Characterizing Impact Induced Hot-Spot Morphology in Granular Solid Explosive

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CHARACTERIZING IMPACT INDUCED HOT-SPOT MORPHOLOGY IN GRANULAR SOLID EXPLOSIVE

A Thesis

Submitted to the Graduate Faculty of the Louisiana State University and Agricultural and Mechanical College in partial fulfillment of the requirements for the degree of
Master of Science in

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Abstract

Deformation induced ignition of heterogeneous solid explosives is believed to originate at hot-spots within the material which are local regions of elevated temperature resulting from dissipative mechanisms such as plastic deformation and inter-particle friction. Inert meso-scale modeling of these materials can principally account for hot-spot formation enabling the characterization of hot-spot size and temperature distributions which are important for ignition but are difficult to experimentally resolve.

The focus of this study is to characterize hot-spot morphology, as well as the distribution of hot-spots, behind quasi-steady compaction waves computed from predicted temperature fields resulting from numerical simulations of rigid planar piston impact on randomly packed, granular HMX ($C_4H_8N_8O_8$). Hot-spots are analyzed from the inert heating predictions of four meso-structures, composed of hexagonal and/or circular shaped particles having average initial solid volume fractions, $\bar{\phi}_{s,0}$, in the range $0.57 \leq \bar{\phi}_{s,0} \leq 0.84$. Predictions indicate that hot-spot temperature distributions are largely insensitive to changes in piston speed, $U_p$, or $\bar{\phi}_{s,0}$ over the ranges $300 \leq U_p \leq 500$ m/s. Higher $U_p$ and lower $\bar{\phi}_{s,0}$ resulted in larger hot-spot sizes. Hot-spot number density, volume fraction, and specific surface area, were shown to be sensitive to variations in $\bar{\phi}_{s,0}$ and are predicted to grow exponentially with piston speed over the ranges considered in this study.

Combustion implications are examined by combining inert heating predictions for uniaxial waves with thermal explosion data and analysis to estimate ignition time distributions and local fractions of ignited mass. These are important first steps in establishing a general statistical theory for early time ignition in heterogeneous solid explosives. Preliminary results indicate number density and size of hot-spots are the major factors which influence the impact and shock sensitivity of these materials over the range of impact speeds considered.
Chapter 1
Introduction

Solid high explosives (HEs) belong to the class of combustibles known as energetic materials, and are often employed in defense, demolition, and mining applications. Early HEs used in munitions were less safe to work with because of their sensitivity to heat, impact, and other conditions [44]. Less sensitive explosive materials have since been developed, such as cyclotrimethylene-trinitramine (RDX, $C_3H_6N_6O_6$) and cyclotetramethylene-tetranitramine (HMX, $C_4H_8N_8O_8$), and are commonly manufactured by either pressing explosive crystals into high-density, granular powder compacts, or are often times mixed with metal grains and a polymer binder to produce a polymer-bonded explosive (PBX).

These materials are highly heterogeneous, containing multiple phases, inter- and intra-particle porosity, surface asperities, and other irregularities which affect how the explosive behaves when shocked. Ignition in these materials occurs at localized regions of elevated temperature called “hot-spots,” which result from shock interactions with the material inhomogeneities. Hot-spots form from a number of different phenomena, such as void collapse, plastic deformation, frictional sliding, and micro-jetting, and those with size and intensity sufficient enough to overcome thermal quenching will ignite and begin to consume the surrounding material. If conditions are favorable, the growth and coalescence of hot-spots can ultimately lead to detonation of the material. A detonation wave is a self-sustaining, reactive wave which propagates through the material at supersonic velocities (typically between 3 - 9 km/s). Relatively insensitive HEs like HMX have been observed to undergo a deflagration-to-detonation (DDT) transition under the proper confinement conditions when subjected to piston impact speeds as low as 100 m/s, raising concerns of safety and payload survivability, and prompting an effort to understand DDT in these materials [37].
In this study, a methodology is proposed for characterizing the morphology of hot-spots in granular explosives using inert temperature field predictions. A comprehensive set of statistics is constructed to investigate the influence of wave strength, initial particle packing density, and particle shape on the distribution of hot-spots formed behind quasi-steady compaction waves in granular HMX. Here, quasi-steady refers to a wave’s average velocity and strength and not its structure, which continues to fluctuates locally. Lastly, the combustion implications are examined by applying thermal explosion analysis to estimate fractions of reactive mass and associated ignition time distributions.

In the remainder of this chapter, a brief literature review is provided, the motivation for this study is discussed, and the model problem considered in this study is summarized. Lastly, the goals of this study are specified and an outline of this thesis is given.

1.1 Background and Motivation

A large body of experimental and computational work is devoted to investigating and understanding the shock sensitivity of solid high explosives. In this section we summarize work particularly relevant to this study and highlight motivations for this research.

1.1.1 Experimental

Shock sensitivity is often measured by a gap test, in which a standard donor explosive produces a shock pressure of uniform magnitude which is transmitted to the test explosive through an attenuating inert barrier or gap [11]. By varying the thickness of the barrier between the donor and test explosives, one can determine the barrier thickness required to inhibit detonation in the test explosive. Gas gun and laser driven flyers are also commonly used to shock load high explosives by firing a high-speed projectile directly into a small sample of explosive material and recording the response. Impact sensitivity tests, such as drop weight and skid tests, measure explosive response to mild impact events. Drop weight tests are performed by dropping a fixed weight onto a prepared sample of the explosive to be tested from a given distance. Skid tests, sometimes called the oblique impact test, simulate a bare explosive charge accidentally hitting a rigid surface at an oblique angle
during handling. Vigorous combustion of the explosive material is observed in both impact sensitivity tests and shock sensitivity tests; however, shock sensitivity tests are generally accompanied by a clear transition to detonation.

There is a large research effort devoted to better understanding the relationship between particular features of the material meso-structure, such as particle size and shape, inter-particle pore size, and particle surface roughness, and the observed shock and impact sensitivity response of the material. Numerous studies into the effect of particle size on the mechanical sensitivity of explosives show that fine grained explosive is less sensitive at lower pressures and more sensitive at higher pressures ([35],[36],[38]), and is believed to be related to the size and number density of hot-spots. In addition, particle size was shown to influence rise time of the shock and compaction wave thicknesses [37].

