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SDRD SITE-DIRECTED RESEARCH & DEVELOPMENT

Dynamic Particulate Behavior in Turbulent Media

NNSS: Clare Kimblin, Ian McKenna, Matt Staska, Paul Taylor, Roy Abbott, Jonathon Rivera, Rick Allison, Chusia Moua

Keystone: Mary O’Neill; LLNL: Jason Sears, Jens von der Linden, Chris Kueny; Univ. of Oregon: Joshua Mendez-Harper, Professor Josef Dufek

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Topics

- Challenge & goals
- Progress in building the new shock tube overpressure apparatus (STOA)
  - *Ian McKenna, Paul Taylor, Matt Staska, Roy Abbott, Rick Allison, Chusia Moua*
- Correlation between experimental results and hydrodynamic and electrostatic simulations
  - *STL experimental work with LLNL modelers: Jason Sears, Jens von der Linden, Chris Kueny*
- University of Oregon particle-to-particle charging results for diamond, graphite, and detonation soot
  - *U. of OR: Joshua Mendez-Harper, Professor Josef Dufek*
- Simulations related to minimizing particle-to-shock tube interactions
  - *Matt Staska, Jonathon Rivera*
- Cloud behavior model and analytical tool development
  - *Keystone: Mary O'Neill*

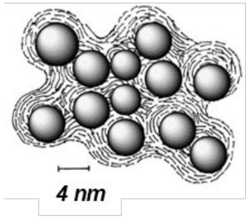
Overarching Challenge: Discrimination of hydrodynamic tests via particulate signatures

- HE events produce measurable temporal RF and optical signatures, as well as sub-micron to micron-scale particulates
  - These may provide insight into HE package design, and formulation
- Large-scale HE tests are costly, and *variables and signatures* difficult to separate
- Modelers believe small-scale, controlled experiments provide the best approach to studying aspects of early-time HE processes
  - Real-time RF and optical signatures can provide validation in the development of predictive HE models
  - Particulate evolution under shock conditions can inform particulate formation models
- The Shock Tube Overpressure Apparatus (STOA) provides a means to support such models

Nonproliferation efforts require improved understanding of the effects of shock on RF and optical signatures, and on particulate formation

Goals

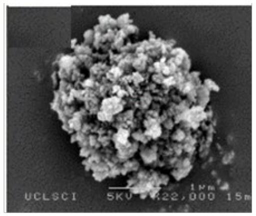
- Build improved STOA and provide well characterized rapid decompression tests and data analysis to help answer questions:
  - Which carbon-based particulates generate RF/optical signatures, and how?
    - Provide data that validates predictive HE models that can ultimately correlate real-time RF and optical signatures, with detonation types
  - How does additional shock impact C particulate evolution?
    - Provide a controlled experimental platform to support models correlating late-time recovered particulates to test conditions
- Leverage collaboration with LLNL modelers to demonstrate correlations between STOA results and hydrodynamic and electrostatic models
- Leverage STOA diagnostics and analysis tools for large scale tests



Model of core nanodiamond (ND) in amorphous soot
Kruger *et al.*, 2005

?

Effect of pressure & electrostatics on C allotrope and aggregation?



Micron-scale agglomerate
Bevilacqua *et al.*, 2008.

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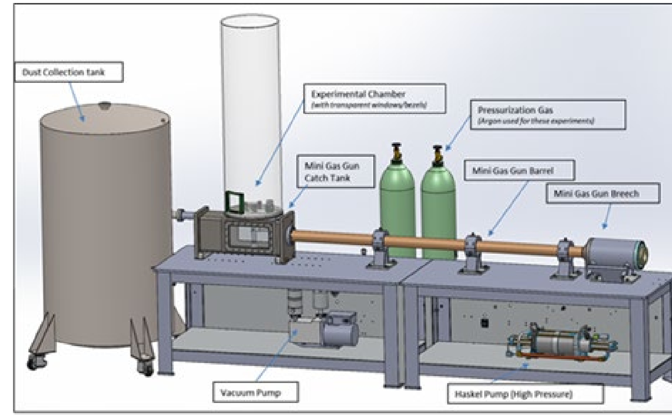
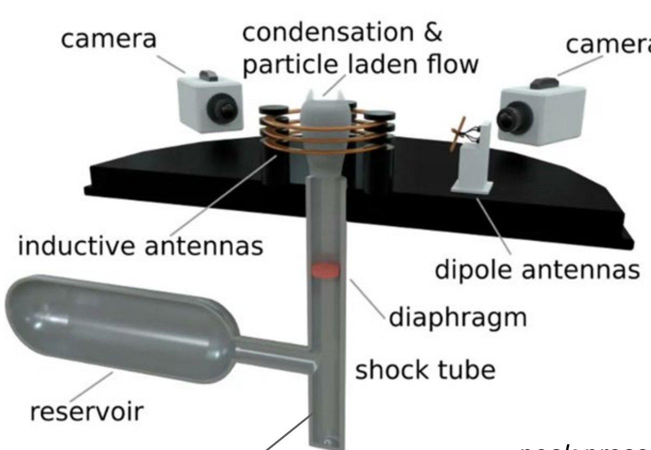
STOA re-build for carbonaceous particulate/shock studies

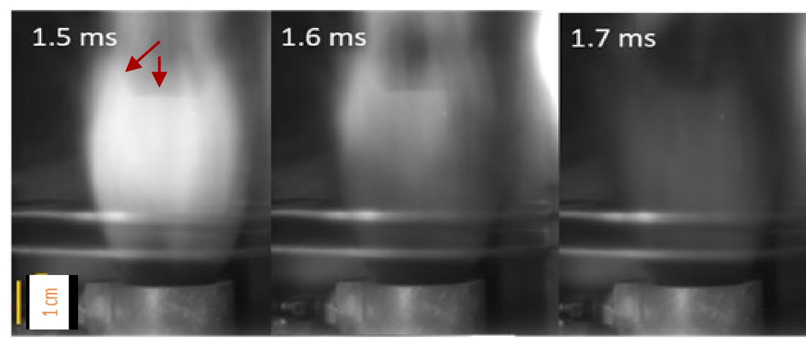
- **Progression of STOA development**
  - Based on design used by LMU volcanologists to study RF associated with volcanic eruptions (Cimarelli, et al., *Geology* (2014) 42 (1): 79–82)
  - STL proof-of-concept system (Aug. 2018, end of FY18 SDRD)
    - Attached to STL's mini gas gun (right)
  - Stand-alone system (non-SDRD funding FY19)
    - Resided in STL's *multi-use* anechoic chamber
  - Revised system being optimized for DS-focused studies
    - Will reside in a newly constructed RF-shielded chamber and be dedicated to STOA experiments



Initial STL incarnation reliant on gas-gun

- **STOA structural modifications:**
  - Infinite reservoir and reduced particle quantities. Permit focus on observable shock interface





TNT detonation soot entrained in standing shock wave (Mach Disc)

1000 psi (70 atm) diaphragm;
peak pressure at side of 2 cm diameter vent ~ 10 atm.

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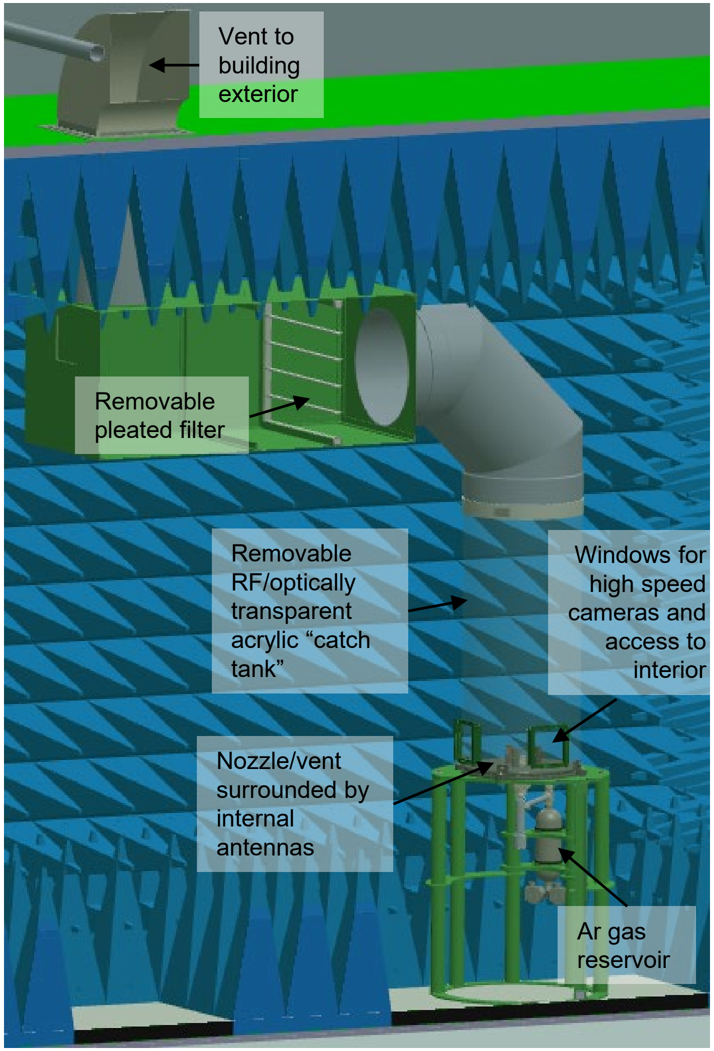
Modifications for improved STOA



RF and Anechoic Chamber SME: Paul Taylor; STOA and exhaust design by Matt Staska and Roy Abbott. Shared effort with mm-wave SDRD.

