to be quantified fragment sizes in the micron range
  - Validation began on the macro-fragmentation (HGDE) model
  - Coupled the macro- and micro- (1-D model) fragmentation models still requires more work.

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