Designing Experiments for Improved Estimation of Particle Size Distributions in Ejecta Clouds

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with contributions from Aaron Luttman (NNSS), Daniel Marks (NNSS), Martin Schauer (LANL), Paul Steele (LLNL), Kasey Bray (University of Kentucky), Clayton Birchenough (Embry-Riddle Aeronautical University), and many others
The Problem with Mie:
A Daunting Story of the Mischievous Parameters

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The Nevada National Security Site (NNSS)

President Harry Truman authorized a partition of the Nellis Air Force Gunnery and Bombing Range in Nevada on December 18, 1950.

The test site is comprised of 1360 square miles.
The Nevada National Security Site (NNSS)

Atmospheric Testing

Operation Plumbbob, a 37 kiloton balloon test.

Underground Testing

Sedan, buried 625ft below ground yielded a 104 kiloton blast and moved 6.5 million cubic yards of earth and rock.

Photos courtesy of National Nuclear Security Administration / Nevada Field Office
Created in 2000, the NNSA is responsible for

- Maintaining and enhancing the safety, security, reliability and performance of the nation’s nuclear stockpile
- Preventing nuclear proliferation
- Nuclear and radiological emergency response, both in the US and abroad
- Powering the nuclear navy

We no longer engage in supercritical thermonuclear detonation, but the Stockpile Stewardship Program involves subcritical nuclear experimentation.
Programs within National Security Technologies, LLC:

- Defense Experimentation and Stockpile Stewardship
- Nuclear Operations
- Global Security
- National Center for Nuclear Security
- Environmental Management
- Site-Directed Research and Development

Cygnus radiography machine
http://nnsa.energy.gov/cygnus

Bowling ball experiment
NNSS One Voice, June 2014

Nevada Test Site Guide
http://www.nv.doe.gov/library/publications/historical/
Basic objective: To study properties of ejected particulates (ejecta) from the surface of a shocked metal.

Examples of possible ejecta
**Basic objective:** To study properties of ejected particulates (ejecta) from the surface of a shocked metal.

**Examples of possible ejecta**

- Scratch
- Grain Boundary
- Inclusion
- Void
- Metal Object
- Shock Wave
Basic objective: To study properties of ejected particulates (ejecta) from the surface of a shocked metal.

Examples of possible ejecta
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Examples of possible ejecta

Features contributing to ejecta:
1. Surface defects
2. Shock pressure
3. Temporal profile
4. Material properties
We are interested in:

1. Amount of ejecta
2. Size of ejecta
3. Velocity of ejecta

Holography can be used to quantify all three, but its size can be cumbersome to field on an experiment.

Mie scattering

- measures scattered light off of particles,
- can be used to solve for particle size distribution,
- has a much smaller footprint than holography.
Mie Scattering

A closed form solution to Maxwell’s equations exists describing light scattering off particles, assuming

- the particles are spherical,
- the particle radii are of the same order of magnitude as the wavelength of the laser light, and
- there is only single scattering.
Model

The Mie scatter model gives the scattered intensity of light as [1,2]

\[ I_s(\theta) = I_i \int_{\alpha_0}^{\alpha_1} |S(\theta, \alpha)|^2 f(\alpha) d\alpha \]

- \( I_i \) is the total light transmission,
- \( f(\alpha) \) is the continuous probability distribution for \( \alpha \),
- \( S(\theta, \alpha) \) is the scatter function,
- \( \alpha = \frac{2\pi nm}{\lambda} r \),
- \( \lambda \) is the wavelength,
- \( r \) is the particle radius, and
- \( n_m \) is the refractive index of the medium.
Model

The Mie scatter model gives the scattered intensity of light as [1,2]

\[
I_s(\theta) = I_i \int_{\alpha_0}^{\alpha_1} |S(\theta, \alpha)|^2 f(\alpha) d\alpha.
\]

We compute the scattering function \(S(\theta, \alpha)\), which is an infinite series comprised of

- spherical Bessel functions of \(\alpha\),
- spherical Hankel functions of \(\alpha\),
- Legendre polynomials in \(\cos(\theta)\), and
- derivatives of Legendre polynomials in \(\cos(\theta)\).

Literature on aerosols generally assume \(\alpha \sim \text{Lognormal}(\gamma_\alpha, \delta_\alpha)\) [6].