Borne et al. [5] examined the role of various kinds of pores on the shock sensitivity of pressed formulations of reduced sensitivity RDX (RS-RDX). In their study, the inter-particle pores (pores in the binder material or pores at the interface of RDX particles and binder) had a limited influence on the shock sensitivity, while intra-particle pores (pores inside the RDX particles) where shown to be important in establishing shock sensitivity. Conversely, in shock sensitivity studies of granular HMX, Czerski and Proud [9] found intra-particle void count to be uncorrelated with sensitivity. The inclusion of binder in polymer bonded explosives (PBXs) serves to homogenize the stress field and enhance the significance of intra-particle pores on the shock sensitivity in these materials.

Czerski and Proud [9] investigated the influence of crystal morphology on the shock sensitivity of granular RDX using gap tests. Their results revealed shock sensitivity was correlated with more angular crystals for particles 100 - 200 μm in size, whereas sensitivity in particles 10 - 30 μm in size correlated with the surface roughness of the particles. Czerski and Proud postulated that viscoplastic work at particle contacts is the most dominate energy localization mechanism for 100 - 200 μm sized material, and suggested jetting from surface dimples as a likely factor influencing the sensitivity of the 10 - 30 μm sized...
Bellitto and Melnik [4] observed that the shock sensitivity of RDX based PBX samples correlated, not with the average surface roughness of the material, but rather the consistency of surface roughness across the particle surface.

Understanding the details of how a shock interacts with these features to form hot-spots and transition to detonation are difficult, if not impossible, to determine experimentally at this time. Therefore, experimental investigations of shock initiation must be supplemented by computational modeling.

1.1.2 Computational

Many computational models have been developed to model shock initiation and failure phenomena in heterogeneous solid explosives by integrating a description, either implicitly or explicitly, of hot-spot formation and growth. Broadly speaking, these models can be categorized as either empirical or mechanistic.

Forest Fire [24], Ignition and Growth [22], and Johnson-Tang-Forest (JTF) [19] are common empirical models that have been successfully used to describe initiation and failure phenomena in large-scale code calculations. These models make no distinction in hot-spot origin. Instead, they assume a small amount of explosive is ignited by the passage of the shock wave, initiating reaction in the remaining material. Ignition and Growth, for example, uses a pressure dependent burn rate to describe the reaction process, achieving good qualitative agreement with manganin pressure gauge data and correlating well with experimentally observed run distances to detonation. These models make extensive use of experimental data to parameterize the reaction rate equations, however, for different initial conditions they must be re-parameterized.

Mechanistic models are based on a micromechanical description of the various phenomena occurring during shock propagation in the explosive and interactions with inhomogeneities. Bowden and Yoffe [6] were the first to show that the rapid compression of a gas filled void entrained in an otherwise homogeneous energetic material could lead to ignition. Mader [23] constructed a two-dimensional hydrodynamic code to model the process
of hot-spot formation and shock initiation due to shock interaction with a void contained in a cylinder of nitromethane. Khasainov et al. [20] were the first to develop a viscoplastic pore collapse model and apply it to hot spot formation resulting from shock propagation in heterogeneous explosives, demonstrating that viscoplastic effects were a potential ignition source. In addition to modeling the dynamics of pore collapse, the model of Kang et al. [19] included processes such as visoplastic heating, finite chemical effects, and heat exchange between the pore gas and surrounding material. The results showed viscoplastic heating to be an effective mechanism for shock initiation of porous, energetic materials, and demonstrated that the initial porosity of the material and the initial pore size strongly influence hot spot formation. Massoni, et al. [27], introduced a mechanistic model which takes into account both the microscopic phenomena of hot-spot formation due to visoplastic pore collapse, and the coupling of these effects with macroscopic waves propagations to predict DDT in pressed solid explosives. Nichols and Tarver [18] likewise considered pore collapse as a dominate formation mechanism, and introduced a statistical hot-spot reactive flow model which considers a distribution of outwardly burning, spherically shaped hot-spots, with an initial hot-spot volume equal to the initial pore volume.

Mechanisms other than viscoplastic pore collapse, such as friction and shear banding, have been investigated as potential sources of ignition as well. Frey [10], Grady and Kipp [14], and Kipp [21], have developed two-step models based on shear banding. In these models, the local temperature increase results from viscoplastic heating generated by localized deformations around discontinuities in the material.

It is unlikely that a single localization mechanism will play the dominate role over the entire spectrum of loading conditions. In addition, numerical simulations of heterogeneous solid explosive at the meso-scale [32] reveal significant fluctuations in the stress and temperature fields, giving rise to far more complex and varied hot-spot morphologies than the simple spherical ones assumed in many of these earlier models. A more recent study has been proposed by Horie and Hamate [17], which attempts to incorporate the wide variety
of hot-spot formation mechanisms into a general framework for modeling shock initiation of heterogeneous solid explosives by coupling a statistical hot-spot model with hydrodynamic flow equations. The model aggregates hot-spot surfaces formed in a representative volume element through void collapse, shear banding, and friction into a thin layer of reactive hot-spot material. Though promising, the model assumes an exponential distribution of hot-spot sizes based on observations of the distribution of contact forces in granular media [41], which may or may not be an accurate description. In addition, Hamate and Horie note, as others have, of the need for informed hot-spot temperature distributions to improve upon current model predictions; however, it remains fundamentally unclear how meso-structure (particle size and shape, packing, porosity, defects, etc.), component thermomechanical properties, and metal and binder mass fractions, affect impact induced heating of the high-explosive component which establishes their impact sensitivity and survivability.

Inert meso-scale modeling of these materials can principally account for hot-spot formation, enabling spatial and temporal characterization of hot-spot size and temperature distributions that are important for ignition but are difficult to experimentally resolve ([1],[3],[32]). Current models predict highly fluctuating stress fields and energy localization due to the effects of shocks interacting with individual material surfaces and contact points. Ultimately, the goal of these models is to quantify localization effects and their relationship to microstructural features. This requires comprehensive knowledge about the distribution of hot-spots formed in the material. Previous attempts at characterizing hot-spots from meso-scale predictions have met with limited success ([2],[32]) and have not, as of yet, attempted to correlate microstructural features with a statistical description of hot-spot morphology.

1.2 Problem Description

The primary focus of this study is to characterize hot-spot morphology as well as the distribution of hot-spots behind quasi-steady compaction waves computed from pre-
dicted temperature fields resulting from the numerically simulated inert impact of randomly packed, granular HMX, illustrated in Fig. 1.1. Here, morphology collectively refers to the geometrical characteristics of a hot-spot, such as its size and shape, as well as other features, such as temperature and proximity to nearby hot-spots. In these simulations, a rigid planar piston impacts the material with constant speed, $v_p$, driving the propagation of a uniaxial deformation wave through the material. The computational domain is of sufficient length to allow a quasi-steady wave to develop. Because particle motion is restricted to the plane, these computations will likely result in slightly higher wave speeds and stresses than real systems, particularly for mild impact.