Above-shock-tube modifications

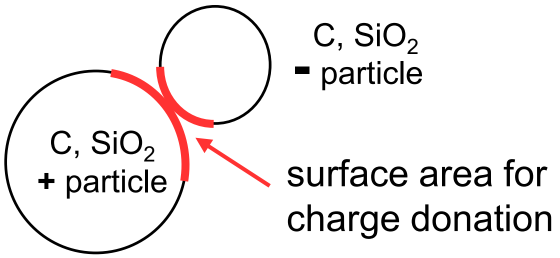
- Better particle exhaust
- Removable catch tank for cleaning or replacement
- Optional nozzle-based sample holder to reduce particulate-to-wall interactions and for improved controlled particulate release

Diagnostic improvements

- DC pressure transducer (P_{trans}) at nozzle to prevent discharges to grounded AC P_{trans}
- Higher frequency RF measurements (40 GHz detectable with block down-conversion method)
- Rogowski coil to determine discharge polarity
- Faraday cups/electrostatic separator to measure particle charge

Rapid decompression experiments

- Fluid dynamics in shock flow provides mechanism for charging, charge separation and discharge
  - Particle charging by contact electrification, and separation by inertia
    - Larger, like, particles thought to donate e's to smaller
    - Similarly sized particles separated into like-charged clusters by their relative Stokes numbers
    - Charge separation generates E-fields
  - Rarefaction may lower breakdown threshold
- Observations suggest that hierarchy of electron discharge (electron avalanche-to-streamer, to-leader) may be disrupted in shock flows (Behnke *et al.* JGR Atm, 2018: VHF RF; Mendez-Harper *et al.* GRL: 2018, barrel shaped discharge)

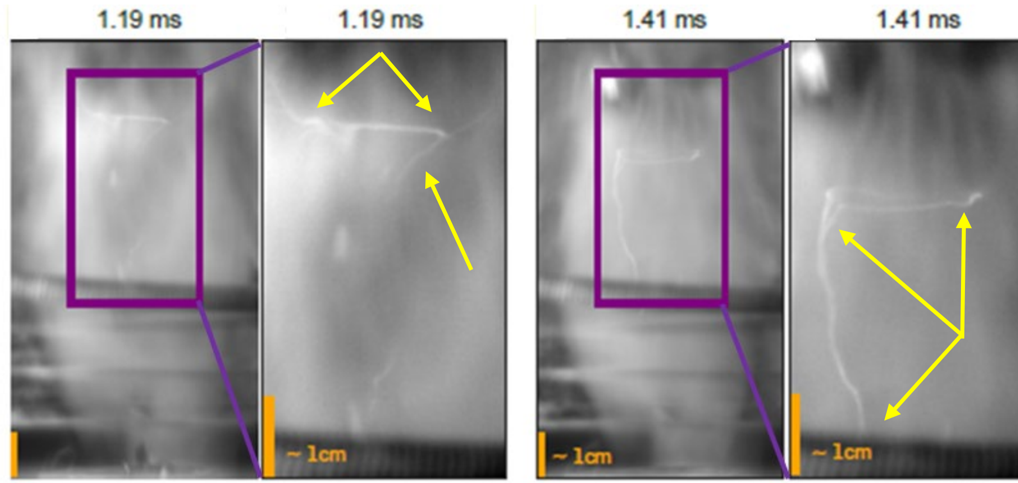


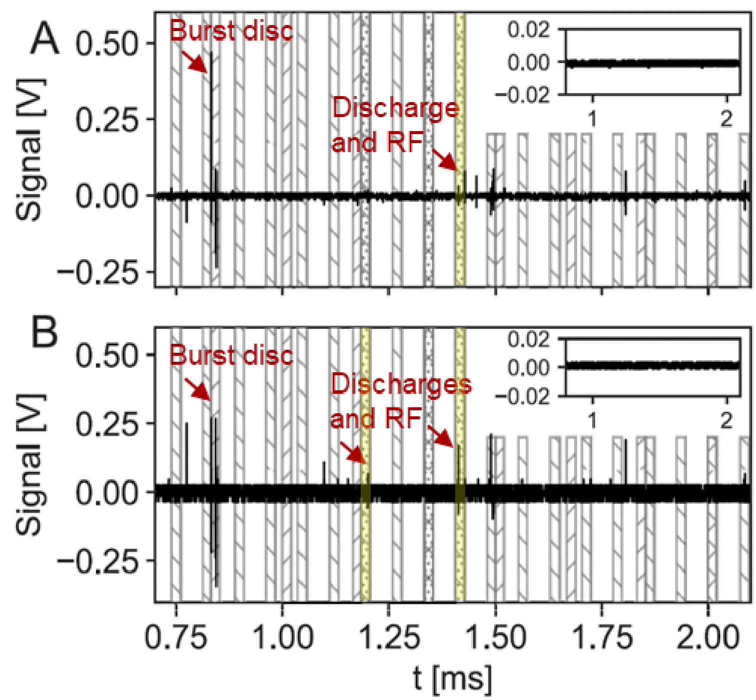
Kok, J. F. and N. O. Renno, "A comprehensive numerical model of steady state saltation (COMSALT)," *J. Geophys. Res.* **114** (2009).

Coincident condensation and discharges observed in decompression with argon-diamond mixture

<100 mg 5 μm diamond, first 3 ms

Peak pressure of 70 atm in tube; and ~10 atm at side of vent





Coincident RF (black lines) and optical emissions (dotted)

Insets = control (no particle, no RF emissions)

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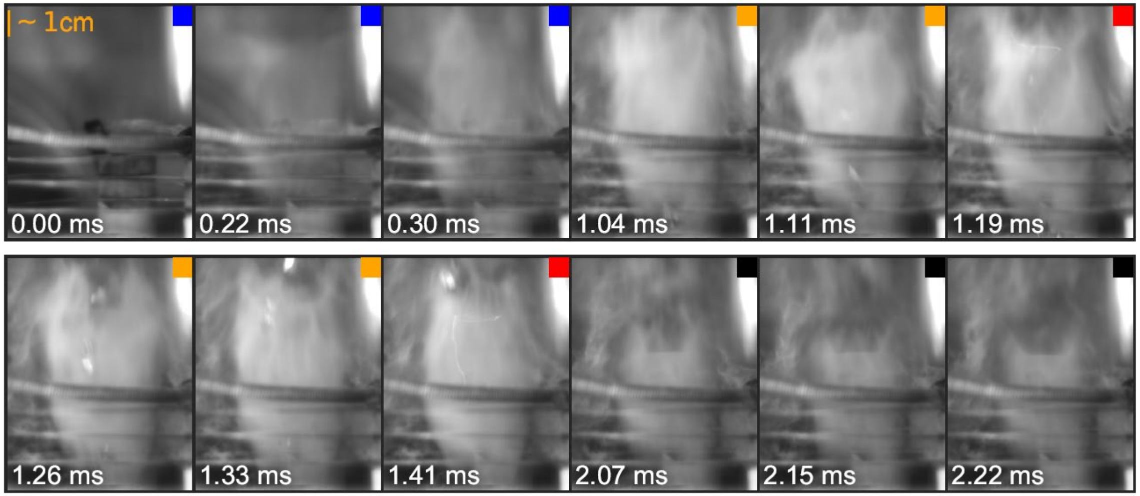
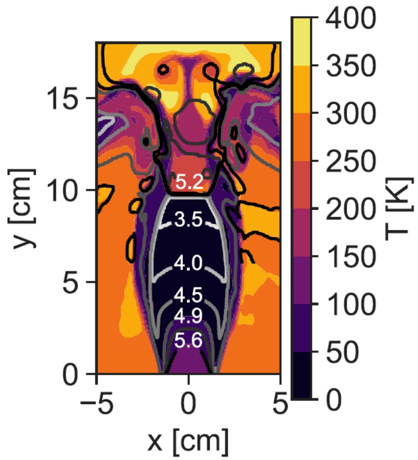
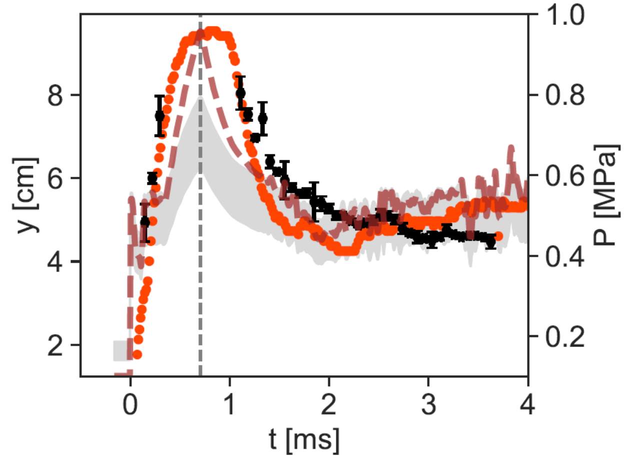
Hydrodynamic model vs. experiment