- \(\alpha \sim \text{Lognormal}(\gamma_\alpha, \delta_\alpha)\) is equivalent to \(r \sim \text{Lognormal}(\gamma_r, \delta_r)\)
The **discretized** Mie scatter model is given as

\[
I_s(\theta_j) = \sum_{k=1}^{K} \frac{l_i}{r_k \ln(1 + \frac{\sigma_r^2}{\mu_r^2})\sqrt{2\pi}} \left| S \left( \theta_j, \frac{2\pi n_m r_k}{\lambda} \right) \right|^2 e^{-\left[ \ln(r_k) - \ln\left( \frac{\mu_r}{\sqrt{1+\sigma_r^2/\mu_r}} \right) \right]^2 \Delta r_k},
\]

where

- \(I_s(\theta_j)\) is the scattered light at probe \(j\),
- \(l_i\) is the total light emitted through the scene,
- \(n_m\) is the complex refractive index of the medium,
- \(\lambda\) is the laser wavelength,
- \(\{\theta_j\}_{j=1}^J\) is the angle discretization,
- \(\{r_k\}_{k=1}^K\) is the discretization of the particle radii,
- \(\mu_r\) and \(\sigma_r^2\) are the mean particle radii and variance of the lognormal distribution on \(r\).
Model

The **discretized** Mie scatter model is given as

\[ I_s(\theta_j) = \sum_{k=1}^{K} \frac{I_i}{r_k \ln(1 + \frac{\sigma_r^2}{\mu_r^2}) \sqrt{2\pi}} \left| S\left(\theta_j, \frac{2\pi nm r_k}{\lambda}\right) \right|^2 e^{-\left[\ln(r_k) - \ln\left(\frac{\mu_r}{\sqrt{1 + \sigma_r^2 / \mu_r}}\right)\right]^2 \Delta r_k}, \]

where

- \( I_s(\theta_j) \) is the **scattered light** at probe \( j \),
- \( I_i \) is the **total light emitted** through the scene,
- \( n_m \) is the complex **refractive index** of the medium,
- \( \lambda \) is the **laser wavelength**,
- \( \{\theta_j\}_{j=1}^{J} \) is the **angle discretization**,
- \( \{r_k\}_{k=1}^{K} \) is the **discretization of the particle radii**,
- \( \mu_r \) and \( \sigma_r^2 \) are the **mean particle radii and variance** of the lognormal distribution on \( r \).
Project Goals

Modeling/Simulation goal:
- Determine the mean $\mu_r$ and variance $\sigma_r^2$ of the particle radii distribution from an experiment.

Experiment design goal:
- Optimize the parameters
  - Number of probes,
  - Probe locations (angles),
  - Discretization of $r$,
  - Wavelength $\lambda$, and
  - Distribution choice.

Transmission
- Data at 7.5°

Physical limitations
$\lambda$ must be on same order of magnitude as particles
Project Goals

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- Determine the mean $\mu_r$ and variance $\sigma_r^2$ of the particle radii distribution from an experiment.

Experiment design goal:
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First approach
1. Fix four of the parameters and allow the fifth one to adjust,
2. Forward model data, and
3. Study sensitivities of $\hat{\mu}_r$ and $\hat{\sigma}_r^2$. 

- Transmission
- Data at 7.5°
Number of probes

Two hundred data sets were generated with 10% added noise, $\mu_r = 2$, and $\sigma_r^2 = 2$, with $n$ linearly spaced angles between -21 and 20 degrees.

The relative percent variation from 95th percentiles are shown for $\hat{\mu}_r$ and $\hat{\sigma}_r^2$.

Reconstruction error of the mean particle radii and its variance stabilize when $|\theta| \geq 12$. 
Probe location

Determined general regions for probe location to minimize reconstruction error:

- Determine an estimate of $\mu_r$ and $\sigma_r^2$,
- Compute angle regions associated with FW10, FW5M, and FW1M,
- Choose least two angles within FW10M, two angles within FW5M, and two within FW1M$^{*†}$.

*The smaller the prior estimates of $\mu_r$, $\sigma_r^2$, the more flexibility we have in choosing angle placement.
† Requires a priori knowledge

Simulated data with $\mu_r = 2$, $\sigma_r^2 = 2$, and the full-width 10%, 5%, and 1% maximums
Relative Intensity

Raw data

<table>
<thead>
<tr>
<th>Intensity</th>
<th>Angles (degrees)</th>
</tr>
</thead>
<tbody>
<tr>
<td>3 \times 10^5</td>
<td>-20 to 20</td>
</tr>
</tbody>
</table>

Normalized data

Truth: $\mu_r = 2, \sigma_r^2 = 2$

Likelihood reconstruction maps

Truth: $\mu_r = 2, \sigma_r^2 = 2$
Future work

- Explore complementary diagnostics, including multi-wavelength extinction with a single, fixed angle but an increased number of wavelengths [5]
- Continue exploring how particle radii discretization affects reconstructions
- Remove the lognormal assumption on particle size distribution
- K2 scattering method for selection of angles and/or wavelengths as from [3]
- Apply the method from Youssef’s talk yesterday
References