Figure 1.1: Computational domain and boundary conditions for a representative meso-scale simulation. The average particle diameter is $\bar{d} \sim 60 \, \mu m$ and the average initial solid volume fraction is $\bar{\phi}_{s,0} = 0.835$ [32].

The meso-scale model initially developed by Panchadhara and Gonthier [32] uses an explicit combined discrete element-finite element method and incorporates a penalty based contact algorithm for interparticle penetration. A finite deformation hyperthermoelastic-viscoplastic constitutive theory is used to model the stress response of the material, and frictional contact between particles is estimated using a stick-slip (Coulomb law) model. A pseudo gravity settling algorithm is used to seed the computational domain with approximately 4000 particles having an average size (radius) of 30 $\mu m$, and between 300 - 400 finite elements per particle. At this time, the simulations are inert, and do not model phase change or fracture of the explosive particles, focusing instead on characterizing the relative importance of volumetric and frictional work in these granular systems.
Figure 1.2: Meso-scale predictions for (a) wave speed as a function of piston speed, and (b) pressure as a function of piston speed. Meso-scale predictions are represented by solid curves and agree well with experiments for $\phi_s = 0.678$ ([25],[33]).

Figure 1.2 shows the predicted Hugoniots for granular HMX with initial solid volume fractions of $\phi_{s,0} = 0.577, 0.678, 0.768, \text{ and } 0.835$. Good agreement is achieved between the model predictions and the experimental results of Sheffield [37] for $\phi_{s,0} = 0.678$. At piston impact speeds $< 300 \text{ m/s}$, the granular bed is “frictionally rigid”, retaining some small amount of porosity after compaction. For impact speeds above 300 m/s, there is a linear relationship between piston speed and wave speed, and all the porosity in the system is removed by the wave. Observations of mass specific energy dissipation indicate mass specific friction work is more significant for mild impact, while mass specific plastic work plays the dominate role for strong impact.

Figure 1.3 shows contours of Von Mises stress predicted by the meso-scale model for three piston impact speeds. Heterogeneity in the meso-structure gives rise to pronounced stress chains at 50 m/s impact and serves to highlight the complex response of these multi-body systems to impact. Figure 1.4(a) gives predicted temperature fields within granular HMX immediately behind a uniaxial wave that is supported by a $U_p = 500 \text{ m/s}$ piston; Figure 1.4(b) gives the predicted temperature rise due to plastic work alone. The predicted temperature rise is due to dissipative heating by plastic and friction work, with compression
Figure 1.3: Contours of Von Mises stress for 50 m/s, 250 m/s, and 500 m/s piston impact speeds [32].

Figure 1.4: Predicted temperature field behind a uniaxial wave for $U_p = 500$ m/s: (a) net temperature rise; (b) temperature rise due to plastic work [32].
Figure 1.5: Ignition evolution begins with the local ignition of hot-spots, followed by hot-spot growth and coalescence which gives rise to an observable ignition event; however, not all observable events need be followed by transition to detonation.

work being largely inconsequential. The most intense heating is predicted to occur in the vicinity of interparticle contacts. Because the thermal conductivity of HMX is low, these predictions are effectively adiabatic.

A significant amount of prior work has been focused on investigating potential hot-spot formation mechanisms, but very little progress has been made to characterize the statistical nature of hot-spots, which may be used to better understand the processes associated with the ignition and growth of reaction. To this end, we mechanistically describe ignition as consisting of two sequential steps, as illustrated in Fig. 1.5: 1) local ignition of thermally isolated hot-spots within the high-explosive component followed by 2) hot-spot growth, coalescence, and flame spread that gives rise to a measurable global ignition event at the macro-scale. Subsequent transition to detonation may occur depending on the degree of material confinement.

Inert meso-scale modeling predictions contain a significant amount of statistical information about the distribution of hot-spots formed in the material. Data-mining meso-scale modeling predictions to obtain hot-spot distributions, which is non-trivial, can lead to the development of macro-scale models which better predict shock initiation of heterogeneous solid explosives. For example, the Ignition and Growth model incorporates a pressure
dependent burn rate model given by

\[
\frac{\partial F}{\partial t} = I (1 - F)^x \eta^r + G (1 - F)^y p^z, \quad (1.1)
\]

\[
\eta = V_o/V_1 - 1, \quad (1.2)
\]

to describe the reaction process. Here \( F \) is the fraction of explosive that has reacted, \( t \) is time, \( V_o \) is the initial specific volume of the explosive, \( V_1 \) is the specific volume of the shocked, unreacted explosive, \( p \) is pressure, and \( I, x, r, G, y, \) and \( z \) are constants. The first term in Eq.(1.1) represents the burning of a small amount of explosive material assumed to have been initially ignited by the passage of the shock wave. The second term in this equation describes the subsequent growth of reaction and contains a constant \( G \), which corresponds to an ignited surface area to volume ratio. These quantities are typically parameterized using experimental data, but may, in principle, be estimated from hot-spot size distributions computed directly from meso-scale predictions. In the statistical model introduced by Horie and Hamate [17], the distribution of hot-spot surface areas throughout the material is assumed to be exponential, and is given by

\[
F_A = \frac{a_{tot}}{\xi} \left( 1 - \alpha \exp \left( -\xi \frac{\epsilon_d}{\epsilon_d^o} \right) \right), \quad (1.3)
\]

where \( F_A \) is the total hot-spot surface, \( \epsilon_d \) is the specific dissipated energy, and \( a_{tot} = F_A(\epsilon_d^o) \) is the incipient reaction area. Other parameters are related by

\[
\xi = 1 - \alpha \exp(-\xi) \quad (1.4)
\]

\[
\frac{a_{tot}}{\xi} (1 - \alpha) = a_o = F_A(\epsilon_d = 0) \quad (1.5)
\]

As previously mentioned, the assumption of an exponential distribution of hot-spot surface areas is based on observations of the distribution of contact forces in granular media [41]. This assumption can be validated through analysis of inert temperature field predictions.
Because inert simulations do not describe the multi-phase physics leading to global ignition, we focus primarily on features relevant to local ignition that are stochastic due to particle-scale variations in material meso-structure and composition, and are difficult to measure. A local ignition analysis is important because it establishes lower-bound impact thresholds needed for global ignition, and it can identify the fraction of ignited mass that partially determines global ignition times. Within the context of this work, it is noted that global ignition does not necessarily imply transition to detonation; rather, it only implies a measurable combustion event.