Simulated pressure, $Log_{10}P$, (Pa) , and T (K) 0.7 ms



Mach disk height (Left axis): experiment (black) vs. LLNL simulation (orange)



Hydrodynamic model confirms that temperatures support Ar condensation, and permit Mach Disk (MD) height comparison

- LLNL model indicates that supersonic flow becomes subsonic at shock boundary, where heating leads to sharp cut-off in Ar condensation
- P at nozzle is high, decreases above nozzle, and rapidly increases at shock front
- Good agreement between experimental MD height (black dots) and hydro-dynamically modeled MD height (red dots) vs. time

First time models of internal phenomena directly validated against experiment

Preliminary electrostatic model

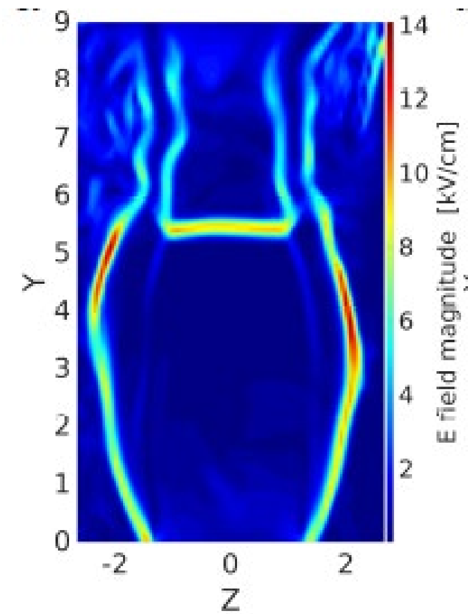
Points of maximum ionization

- ***Input:*** P, T, density from hydrodynamic model (1.41 ms), and E-field (assumed to be proportional to velocity gradient, where collisional charging expected to be greatest)
- ***Output:*** points of maximum ionization, α, and possible breakdown paths through local maxima

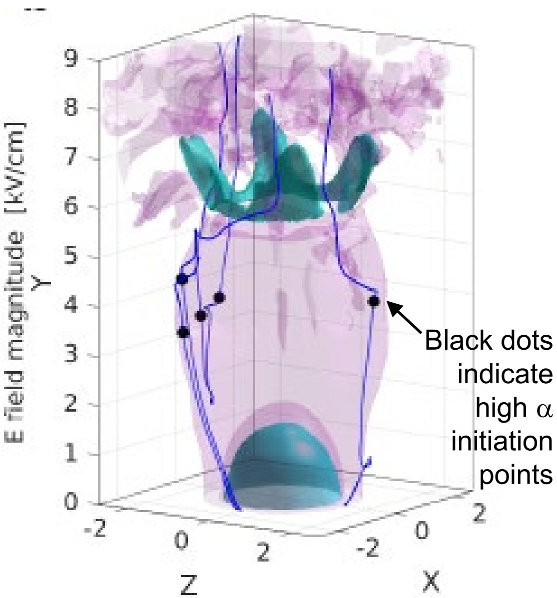
Model supports the theory that **standing shock cuts off discharge**, leading to spatially confined streamers; and suppression of longer λ, lower f emission leaders

- Higher frequency RF measurements to be made at future STOA tests

Simulated electric field estimated as function of velocity gradient



Simulated electrical discharge



Raether-Meek criterion to determine the # of ionization lengths($1/\alpha$) along discharge path for N_e to support avalanche to streamer transition.

For Argon:

$$\ln(N_e) = \int_0^l \alpha(E/n_0)\,dl \gtrsim 10$$

α = **#e's freed per unit length**, l = e drift length,

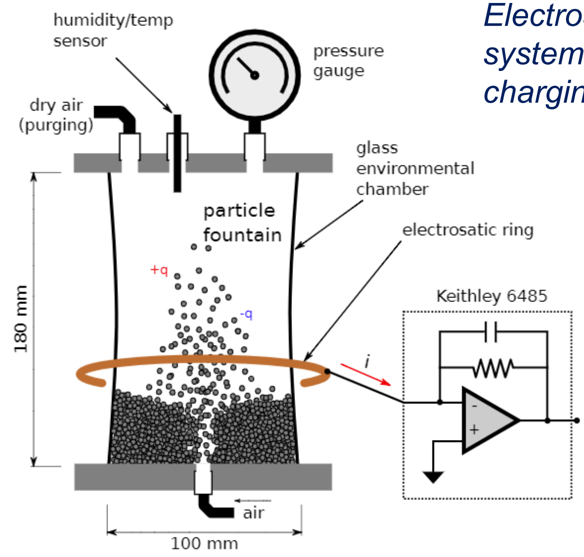
E = electric field, n_0 = local neutral gas number density

Experiment combined with models suggests condensation and discharge regulated by standing shock height

University of Oregon – Diamond particle charging

Means to support STOA studies and better understand C particle behavior

- Fluidized bed studies designed to measure *interparticle* charging of ~90 μm diamond (D), ~60 μm graphite (GR), and Comp B detonation soot (DS)
- Measure charging rate, charge magnitude, and polarity at fluidization energies of 0.055–0.062 L/s in dry air
  - No aggregation readily observable with diamond
- UPPER = System for **bulk** charging rate using electrostatic ring *(No perpendicular gas stream because diamond was hitting glass walls).*
- LOWER = Larger system required for **per particle** charge measurements with Faraday cup (FC) and electrostatic separator (ES)



Electrostatic ring system used for bulk charging rates

Particle fountain for Faraday Cup and Electrostatic Separator particle charging measurements:

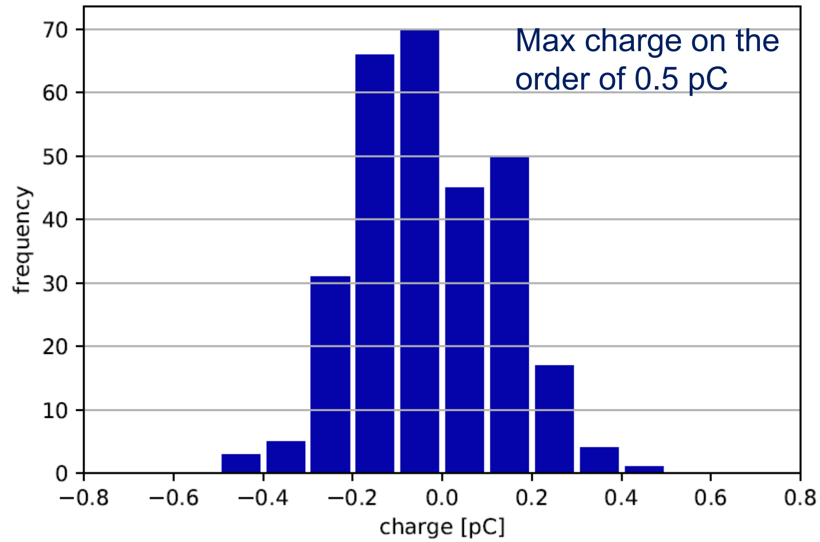
Zoom-in on diamond fountaining, with gas stream to sample particles

