R2-A.3: A Novel Method for Evaluating the Adhesion of Explosives Residues

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II. Project Description

A. Project Overview

The goal of this project is the application of a new interpretation and modeling approach to a traditional experimental method, the centrifuge method, for measuring the adhesion of explosives residues to surfaces. The approach will yield look-up tables containing force constants for the residue-surface systems that are indexed to the particle sizes of a residue. These constants are used in a simple, closed-form algebraic model that can be evaluated on a hand-held calculator to predict the adhesion force of the residues.

Figure 1 shows the configuration of the centrifuge, with emphasis on the orientation of the residues on the surface relative to the axis of rotation. The residues adhere to the surface primarily through van der Waals forces, while the inertial force from the centrifuge's motion acts to dislodge them. By monitoring the rotational speed required to remove residues of a given size, it is possible to determine the residue adhesion force. From the adhesion force and residue size distribution, the distribution of effective Hamaker constants (the force constants in van der Waals adhesion force descriptions) of model spherical particles against a flat substrate was calculated using the well-established approximate relationship [1]:

\[ F_{vdW}(D) = \frac{A_{eff} R}{6D^2} \]  

where \( F_{vdW}(D) \) is the van der Waals adhesion force, \( A_{eff} \) denotes the Hamaker constant of the system, \( R \) is the radius of the particle, and \( D \) represents the separation distance between the two surfaces, which is generally regarded to be 0.4 nm for particles or residues in contact with a surface. Figure 2 shows how the modeling and simulation approach developed here can be used to describe the adhesion force distribution of a population of particles against a surface.
In addition to our work identifying the force of adhesion holding explosives residues to surfaces, it is necessary to understand the process by which a residue fails when a load is applied during the contact sampling process. For this purpose, we are interested in measuring and modeling the failure of composites that mimic C-4 and Semtex, which are common compounded explosives. To perform these studies, a combined Finite Volume and Discrete Element Method (FVM-DEM) framework is used. This approach uses the DEM method to track the behavior of particles in a fluid medium, and uses FVM to track the behavior of the flowing fluid.

To illustrate how this approach works, the behavior arising when a 125 μm glass particle flows through a constriction between four stationary 250 mm particles in a non-Newtonian shear thinning liquid is evalu-
ated in Figure 3. As the particle moves past the others, there is a reduction in the viscosity, which increases the velocity around the large particles. This, in turn, channels the smaller particles to move between them. Experimental work in our lab has determined that the binders in C-4 and Semtex are shear-thinning. When flow occurs, the locations in the binder where the velocity gradients are the largest will see rapid reductions in viscosity. This is shown in Figure 3. In this figure, the fluid flows from right to left. As can be seen, the viscosity of the fluid drops immediately ahead of the particle, as the fluid accelerates to pass around the particle. Similarly, after emerging from the space between the two larger particles, the fluid again accelerates into the larger space, resulting in yet another reduction in viscosity. Because the viscosity of the fluid drops with increasing shear, the viscosity drops in the regions where the fluid accelerates, as shown.

![Figure 3: Viscosity profile as a shear-thinning fluid moves from right to left around a 125 μm particle that will move between two 250 μm particles. As can be seen, the viscosity drops (blue) where the fluid accelerates around and between the particles.](image)

In Figure 4, the velocity profile corresponding to the profile in Figure 3 is shown. As can be seen, the velocity is highest where the fluid flows through the constriction, resulting in the low viscosities in this region seen in Figure 3.

![Figure 4: Velocity profile of shear-thinning fluid flowing around a 125 μm particle and between two 250 μm particles, corresponding to the viscosity profiles shown in Figure 3.](image)
The result indicates that, when a swiping load is applied to a residue of energetic material, it is likely that the material will form one or more “ribbons” of inviscid (low viscosity) binder, and large “chunks” of binder containing energetic material that are adjacent to the ribbons will move as a unit. This is shown in the top right of Figure 5. Alternatively, in the case where the adhesion between the binder and energetic material particles is the weak link in the adhesion, the failure will occur along the yellow line at the binder-particle interface (see the bottom left of Fig. 5). Finally, if the weak link in the adhesion is at the binder-surface interface, the removal will occur along the yellow line (see bottom right of Fig. 5).