1.3 Objectives of This Study

The primary objective of this study is to formulate a methodology for characterizing hot-spots that can be used to examine the influence of meso-structure on impact induced heating of solid high-explosive. In this study, we are primarily interested in describing hot-spots formed by plastic and friction work behind quasi-steady compaction waves in granular HEs, though the approach is applicable to hot-spots created by other localization mechanisms, in both granular and polymer-bonded systems. Analysis of granular systems is important in establishing baseline predictions. The method uses standard image processing techniques to identify and quantify hot-spots and their corresponding features from digital renderings of temperature fields predicted by inert meso-scale modeling which has not been considered by others. Specific objectives of this work are:

1. Present a methodology for quantitatively characterizing hot-spot morphology (intensity, size, shape, and proximity) based on inert meso-scale temperature field predictions.

A fundamental understanding of the early time ignition response of these materials rests on the ability to characterize, quantitatively, the morphology of hot-spots and their dependence on initial meso-structure. Ignition in hot-spots depends on a balance between energy generated by the reaction process, and energy lost to the surrounding environment through heat transfer. Hot-spot size, shape, and intensity are important
in establishing these critical conditions for local ignition [39]. The proximity of hot-spots is important in establishing the rate of hot-spot coalescence and growth, which is believed to be necessary for a transition to detonation. In addition, Objective 1 can provide meso-scale justification for many of the parameters used in shock ignition and growth models, such as hot-spot size and temperature distributions, number density, and reactive surface-to-volume ratio, aiding in the development of better macro-scale models.

2. *Investigate the influence of wave strength, packing density, and particle shape on the distribution of hot-spots formed by quasi-steady compaction waves in granular HMX.*

This objective promotes a more sophisticated understanding of the connection between local non-uniformities within the material and the mechanisms of hot-spot formation that are difficult to realize experimentally. This study intends to provide information on the correlation between characteristics of the undeformed material and the statistical nature of hot-spots.

3. *Investigate the ignition implications of inert heating predictions.*

Inert heating predictions can be combined with thermal explosion analysis ([16],[39]) to provide estimates for the fraction of locally reactive mass and the associated ignition time distribution. These are important first steps in establishing a general statistical theory for ignition, based on an approach formulated by Terao [40] to model shock induced ignition in reactive gases.

An outline of the remainder of the paper is as follows: Chapter 2 contains a summary of the constitutive equations and boundary conditions for the meso-scale model, developed by Panchadhara and Gonthier [32], and used in this study. In addition, the methods for hot-spot identification and feature quantification are posed, and a general approach is proposed for estimating hot-spot ignition time distributions and ignited mass fractions from the joint distribution of hot-spot size and temperature. The chapter concludes with
a discussion of the image processing algorithms used to compute hot-spot morphological features. Chapter 3 presents results for predicted hot-spot morphological distributions, and investigates the sensitivity of these distributions to impact speed, initial porosity, and initial particle shape, as well as the parameter used to identify with hot-spots. Conclusions and recommendations for future work are given in Chapter 4.
Chapter 2
Computational Technique

In this chapter, we first briefly summarize the mathematical model and numerical technique used to obtain meso-scale predictions for the inert temperature fields analyzed in this study. Next, a discussion of random heterogeneous materials is given, followed by a description of the technique used to select potential hot-spot material directly from the predicted temperature fields. After establishing the definition of a “hot-spot”, the quantities used in this study to characterize their morphology and statistics are defined and discussed. Following that, we introduce an approach for identifying chemically significant hot-spots and estimating ignition time distributions by combining joint distributions of hot-spot intensity and size with thermal explosion analysis. Explosion time distributions can be used to facilitate the development of statistical tools to estimate the relative shock sensitivity of different materials. Finally, the basic digital image processing techniques used to evaluate hot-spot features from digitized temperature fields are summarized.

2.1 Meso-scale Model

Multi-body contact induced by dynamic deformation is posed as a coupled initial-boundary-value problem (IBVP) for the displacement field $u$ and temperature field $T$ within particles. These fields are described by the following momentum and energy evolution equations within each particle:

$$\rho \ddot{u} = \nabla \cdot \sigma,$$

$$\rho c_v \dot{T} = -\nabla \cdot q + \rho r.$$  

Here, $\rho$ is the local mass density, $\sigma$ is the Cauchy stress tensor, $r$ is the deformation induced heating, $q$ is the heat flux, $c_v$ is the specific heat at constant volume, and $\nabla \equiv \partial(\cdot)/\partial x$ is the spatial gradient operator. Body forces are ignored in these equations as
they are inconsequential compared to impact induced deformation forces. All particles are initially stationary, stress free, and at a uniform ambient temperature of 300 K. Only contact boundary conditions are imposed on the displacement and temperature fields of the particles:

\[ \sigma \cdot n = t_c \text{ on } \Gamma \forall t, \]  
\[ (-k_T \nabla T) \cdot n = q_f + q_c \text{ on } \Gamma \forall t, \]  

where \( \Gamma \) is the particle boundary, \( n \) is the unit normal to \( \Gamma \), \( t_c \) is the contact traction, \( k_T \) is the thermal conductivity, \( q_f \) is the heat flux due to frictional heating, \( q_c \) is the heat flux necessary to impose ideal thermal contact, and \( t \) is time. The system of equations is closed by prescribing a constitutive theory for the stress response. To this end, a hyper-elastic, multiplicative, finite strain constitutive theory is used to model stress-strain behavior. A Perzyna over-stress model, coupled with an associative flow rule and a Von-Mises type yield criterion with isotropic hardening, are used to prescribe the evolution of inelastic strain. Material properties used in this study are chosen to be representative of the secondary high explosive HMX. Details about the mathematical model and constitutive theory can be found in Ref. [32].

Computations are performed using a combined finite and discrete element method that is well-suited for problems involving heterogeneity. This combined method uses the finite-element method (FEM), coupled with a radial return stress update algorithm, to numerically integrate the time-dependent, 2-D conservation principles and viscoplastic flow rule governing deformation of individual particles, and uses the discrete-element method (DEM) to account for interactions between particles. The DEM is based on a distributed, conservative potential based penalty method whereby the normal contact traction between particles is estimated by penalizing their penetration, and frictional tractions are estimated using a penalty regularized Amonton’s Coulomb law. Particles are discretized using con-
stant strain, triangular finite elements, where each particle consists of 400-800 elements for all computations performed in this study. A temporally second-order accurate, explicit numerical technique is used to integrate the finite element equations for nodal displacements and temperatures. For these computations, hot-spot size is limited to the size of a single finite element, \( \approx 0.1\% \) the size of an average particle. Additional details about the numerical technique can be found in Ref. [31].