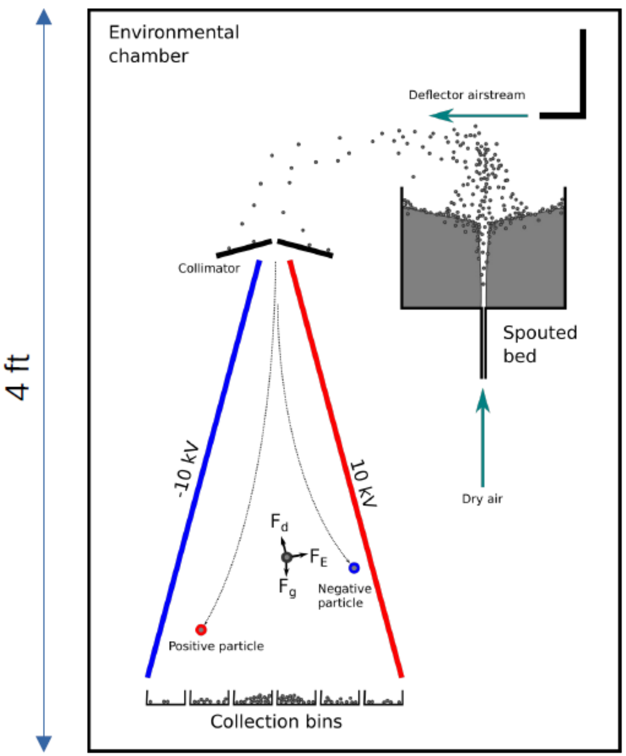
U of OR – Fluidized bed with ~90 μm diamond

Charge magnitude and polarity measured with Faraday cup (FC) and electrostatic separator (ES)

- Conservation of charge (upper RHS, FC)
  - Distribution has mean charge of ~0
- Charge polarity and particle size measured using ES (below) and optical microscope
  - Size dependent bipolar charging not observed (lower RHS)

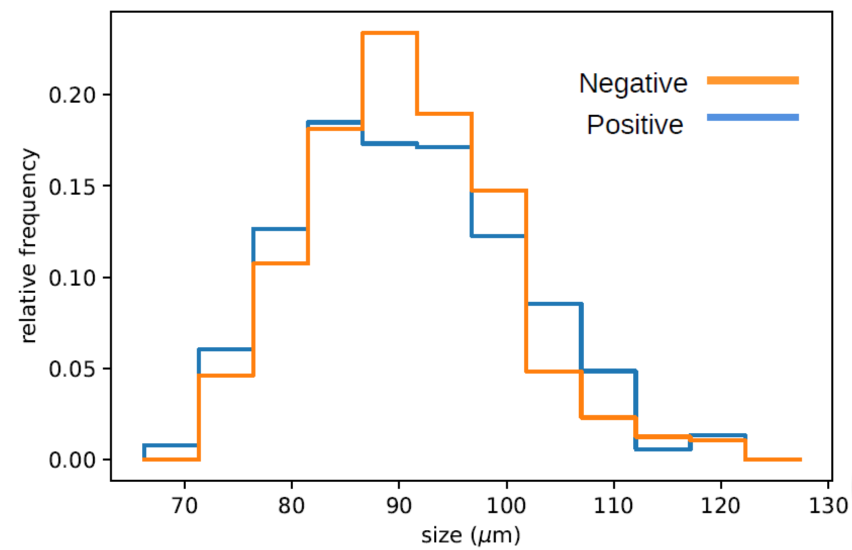
Charge distribution on diamond particles (0.0554 L/s)





Electrostatic separator: positive particles deflect toward negative plate and vv. Particles then sized

Charging (w ES) based on size (with optical microscope)

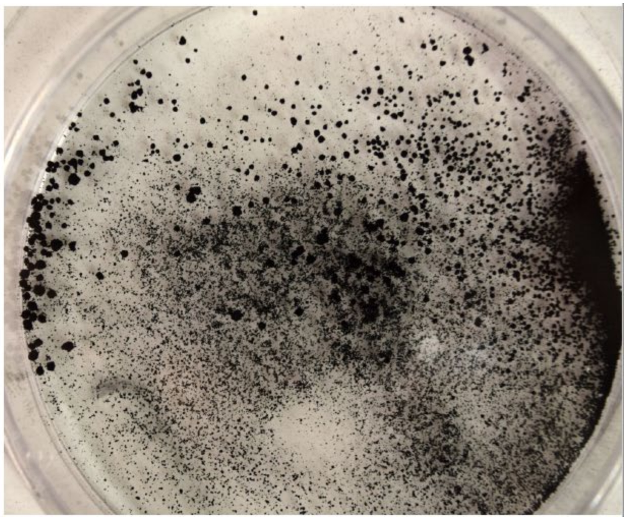


U of OR – Graphite (GR) and detonation soot (DS)

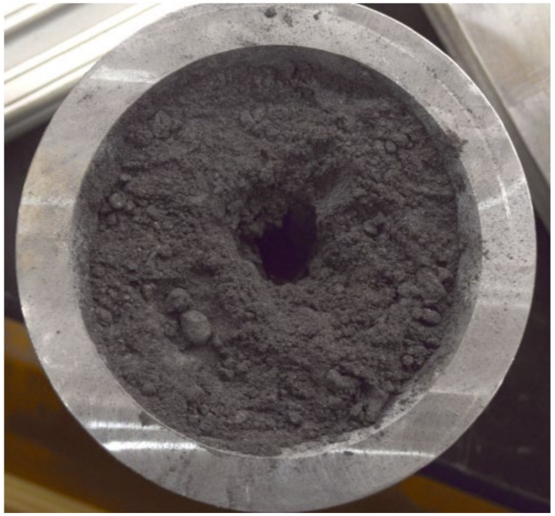
- GR and DS highly prone to aggregation
  - Material self channelizes after few seconds of attempted ‘fountaining’ in fluidized bed
  - Measurement of single particles from fluidized bed with Faraday cups not possible
- Alternative strategy required

Graphite

Detonation soot



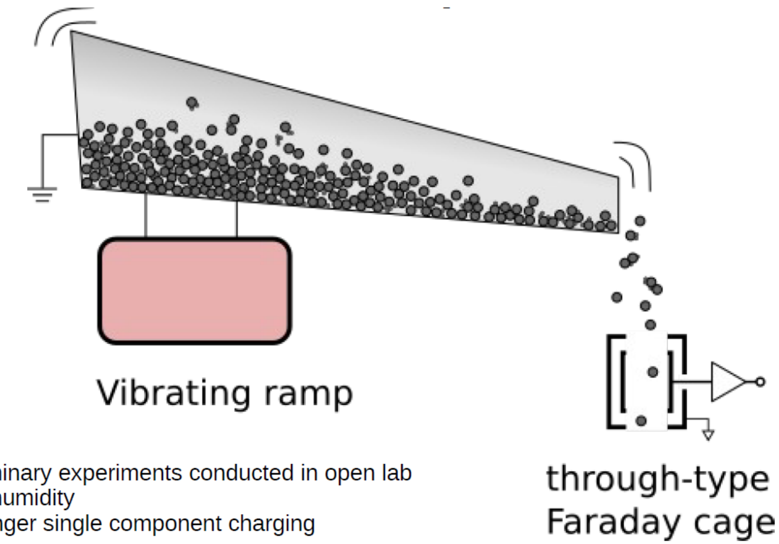
Fluidization behavior of DS



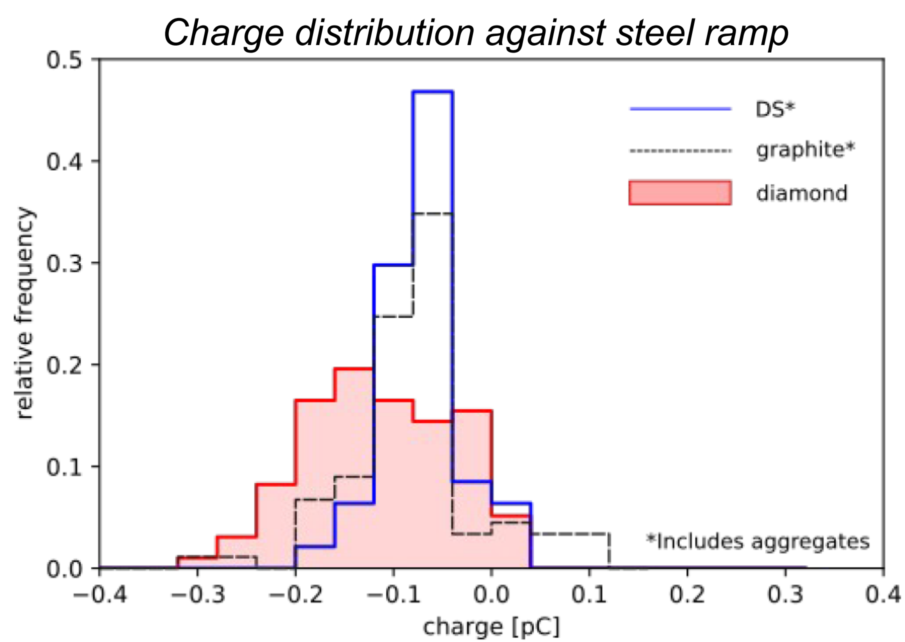
U of OR – Vibrating ramp

Vibrating ramp (top right) helps to break up aggregates and separate material, but difficult to isolate particle-particle collisions