Figure 5: Schematic showing possible routes of residue removal from a surface by the swab during contact sampling. Residue under load during swiping (top left). Residue under load showing ribbon (failure line) where the binder has low viscosity resulting from local fluid motion in non-Newtonian fluid (top right). Residue under load in which the binder-residue interface is the weak link in the chain, as shown by the yellow failure line (bottom left). Residue under load in which the binder-surface interface is the weak link in the chain, as shown by the yellow failure line (bottom right).

The goals of this project are to:

- Perform modeling studies to simulate the behavior of the compounded explosives residues of C-4 and Semtex, including to see if they will deform under swiping load during contact sampling.
- Validate the modeling results using live and simulated C-4 and Semtex with commercial swabs under representative swiping conditions.
- Transfer the results of this research to commercial partners who will use it to develop optimal swabs that most effectively remove residues from surfaces.

When this project succeeds, the knowledge that we generate will be used by swab manufacturers to optimize the design and application of the swabs so that they most effectively remove the residues from the surfaces of interest, facilitating the detection of explosives at checkpoints.
B. State of the Art and Technical Approach

The state of the art in contact sampling is well developed. Virtually all contact sampling protocols used in conjunction with ion mobility spectrometry (IMS) detection involve swabs made of Teflon-coated fiberglass, Nomex, paper, or muslin. These materials are provided by the manufacturers of the IMS equipment, and are designed to be compatible with a specific device. The swabs are optimized to endure repeated exposure to the thermal cycling in the IMS, but not for their effectiveness in removing residues from surfaces. The technical approach pursued here involves fundamental studies of the way that residues deform and yield under the swiping load applied during contact sampling. By developing this understanding, it is possible to elucidate how a swab must contact a residue in order to remove the maximum amount of residue from a surface. With particulate solid residues, this is relatively straightforward to understand: it is necessary to come into contact with the particles. If the adhesion force between the particles and the swab is greater than between the particle and the surface, then it will be collected. In the case of the compounded residues, the behavior is substantially more complex. Specifically, these residues will deform under the sampling load, and it is not clear where they may yield when the swab attempts to lift them from the surface. There have been virtually no studies of this phenomenon, although there has been work on the deformation of compounded, highly-filled composites, primarily for work in granular solids [2-11]. In the first part of this work, our approach is to adopt these existing methods and to understand how the residues will behave under the mechanical stresses associated with contact sampling.

In the second part of this work, we will adapt the centrifuge method to evaluate the force required to remove residues of particulate and compounded explosives from surfaces [12-18]. This method allows for the direct measurement of the force required to remove large numbers of particulate explosives, or populations of compounded explosives residues, from surfaces. When these measurements are made, we characterize the adhesion of a sufficiently large number of particles or compounded residues so that the results can be readily generalized to all systems of interest. Moreover, the measurements specifically capture the effects of the topography, shape, and deformation of the explosives particles or residues, as well as the effects of the topography and deformation of the surface to which they adhere. When the two parts of this project are combined, we obtain a comprehensive understanding of the force required to remove residues of explosives, both particulate and compounded, from surfaces, in addition to a first principles understanding of the way that the explosives deform and fail during removal. This understanding enables the development of improved residue sampling protocols and materials.

C. Major Contributions

The outcomes produced in Year 4 include:

1. A first generation model for fluid and particle motion: We finished a first generation model for the behavior of particles and fluid moving through an array of fixed particles by using particles of the same size scale as those found in energetic materials compacts and fluids with similar mechanical properties to compounded explosives.

2. A method for measuring forces required to remove residues from surfaces: We developed and validated a revolutionary interpretation of classical adhesion force measurements using the centrifuge technique. This method allows us to measure the adhesion force of a large population of residues or particles and to include the effects of the size, shape, topography, and deformation of the particles or residues, as well as the shape and deformation of the surface to which they adhere.

The outcomes produced in Year 5 include:

1. We validated the centrifuge method and create a customer-friendly code to interpret the measured adhesion force distributions and translate them into look-up tables that can be readily used
to describe residue adhesion. This is essential if the work will be translated to customers in the community.

2. We developed a fluorescent microscopy method for evaluating the removal of residues from surfaces using the centrifuge method.