2.2 Hot-Spot Characterization

The production of solid explosives introduces a degree of randomness into the material. In most instances, a statistical description is the only means of characterizing the microstructural features of these materials, which may be classified as random heterogeneous materials. A random heterogeneous material rests on the assumption that any sample of the medium is a realization of a specific random or stochastic process. An ensemble is a collection of all the possible realizations of a random medium generated by a specific stochastic process. Details on the characterization of heterogeneous materials can be found in Ref. [42].

Following the terminology of set theory, let \( \Omega \) be the outcome space corresponding a material’s ensemble, and \( \omega \in \Omega \) be the event corresponding to a single realization of that material occupying some space \( \mathcal{V}(t) \in \mathbb{R}^3 \). Because this study analyzes 2-D temperature fields, the approach presented herein will be restricted to \( \mathbb{R}^2 \), though extension to \( \mathbb{R}^3 \) is straightforward.

In this study, we are interested in identifying hot-spots resulting from planar piston impact through the use of inert temperature field predictions, which are sensitive to features of the microstructure. The temperature field, \( T(x, t; \omega, U_p) \), resulting from deformation induced heating for a given material realization \( \omega \) and a given piston speed \( U_p \) will in general depend upon the position vector \( x \in \mathcal{A} \) and time \( t \), where \( \mathcal{A} \) is the computational domain.
Figure 2.1: (a) Temperature field resulting from a 500 m/s piston impact. (b) Temperature distribution extracted from points along the section line in (a). Potential hot-spot material is identified as any material above a predetermined $T_{th}$, illustrated above.

Hot-spot material is selected by performing a level-cut through the predicted temperature fields, $T(x, t)$, at a predefined threshold temperature, $T_{th}$, where the parametric dependence $\omega$ and $U_p$ has been omitted for clarity. In what follows, the term *hot-spot* will refer to any material existing above the predetermined temperature threshold, $T_{th}$, while the term *critical hot-spot* is reserved for material actively participating in early time ignition, a distinction which will be discussed in greater detail in Section 2.4.

The resulting level-cut, illustrated in Fig. 2.1, produces a *hot-spot temperature field*, shown in Fig. 2.2, which contains $N$ hot-spots, $\hat{A}^1(x, t), \hat{A}^2(x, t), \ldots, \hat{A}^N(x, t)$, enclosed by contours $\Gamma^1(x, t), \Gamma^2(x, t), \ldots, \Gamma^N(x, t)$. This thresholding partitions the domain $A(x, t)$, into two disjoint sets, $A_{HS}(x, t)$ and $\overline{A_{HS}(x, t)}$, such that

$$A_{HS}(x, t) \cup \overline{A_{HS}(x, t)} = A(x, t)$$  \hspace{1cm} (2.5)

and

$$A_{HS}(x, t) \cap \overline{A_{HS}(x, t)} = \emptyset,$$ \hspace{1cm} (2.6)
Figure 2.2: Hot-spot temperature field generated in a small region behind a quasi-steady wave corresponding to $U_p = 500$ m/s and $T_{th} = 500 K$. Hot-spots are indicated by the shaded regions. The appearance of finite element sized hot-spots and jagged boundaries is the result of resolution limitations.

where

$$A_{HS}(x, t) = \hat{A}^1(x, t) \cup \hat{A}^2(x, t) \cup \ldots \cup \hat{A}^N(x, t).$$

(2.7)

The region $A_{HS}(x, t)$ contains the total amount of hot-spot material in $A(x, t)$ for a given material realization and piston speed, while the region $\overline{A_{HS}}(x, t)$ contains lower temperature material. Such an approach filters out cooler material, allowing for a quantitative description of hot-spot characteristics. It should be noted that the morphology of hot-spots in the domain is sensitive to the numerical resolution of the meso-scale simulations, as well as the choice of $T_{th}$. The resolution limitation is is evident in Fig. 2.2. In many cases, hot-spots at particle interfaces are not well resolved, and size predictions must be carefully interpreted. A discussion on the sensitivity of these features to threshold temperature is given in Chapter 3.
A complete statistical description of the hot-spot morphology in these systems requires that we analyze the hot-spot temperature field for every realization $\omega \in \Omega$ and average over all possible realizations. This is not possible in practice, and so we make an assumption of ergodicity. That is, averaging over all realizations in the ensemble is equivalent to averaging over the volume of a single realization in the infinite volume limit [42]. Though computational domains used in this study are not infinite, they are large enough so that the ergodic assumption remains a reasonable approximation, and the hot-spot temperature fields are independent of $\omega$.

In the remainder of the chapter we define quantities used in this study to describe hot-spot morphology which are important in the ignition stage of impact and shock induced combustion. This is followed by a discussion on integrated hot-spot quantities and hot-spot proximity which are important to the growth and coalescence of hot-spots. Next, we introduce the concept of a critical hot-spot and discuss their importance. Lastly, we discuss the image processing tools used to perform analysis of hot-spot temperature fields.

2.3 Hot-Spot Morphology

Hot-spot intensity, size, surface area, and shape are collectively referred to in this study as hot-spot morphology. These features are likely to be most sensitive to variations in microstructure, and are therefore useful from a modeling perspective. For example, numerical studies on spherical interparticle void collapse as an energy localization mechanism have shown that the resulting hot-spots tend to be spherical in shape [24]. A hot-spot’s shape, then, may be indicative of the primary mechanism responsible for its formation.

The distribution of hot-spots in a small region $\delta A$ centered at $x$ at time $t$ can be statistically characterized by a multivariate probability density function (PDF), $h(\xi, x, t)$, where $\xi = \{\text{intensity, size, surface area, shape}\}$ is the collective set of morphological features. The quantity $h(\xi, x, t)\, d\xi$ represents the probability that a hot-spot in $\delta A$ will have a morphology in the range $\xi$ to $\xi + d\xi$ at time $t$ for a given piston speed. The cumulative
distribution function (CDF) is given by

\[ H(\xi, x, t) = \int_0^\xi h(\alpha, x, t) \, d\alpha, \]  

such that \( H(\infty, x, t) = 1 \). Although the random variables are defined on the domain \((0, \infty) \times (0, \infty)\), their upper limits will be capped in practice by initial particle size specifications and thermal conductivity. The quantities which characterize hot-spot morphology and the marginal distributions of \( h(\xi, x, t) \), which are the focus of this study, will now be defined and discussed.