- Results:
  - D, GR, and DS charge negatively against stainless steel (below)
    - work functions of the C-particulates (est. *Φ~4.8)* are higher relative to steel (*Φ~4.4)*
  - **Narrower** charge distribution for GR and DS
  - Studies to be repeated in controlled atmosphere
- *Vibrating ramp studies could be used to guide selection of shock tube and nozzle surfaces*
  - *Al Φ~4.1-4.4; Anodized Al Φ~4.8*



* Preliminary experiments conducted in open lab
* 40% humidity
* No longer single component charging



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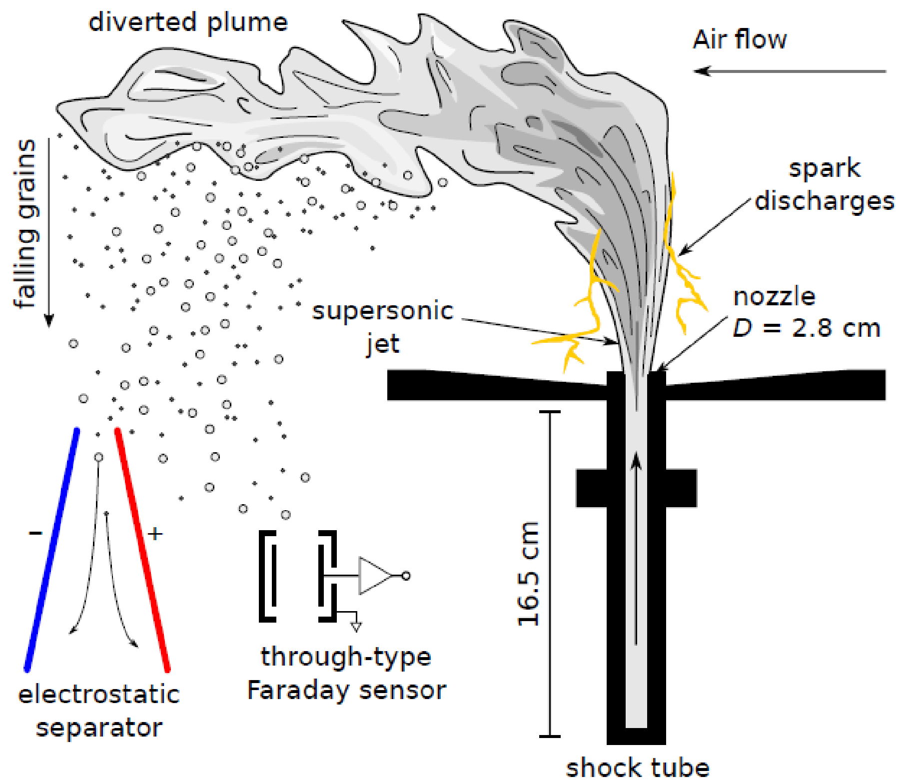
In-situ charge measurements

- Would be significant to be able to model charging of particulates
  - Fluidized bed results proposed for preliminary validation of charging models
- Faraday cups and electrostatic separator to enable **measurement of ~in-situ particle charge** resulting from STOA ejection

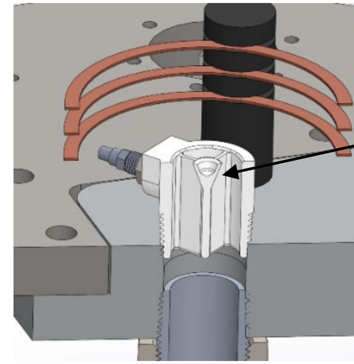


Not to scale

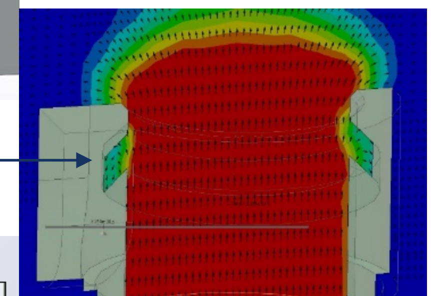
Introduction of small sample quantities from nozzle

In-nozzle sample holder

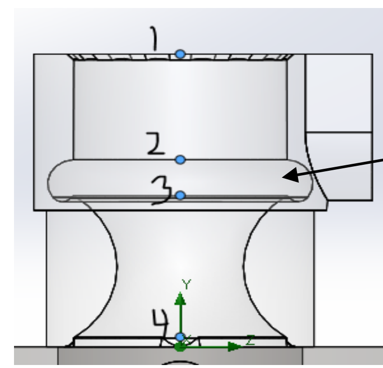
- For reduction in particle-to-wall charging relative to particle-to-particle charging
  - Important for small (~100 mg) sample quantities
- For controlled release of sub-gram sample quantities into standing shock wave
  - Restricted quantity may be due to limited sample availability, or desire to create low particulate concentration conditions for modeling
  - May allow for sequential ejection of different types of particles (ex. micro-diamond into soot)
- Design considerations
  - Sufficient volume for sample (~0.25 mL)
  - Sufficient particle evacuation rate for particle-to-particle charging
  - Does not alter flow so as to prevent Mach Disk from forming above nozzle
- FlowSim to guide 3D printing of optimal PMMA nozzle(s)
  - Focus on Convergent-Divergent (C-D) nozzle



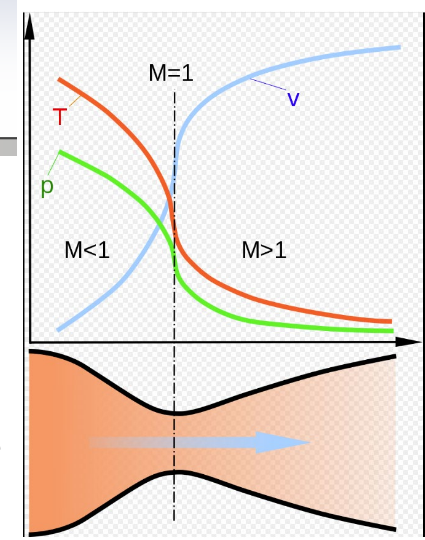
Conical in-nozzle sample holder



Recessed ring, straight nozzle



Recessed ring in C-D nozzle



C-D nozzle behavior (Wiki)

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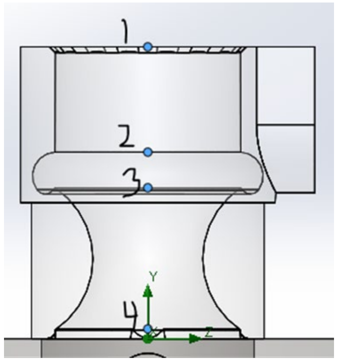
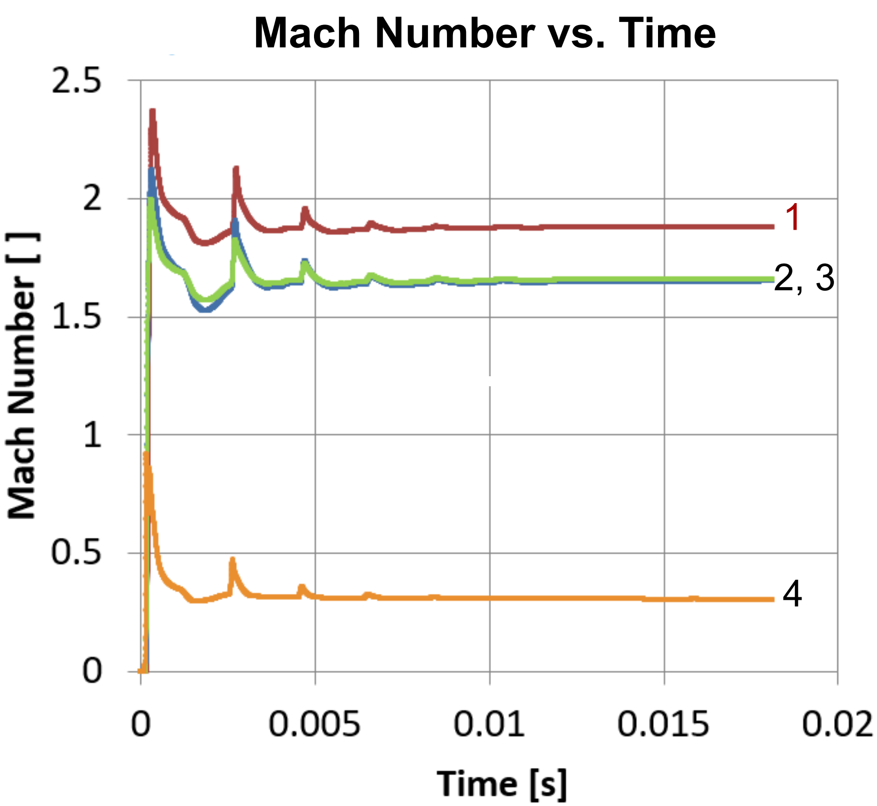
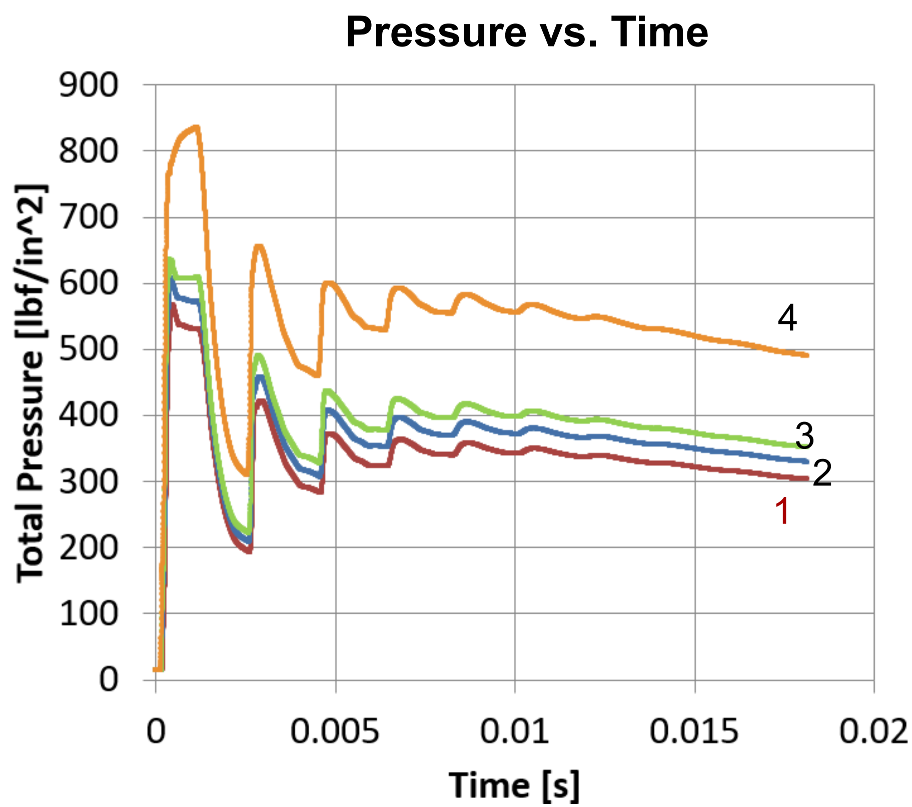
C-D in-nozzle sample holder FlowSim simulations