The outcomes still to be attained include:

1. We must produce lookup tables for the adhesion of TNT, RDX and other model particulate explosives.
2. We must develop a first generation approach for describing the removal of compounded explosives.
3. We must extend the work to include capillary forces, in the case of particulate explosives

D. Milestones

In Year 5, we planned to address the following project milestones:

• Create a look-up table documenting the adhesion forces between particles of explosives and a range of surfaces encountered in air transportation security settings that includes both particulate explosives and compounded explosives residues.

○ Risks: The use of optical microscopy to track particles adhering to the various surfaces of interest may be challenged by the textures of the surfaces. We have a range of microscopes at our disposal that will allow us to address this problem. The removal of compounded residues will not be able to be tracked and interpreted using the same methods as for particulate explosives. Since we have determined that the mechanical properties of the binder are controlling, and not its composition, we can spike the binder with fluorescent dye and use a spectrophotometer to assess the progress of the removal.

• The Year 5 milestones were not accomplished due to the excessively strong adhesion between the explosives and the stainless steel; however, the method of measuring adhesion of the compounded explosives was developed, which is an important milestone in understanding the adhesion between the compounded explosives and various surfaces.

Expected milestones for Year 6 include:

• Measurements of the adhesion between fluorescent spheres and steel using the centrifuge method, which confirms that the method can be executed properly.

• Measurements of the adhesion between particulate explosives and steel.

• Modeling of the adhesion between the particulate explosives and the steel.

• Preparation of look-up tables demonstrating the adhesion constants that are appropriate for the steel adhesion to the particulate explosives.

• Translation of the experimental method, modeling and look-up tables to commercial partners for use in estimating explosive adhesion to surfaces.

○ Risks: The primary risk is that the explosives will adhere too strongly to the surfaces to be removed by the centrifuge method. A new centrifuge with an expanded operating range compared to our existing centrifuge has been purchased. This should allow adhesion forces to be measured over a wide range of forces. The next risk is the challenge of the contrast between the explosive residues and the surfaces onto which the residues adhere. We have a wide range of light microscopy methods available for overcoming this challenge.
E. Future Plans (Year 6)

Year 6 will focus on transition. We will build look up tables of the adhesion of particulate explosives against steel, a representative surface of interest to the air transportation community. We will also hold a workshop at Purdue to teach the community how to execute the method. We will perform Generation 1 experiments and modeling of the removal behavior of compounded explosives from surfaces. Such removal will be driven by deformation in the residue, not by failure at the interface between the residue and the surface onto which it adheres.

III. RELEVANCE AND TRANSITION

A. Relevance of Research to the DHS Enterprise

The new centrifuge method provides a direct measurement of what is required for a trap to remove residues from specific surfaces. The development of new traps with a superior ability to harvest explosive residues requires that the process for removing a residue be understood.

1. Metric 1: New traps will be developed with improved configurations to more effectively remove residues from surfaces. The improved configurations will be based upon the results of this work.

2. Metric 2: New methods will be developed for using traps to more effectively remove residues from surfaces. The improved methods will be based upon the results of this work.

B. Potential for Transition

The purpose of this work is to develop essential understanding that does not currently exist on the way that residues deform and fail when under a swiping load. This knowledge will enable the fabrication of improved swabs and swabbing protocols. In this context, the transition is the dissemination of the knowledge to the community via teleconferences and workshops. This includes disseminating the understanding of the energetics removal and also disseminating the method and the code used to interpret the data.

C. Data and/or IP Acquisition Strategy

Not applicable.

D. Transition Pathway

Technical results documenting how residues deform and fail under sampling load will be transitioned to the community via teleconferences and workshops, including the Trace Explosives Detection workshop in April 2019. We also hope to host at least one workshop at Purdue to teach members of the community the methods we use to make the measurements.

E. Customer Connections

We will conduct quarterly teleconferences with the following:

- Erin Tamargo, CTTSO/TSWG
- Richard Lareau, TSL
- Kerin Gregory, 908 Devices
- Cindy Carey, Bruker
IV. PROJECT ACCOMPLISHMENTS AND DOCUMENTATION

A. Education and Workforce Development Activities

1. Student Internship, Job, and/or Research Opportunities
   a. Trained two domestic PhD students, one MS student, and three domestic undergraduate students on this project.

B. Peer Reviewed Journal Articles


C. Software Developed

1. Models
   a. Model for describing adhesion distribution of powders on a surface using idealized van der Waals forces.

V. REFERENCES


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