A hot-spot’s intensity is represented by its temperature; however, a hot-spot possesses a continuous temperature field which can be spatially complex and difficult to characterize, as illustrated in Figs. 2.7(a) and (b). To quantify the intensity of a hot-spot, we define a mean temperature \( \bar{T} \), a peak temperature \( \hat{T} \), and a temperature deviation \( \tilde{T} \) given by

\[ \bar{T} \equiv \frac{\int_\mathcal{A} T(x, t) \rho(x, t) \, d\mathcal{A}}{\int_\mathcal{A} \rho(x, t) \, d\mathcal{A}}, \]  

\[ \hat{T} \equiv \max \{ T(x, t) \}, \]  

\[ \tilde{T} \equiv \left( \frac{\int_\mathcal{A} (T(x, t) - \bar{T})^2 \rho(x, t) \, d\mathcal{A}}{\int_\mathcal{A} \rho(x, t) \, d\mathcal{A}} \right)^{1/2}, \]

respectively, for \( x \in \mathcal{A} \). The mean temperature \( \bar{T} \) is simply a mass-weighted average of the temperature distribution within the hot-spot. In this study, density variations are assumed to be small, in which case the mass-weighted average reduces to an area-weighted average in \( \mathbb{R}^2 \).

The distribution of mean hot-spot temperatures in a region \( \delta \mathcal{A} \) can be characterized by the marginal distribution \( h_\bar{T}(T, x, t) \). The associated CDF, \( H_\bar{T}(T, x, t) \), gives the probability that a hot-spot in \( \delta \mathcal{A} \) will have a mean temperature \( \bar{T} \leq T \). The same approach can be used to describe the the peak hot-spot temperatures and temperature deviations. The probability of ignition, as well as the time scale of reaction, will depend upon the tempera-
Figure 2.3: Spatial temperature variations in hot-spots resulting from a 500 m/s piston impact. (a) A single hot-spot resulting from highly localized deformation of a particle corner (b) A cluster of hot-spots formed by a combination of friction and plastic work at particle interfaces.

The size of the hot-spot is given by its volume in $\mathbb{R}^3$, or a volume per unit depth in $\mathbb{R}^2$, which is equivalent to its area, $\tilde{A}$. For simple hot-spot geometries, it is useful to identify a characteristic length scale (typically a diameter, in the case of circular or spherical hot-spots [18],[22]) to simplify the analysis, though it is not done in this study. The distribution of hot-spot sizes can be characterized by the marginal distribution $h_{\tilde{A}}(A, x, t)$, and $H_{\tilde{A}}(A, x, t)$ gives the probability that a hot-spot in $\delta A$ will have a size $\tilde{A} \leq A$, such
that \( H_A(\infty, x, t) = 1 \). The size of a hot-spot is an important quantity in determining the critical temperature at which reaction will occur.

The **surface area** of a hot-spot is defined by the isothermal surface \( T(x, t) = T_{th} \) for \( x \in \hat{A} \), and is denoted by the symbol \( \Gamma \). In \( \mathbb{R}^2 \), \( \Gamma \) is a surface area per unit depth, which is equivalent to the perimeter of the hot-spot. The marginal distribution \( h_\Gamma(\ell, x, t) \) describes the distribution of hot-spot perimeters in the region \( \delta A \), which is important in the growth stage of impact induced ignition. Regions with greater reactive surface area will burn more rapidly than those with a smaller amount of reactive surface.

The **shape** of a hot-spot is characterized by an eccentricity, \( \epsilon \), and a surface area-to-size ratio, \( L \). The eccentricity of a hot-spot is the ratio of the distance between the foci of an ellipse with the same second-moments as the hot-spot region, and its major axis length. It can take on values between 0 and 1, where \( \epsilon = 0 \) describes a circle and \( \epsilon = 1 \) a line segment. It has already been mentioned that different hot-spot formation mechanisms may produce distinct hot-spot shapes; therefore, obtaining the distribution of hot-spot eccentricities, characterized by the marginal distribution \( h_\epsilon(\nu, x, t) \), can provide insight into the role particular hot-spot formation mechanisms play in the ignition of solid explosives under different loading conditions.

The second measure of hot-spot shape is given by its surface area-to-size ratio, which in \( \mathbb{R}^2 \) is equivalent to a perimeter-to-area ratio, and can be characterized by the marginal distribution \( h_L(\zeta, x, t) \). This parameter is commonly observed in combustion models [7] and is important for local ignition of the hot-spot. This is demonstrated by considering the simple case of a hot-spot at uniform temperature with conduction, illustrated in Fig. 2.4. A energy balance of the system is given by

\[
\dot{q}_{HS}\hat{A} = \dot{q}_R(T)\hat{A} - \dot{q}_c(T)\Gamma
\]  

(2.12)

where \( \dot{q}_R(T)\hat{A} \) is the rate of energy generation by chemical reaction, \( \dot{q}_c(T)\Gamma \) is rate of energy
lost to the surrounding environment through conduction, and $\dot{q}_{HS} A$ is the rate of change of internal energy of the hot-spot. This can be rearranged to yield

$$\dot{q}_{HS} = \dot{q}_R(T) - \dot{q}_c(T) \frac{\Gamma}{A}. \quad (2.13)$$

If $\dot{q}_R(T) \approx \dot{q}_c(T)$, then ignition will depend on the value $\frac{\Gamma}{A}$. Note that if $\dot{q}_R(T)$ is sufficiently large, $\frac{\Gamma}{A}$ will be largely inconsequential in determining local ignition.

### 2.3.1 Integrated Quantities and Hot-Spot Proximity

A system is said to be strictly *statistically homogeneous* if the probability density functions which characterizes it are *translationally invariant*, i.e., constant under a shift of origin. Mathematically, we can express this condition as

$$h(\xi, t) \, d\xi = h(\xi, x_1, t) \, d\xi = h(\xi, x_2, t) \, d\xi \ldots = h(\xi, x_m, t) \, d\xi \quad (2.14)$$

for all regions $\delta A_i \in A$ centered at locations $x_i$ for $i = 1 \ldots m$. Systems which are strictly *statistically isotropic* posses density functions which are *rotationally invariant*, i.e.,
invariant under rigid body rotation of the spatial coordinates. A *statistically stationary* system is one in which the random variables of interest are independent of time. That is

\[ h(\xi, \mathbf{x}) \, d\xi = h(\xi, \mathbf{x}, t_1) \, d\xi = h(\xi, \mathbf{x}, t_2) \, d\xi = \ldots = h(\xi, \mathbf{x}, t_p) \, d\xi \]  

(2.15)

for all \( t \geq 0 \).