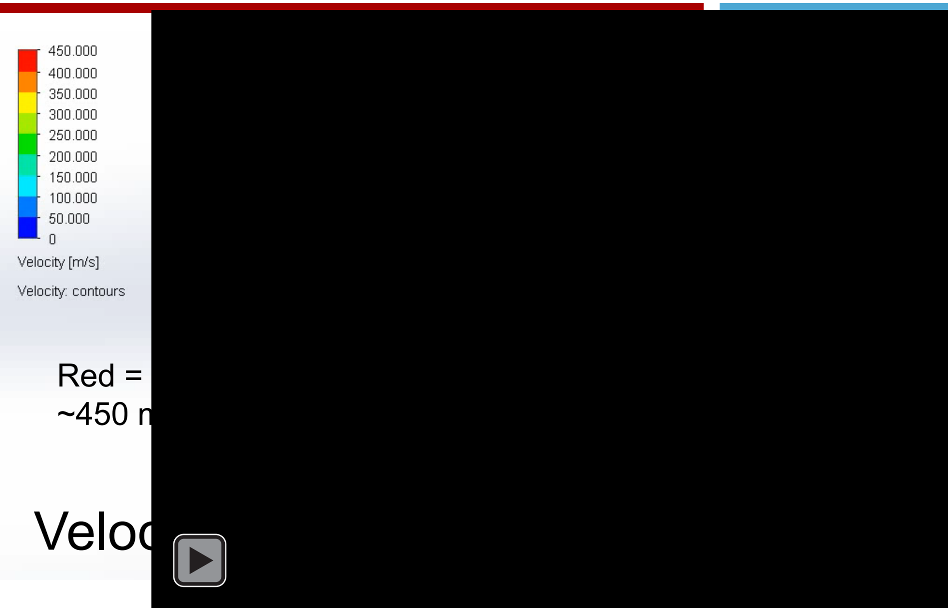
Convergent-Divergent design

- Preliminary results indicate it is best geometry to achieve and maintain supersonic flow
- Peak pressure reduced above convergence, but supersonic velocities sustained
- Most stable sustainment of high velocity compared to other nozzle designs simulated





CD nozzle velocity & vorticity simulations (0-~18 ms)



Impact on standing shock wave?

- Will compare predicted velocity flow above nozzle to that for straight nozzle
  - Initial ECOs with cameras and argon-only to determine effect of C-D on stable MD formation

Particle release rate?

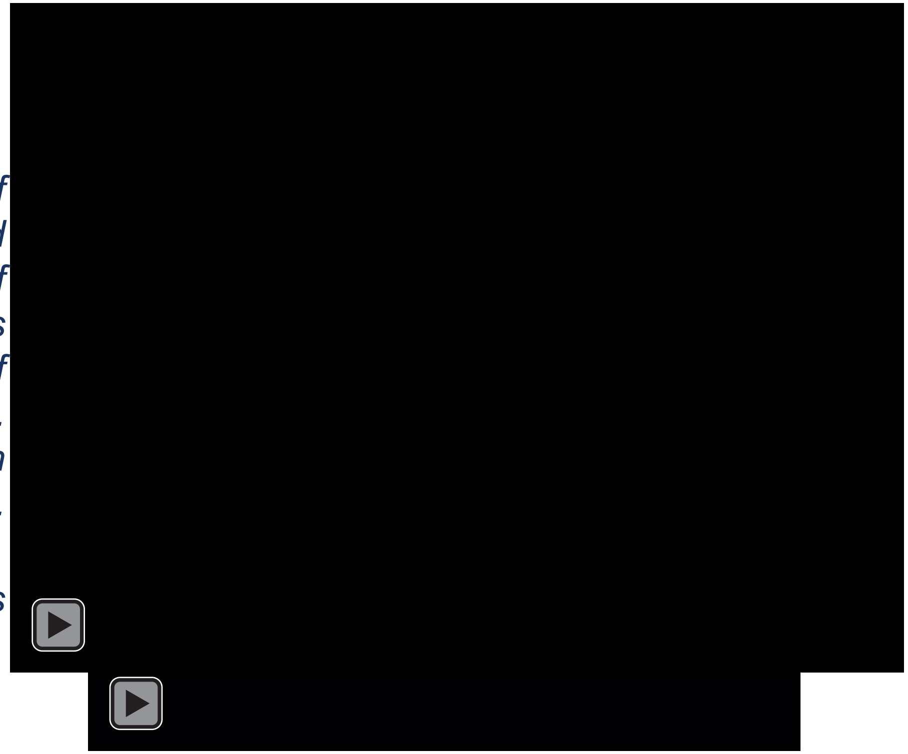
- Vorticity is **highest** in recessed ring
- Iterate 3-D printing, testing and simulations to obtain *sufficient* particle-to-particle interaction and rate of release into standing shock

Cloud behavior model

Transmission through cloud vs. λ: Diamond

Large quantity of fine-grain-sized diamond (47 g of 5 ±2 μm) obscures meaningful view of particles-in-shock. Low transmission and high reflectivity.

Video = 0.2 − 3 ms

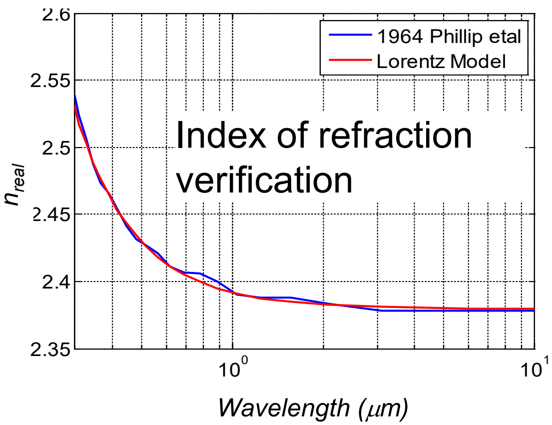


Can we leverage Mie scattering model to inform experimental parameters, and diagnostics used to observe discharges?

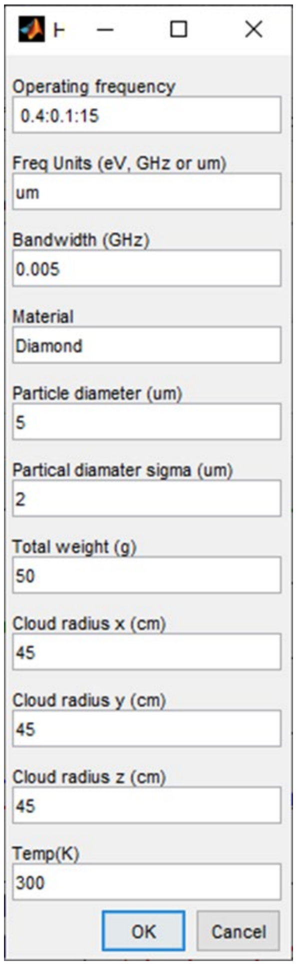
Transmission through cloud vs. λ: Diamond

- Transmission through cloud calculation (Bohren, et al.)
  - *Lorentz dispersion model* implemented to calculate dielectric constant (n^2) over all wavelengths (mmWave to UV-Vis-NIR)
    - Lorentz dispersion model verified against measured data (A)
  - Used as input to *Modified Mie attenuation* model, which allows calculation of attenuation (transmission) through particulate cloud using extinction coefficients
- Model input (B) for STOA release of 50 g of 5 ±2 µm diamond
  - And cloud transmission output (C)

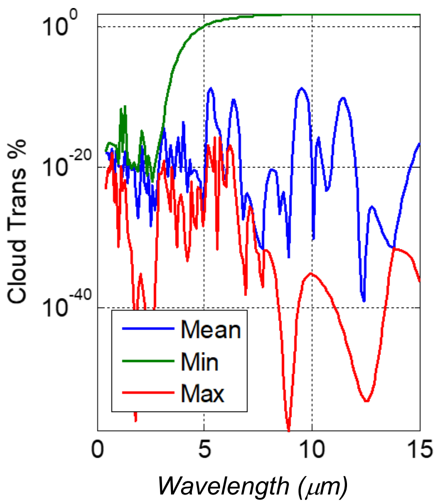
***A.** Measured vs. modeled for diamond*



***B.** MATLAB GUI*



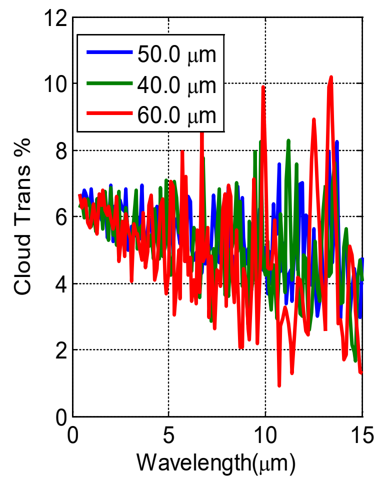
***C.** Mie attenuation using dielectric constant from dispersion model*

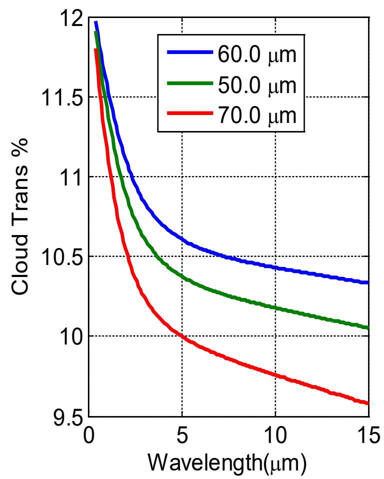


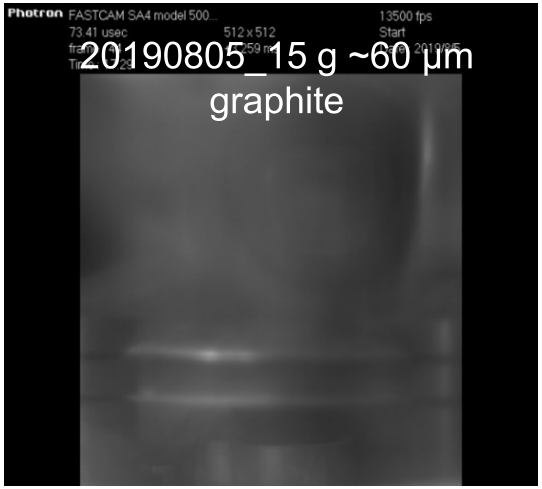
Bohren, C. F., and Huffman, D. R., *Absorption and Scattering of Light by Small Particles*. John Wiley & Sons, Inc. 1983.
https://refractiveindex.info/?shelf=main&book=C&page=Phillip
H. R. Phillip and E. A. Taft. "Kramers-Kronig Analysis of Reflectance Data for Diamond," Phys Rev.136, A1445-A1448 1964; MDO2019-TN005, MDO2020-TN005

Extinction by diamond and graphite

- Extinction from modified Mie model includes calculation of scattering and absorption: $Q_{ext} = Q_{sca} + Q_{abs}$
  - Diamond cloud dominated by scattering (top)
  - Graphite cloud is dominated by absorption (bottom)
- *Separation of extinction into scattering and absorption will aid in*
  - *Predicting sample quantity (per particle type) that permits through-cloud observation of discharges*
  - *Determining ambient light levels for scattering particles like diamond*
    - Scattered light can saturate image, making discharges impossible to see
    - Appropriate room light dimming for imaging of Mach disk and discharges
  - *Selecting detector types (λ) for optical diagnostics (at STOA and for fieldwork)*







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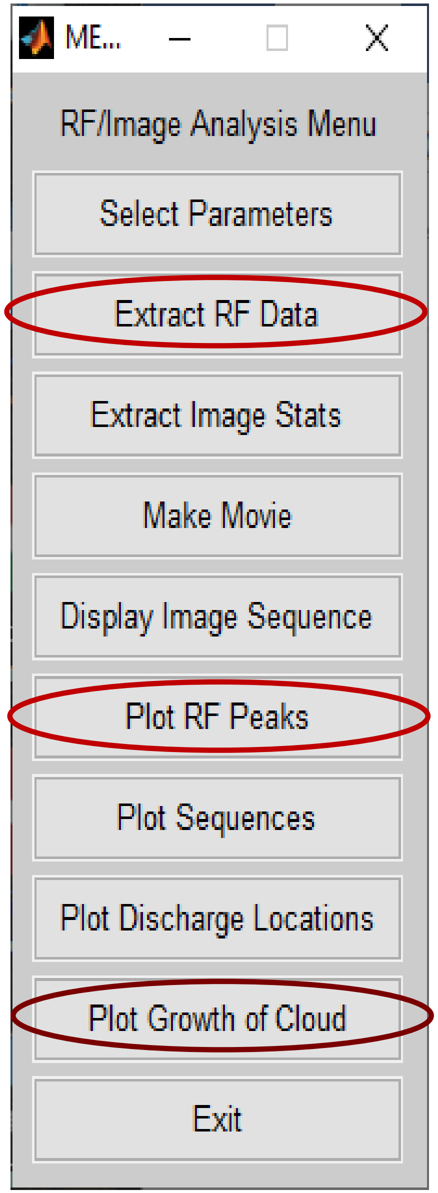
RF/Image analysis tool updates

- RF/image analysis tool updated to handle large events for SSig
  - Leverages Year 1 SDRD MATLAB code for improved image processing and data analysis
- Image analysis updated to
  - Automatically determine the appropriate scale for image axes
  - Include cloud growth analysis function



Menu Function
selectParamsR1.m - user can modify run parameters via sub menus
Extract Detections from RF data – may be csv, wfm, dig or tdms files
Extract Detections from High speed (HS) imagery
Make a movie from HS imagery
Display an image sequence
Plot individual peaks spectra and time sequence
Plot the peaks in different sequences on a single plot
Plot the discharge height and show corresponding image
Plot the cloud growth vs time using Image stats
Exit the program