For all the computations performed in this study, the hot-spot fields in the domain are assumed to be statistically homogeneous, isotropic, and stationary. For these computations, statistical stationarity is a reasonable assumption due to the low thermal conductivity of HMX. Because of this assumption, the dependency of \( h(\xi) \) and its associated marginal distributions on \( \mathbf{x} \) and \( t \) is eliminated. Under these assumptions, it makes sense to identify and define integrated hot-spot quantities of interest.

**Hot-spot volume fraction**, **specific surface area**, and **number density** are quantities which describe the aggregate hot-spot characteristics of a region, and have a tendency to appear as parameters in Ignition and Growth type macro-scale models, accounting for the fraction of explosive material initially ignited by the passage of a deformation wave ([17],[19],[22]). Let \( N \) be the number of hot-spots in \( \mathcal{A} \). Then the local hot-spot volume fraction, \( \phi_{HS} \), specific surface area, \( s_{HS} \), and number density, \( n_{HS} \), are defined by the following expressions:

\[
\phi_{HS} \equiv \frac{\sum_{i}^{N} \mathring{A}_{i}^i}{\mathcal{A}} \quad \text{(2.16)}
\]

\[
s_{HS} \equiv \frac{\sum_{i}^{N} \Gamma_{i}^i}{\mathcal{A}} \quad \text{(2.17)}
\]

\[
n_{HS} \equiv \frac{N}{\mathcal{A}} \quad \text{(2.18)}
\]

For statistically inhomogeneous systems, it is possible to compute these quantities locally within a region \( \delta\mathcal{A} \) to estimate their spatial variation; however, they will be sensitive to the size and shape of \( \delta\mathcal{A} \).
Figure 2.5: Events contributing to the surface-surface, $p_{s,s}$, and point-surface, $p_{p,s}$, probability density functions.

The rate which hot-spots grow and coalesce is believed to be especially important to the transition from deflagration to detonation. As hot-spots react and grow they produce hot gases, causing pressure waves to propagate through the domain and strengthen the lead shock wave to the extent that it transitions into a detonation wave. The proximity of nearby hot-spots is likely to play a role in determining the rate at which growth and coalescence occurs by affecting thermochemical interactions between neighboring hot-spots.

The proximity between hot-spots is represented by nearest neighbor distances commonly used to investigate the spatial dependence between events in a region [26]. Because hot-spots may have complex shapes, it is important to consider the distance between hot-spot surfaces, rather than their mass centers, which may be far removed from the hot-spot boundary. In this study, we incorporate two nearest neighbor distances to examine the spatial proximity and clustering of hot-spots: (1) a hot-spot surface-to-surface distance, $r_{s,s}$, which is the distance between the surface of a hot-spot and the surface of its closest neighbor, and (2) a hot-spot point-to-surface distance, $r_{p,s}$, which is the distance between a random point, $p \in \mathcal{A}_{HS}$, and the surface of the closest neighboring hot-spot. These events,
illustrated in Figure 2.5, provide information about the short range spatial dependency of hot-spots, and can be characterized by distribution functions $P_{s,s}(r)$, which provides information about hot-spot proximity, and $P_{p,s}(r)$, which is used in conjunction with $P_{s,s}$ to determine if hot-spot clustering is present in the domain. Specifically, $P_{s,s}(r)$ gives the probability that the distance, $r_{s,s}$, between the surface of a randomly chosen hot-spot in $A$, and the surface of the closest neighboring hot-spot is $\leq r$. $P_{p,s}$ gives the probability that the distance, $r_{p,s}$, between a randomly selected point in $A_{HS}$ and the closest neighboring hot-spot is $\leq r$. A plot of $P_{s,s}(r)$ and $P_{p,s}(r)$ provides evidence of inter-event interactions. If hot-spots are clustered in the domain, then $P_{s,s}$ would increase steeply for small values of $r$, and plateau as the distances get larger. The opposite interpretation holds true for $P_{p,s}$, which would plateau for small values of $r$, and rise sharply with increasing $r$. In the event that clustering is not present, the distributions would collapse to a single curve.

2.4 Critical Hot-Spots and Ignition Implications

Ignition is a thermally activated phenomenon that depends on the distribution of hot-spots within the material meso-structure that are sufficiently intense to trigger reaction. By combining inert hot-spot distribution predictions with thermal explosion data and analysis, it is possible to estimate corresponding hot-spot ignition time distributions and fractions of ignited mass for a material having a prescribed composition and meso-structure. This information can provide the foundation for future work in a statistical theory to estimate the early time deformation-induced ignition (or local ignition) probability of the material as a function of wave strength.

We stipulate two propositions about impact induced hot-spots and ignition: 1) ignition depends on the thermal intensity of critical hot-spots; and 2) ignition depends on critical hot-spot size and cumulative mass which are measures of its capability to overcome quenching. An increase in critical hot-spot intensity, size, and cumulative mass will increase the probability of ignition. As already discussed, inert temperature field predictions provide a means of characterizing the morphology of hot-spots in the material. Based on these
features, we define a joint density function for hot-spot intensity and size \( q(\hat{T}, \hat{A}) \), where the product \( q(\hat{T}, \hat{A}) \, d\hat{T} \, d\hat{A} \) gives the fraction of a hot-spot mass having a peak temperature and size within the interval \( (\hat{T}, \hat{T} + d\hat{T}) \times (\hat{A}, \hat{A} + d\hat{A}) \). In general, this joint distribution varies spatially and temporally, but because of assumptions of statistical homogeneity, isotropy, and stationarity, their dependence is ignored in this discussion. The cumulative joint distribution is then given by

\[
Q(\hat{T}, \hat{A}) = \int_0^{\Delta \hat{T}} \int_0^{\Delta \hat{A}} q(\alpha, \beta) \, d\alpha \, d\beta
\]

(2.19)

which gives the fraction of hot-spots having a peak temperature \( \leq \hat{T} \) and a size \( \leq \hat{A} \) such that \( Q(\infty, \infty) = 1 \).