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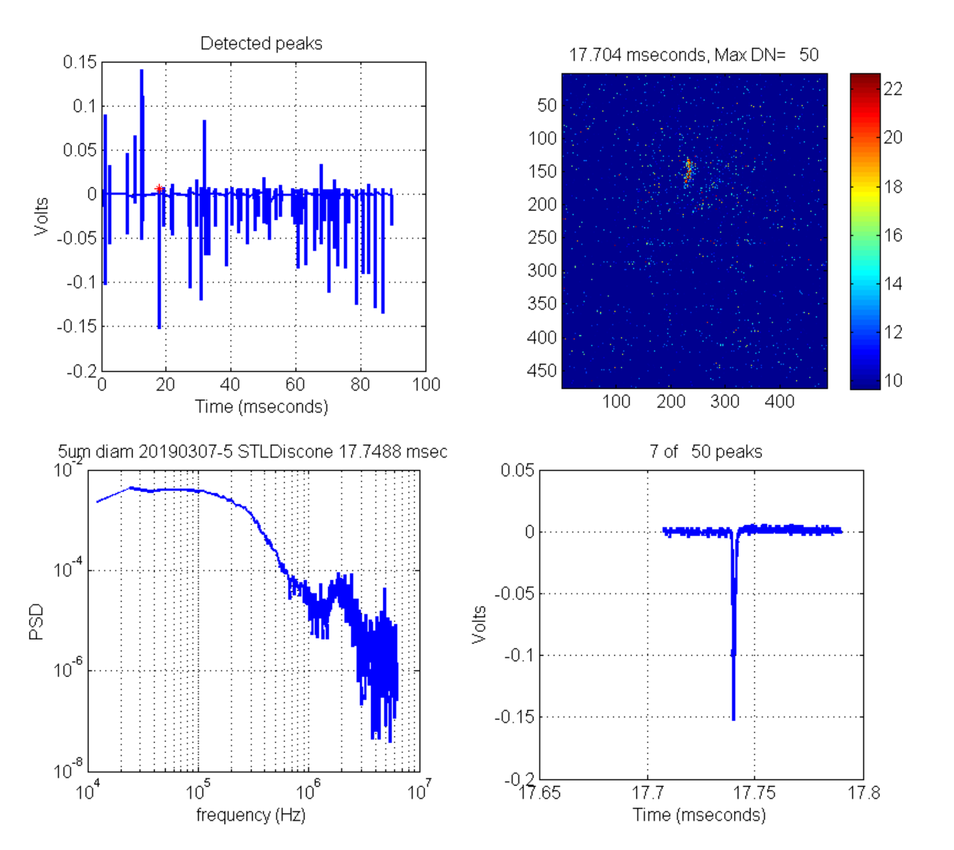
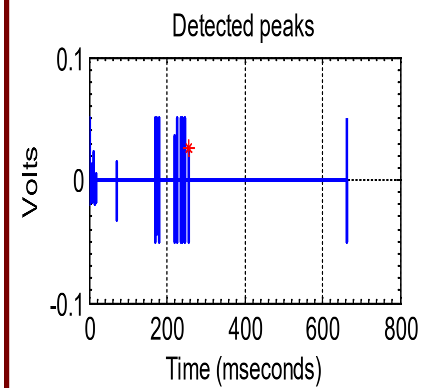
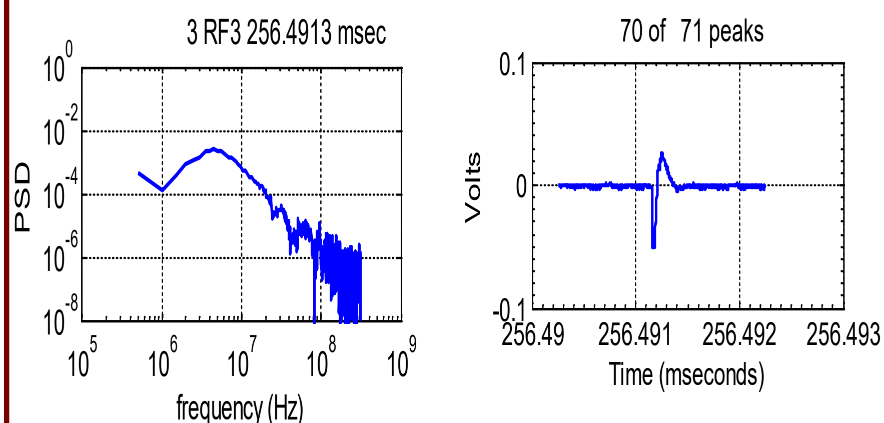
Previously presented STOA data (left) vs. recent field data (right)





No equivalent high speed image data available.
Fireball emissions dominate at early time.

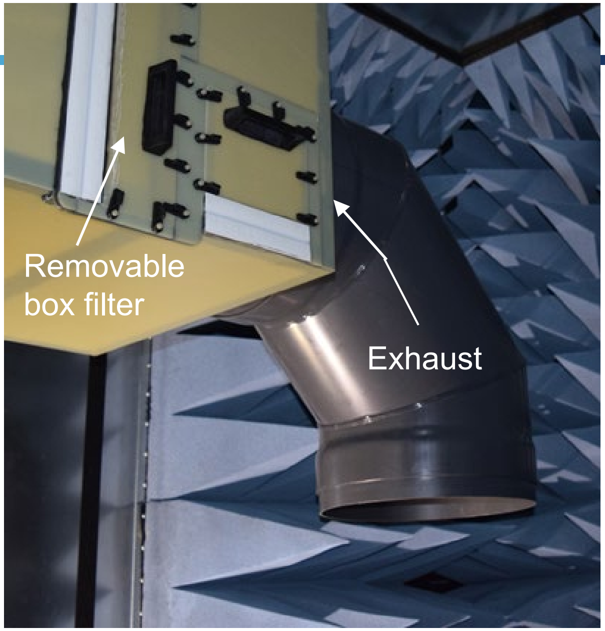


- *Significant similarities in RF output, despite field data signal amplitude being higher*
- *Field data were collected with a faster O-scope: higher frequency PSD*

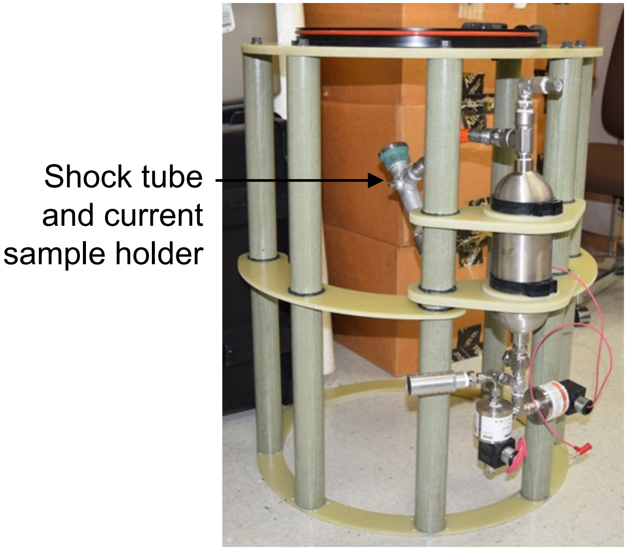
RF emissions occurring on a large scale can be mimicked on the small scale

Next Steps

- FY 2021 Q2−Q4
  - Complete STOA set-up and begin using
    - Test nozzle-based sample delivery. Iteratively revise as needed
  - Employ new diagnostics and analysis software, including 40 GHz antennas, Faraday cups and/or electrostatic separator, LWIR detectors (if indicated)
  - Perform experiments with graphitic vs. mixed diamond-graphitic detonation soots
    - Is there a distinction in RF/optical emission as a function of detonation soot type?
  - Determine scope for possible U of OR subcontract *continuation*
  - Share data with modelers



Acrylic catch tank will connect between STOA baseplate and exhaust



Summary of Results, Path Forward

- STOA Benefits
  - Large scale tests are a "black box" where RF and optical phenomena are concerned — only external observations can be made
    - STOA reproduces essential hydrodynamic and electrostatic aspects of HE test events in a well-characterized environment
    - Allows for direct comparison between modeled processes and experimental results *(not possible before)*
      - Manuscript submitted with LLNL *et al*. demonstrating consistency between experiment and hydrodynamic and electrostatic models
  - Leverage of algorithms and STOA diagnostics for large-scale tests
    - SDRD developed RF and optical analysis tools recently leveraged for analysis of large-scale test data
  - Revised STOA and diagnostics will allow for:
    - Introduction of small particle quantities in a more controlled manner and with reduced particle to wall charging
    - Better understanding of RF associated with DS, with improved diagnostics
    - Exploration of the effect of additional shock on DS particulates
    - Inclusion of particle charge measurements to support charging simulations

Questions?

Impact

- Manuscript demonstrating consistency between experiment and hydrodynamic and electrostatic models submitted with LLNL, U of FL, LMU: “Standing Shock Regulates Sparks in Explosive Flows,” J. Von der Linden, C. Kimblin, I. McKenna, et al.
- APS Conference: “Standing Shock Regulates Sparks in Explosive Flows,” APS Division of Fluid Dynamics, November 22, 2020, presentation given by J. Von der Linden
- APS Conference: “The Effect of Particles on Standing Shockwaves Regulating Spark Discharges in Volcanic Eruptions,” 61st Annual Meeting of the APS Division of Plasma Physics, October 24, 2019, presentation given by J. Von der Linden
- 2019 Fall AGU Meeting: “The Effect of Particles on Standing Shockwaves Regulating Spark Discharges in Volcanic Eruptions,” Dec. 2019, poster presented by J. Von der Linden
- New collaborations
  - Josef Dufek and Joshua Mendez-Harper (U. of OR)
- The SDRD-funded work allows us to participate in further DOE funded work