Thermal explosion data and analysis can be used to estimate the fraction of hot-spots that are chemically significant, termed critical hot-spots in this study. For example, thermal explosion analysis has shown that the complete reaction threshold for hot-spots in energetic solids depends on both their size and initial temperature, and may be described by a manifold \( I(\hat{A}, T) \) on \((0, \infty) \times (0, \infty)\) such that complete reaction results for \( I \geq 0 \). The corresponding thermal explosion time may be generally expressed by \( \tau = \tau(\hat{A}, T) \). The cumulative mass fraction of hot-spots within the interval \((0, \hat{A}) \times (0, \hat{T})\) that locally undergoes complete reaction (referred to as locally ignited mass fraction in this study) is given by

\[
R(\hat{A}, \hat{T}) = \int_0^{\hat{T}} \int_0^{\hat{A}} H(\alpha, \beta) \, q(\alpha, \beta) \, d\alpha \, d\beta
\]

(2.20)

where

\[
H(\alpha, \beta) = \begin{cases} 
1 & \text{if } I(\alpha, \beta) \geq 0, \\
0 & \text{otherwise.}
\end{cases}
\]

Thus, the total fraction of locally ignited mass is given by \( R(\infty, \infty) \). Moreover, an expression for the expected (or average) explosion time of locally ignited mass fraction is simply
given by
\[ \tau = \frac{1}{R(\infty, \infty)} \int_0^\infty \int_0^\infty \tau(\alpha, \beta) \ H(\alpha, \beta) \ q(\alpha, \beta) \ d\alpha \ d\beta. \tag{2.21} \]

It is possible to obtain a probability distribution function for \( \tau \) based on the marginal and joint probability functions \( H_A \) and \( H_B \) [15]. If this distribution function is given by \( g(\tau) \), then the cumulative mass fraction of critical hot-spots defined on \((0, \tau)\) is given by

\[ S(\tau) = \int_0^\tau g(\gamma) \ d\gamma; \tag{2.22} \]

where \( \int_0^\infty g(\gamma)d\gamma = 1. \)

### 2.5 Digital Processing of Hot-Spots

The level-cut approach is applied to temperature field predictions from meso-scale simulations of planar impact events. Temperature fields are first converted into high resolution digital images and image segmentation and regional descriptors are then used to detect hot-spots amid the background pixels. Hot-spot morphological and spatial statistical information can then be computed with little loss in accuracy. The following sections briefly describe these methods, which have been implemented using the Image Processing Toolbox, a robust set of MATLAB® functions useful for image processing applications [28].

#### 2.5.1 Image Segmentation

A simple global thresholding algorithm is implemented to isolate hot-spots in the image from background material, converting the RGB image, \( f(x,y) \), to a binary one in the process. The thresholded binary image \( b(x,y) \) is defined as

\[ b(x,y) = \begin{cases} 
1 & \text{if} \ f(x,y) > \lambda \\
0 & \text{if} \ f(x,y) \leq \lambda
\end{cases} \tag{2.23} \]

where \( \lambda \) is a constant.
Figure 2.6: Vertical and horizontal neighbors of $p$ are shown shaded in blue, while diagonal neighbors are shaded in pink. The 8-neighbors of $p$, $N_8$, are used to determine the type of adjacency shared between neighboring pixels.

Once isolated, hot-spot pixels are assigned a unique identity by utilizing the Toolbox function \texttt{bwlabel}, which identifies connected components (hot-spots) in a binary image. The algorithm can be summarized as follows:

A pixel $p$ at coordinates $(x,y)$ has two horizontal and two vertical neighbors, denoted $N_4(p)$, whose coordinates are $(x+1,y),(x-1,y),(x,y+1)$. The four diagonal neighbors of $p$ have coordinates $(x+1,y+1),(x+1,y-1),(x-1,y+1)$, and $(x-1,y-1)$ and are denoted by $N_D(p)$. $N_4(p)$ and $N_D(p)$ are shown in Figure 2.6. The union of $N_4(p)$ and $N_D(p)$ are the 8-neighbors of $p$, denoted $N_8(p)$. Two pixels $p$ and $q$ are said to be 4-adjacent if $q \in N_4(p)$. Similarly, $p$ and $q$ are said to be 8-adjacent if $q \in N_8(p)$. A path between pixels $p_1$ and $p_n$ is a sequence of pixels $p_1, p_2, ..., p_{n-1}, p_n$ such that $p_k$ is adjacent to $p_{k+1}$ for $1 \leq k < n$, and is referred to as either 4-connected or 8-connected, depending on the type of adjacency used. Two foreground pixels $p$ and $q$ are said to be 4-connected if there exists a 4-connected path between them, consisting entirely of foreground pixels. They are 8-connected if there exists an 8-connected path between them. For any foreground pixel, $p$, the set of all foreground pixels connected to it is called the connected component containing $p$. In this study, 8-adjacency was used to identify connected components.

The output of the function \texttt{bwlabel} is a label matrix, which assigns a unique integer, ranging from 1 to the total number of connected components found, to pixels of the same connected component. Thus, each hot-spot in the image is given a unique identity, allowing
additional analysis to be performed. The results of the image segmentation algorithm are illustrated in Figure 2.7, which shows hot-spot identified from an RGB image. Additional information on MATLAB’s Image Processing Toolbox and general image analysis can be found in Ref. [13].

2.5.2 Estimating Hot-Spot Morphology and Proximity

Hot-spot intensity is estimated from an RGB color image of the hot-spot temperature field. An RGB color image is an array of color pixels, where each pixel is a triplet corresponding to the red, green, and blue components of an RGB image at a specific spatial location. A color pixel at location \((x, y)\) can be represented by a vector in RGB space given by

\[
c(x, y) = \begin{bmatrix} c_R(x, y) \\ c_G(x, y) \\ c_B(x, y) \end{bmatrix} = \begin{bmatrix} R(x, y) \\ G(x, y) \\ B(x, y) \end{bmatrix},
\]

(2.24)

where \(R(x, y), G(x, y), \) and \(B(x, y)\) are the corresponding red, green, and blue components of the pixel, respectively, and vary from 0 to 255. In this study, only the red and blue components where used to represent hot-spot temperatures, with the green component set
to zero. A value of \( c = [255 0 0] \) corresponded to the lowest temperature observed in the
domain \( T_{\text{min}} \) and a value of \( c = [0 0 255] \) corresponded to the highest temperature in the
domain \( T_{\text{max}} \). The temperature of a pixel is given by

\[
T(x, y) = \frac{1}{2} [T_R(x, y) + T_B(x, y)],
\]

(2.25)

where

\[
T_R(x, y) = T_{\text{max}} - \frac{T_{\text{max}} - T_{\text{min}}}{255} c_R
\]

(2.26)

\[
T_B(x, y) = \frac{T_{\text{max}} - T_{\text{min}}}{255} c_B + T_{\text{min}}
\]

(2.27)

The peak temperature, \( \tilde{T} \), is determined by locating the pixel with maximum temperature.
The average hot-spot temperature, \( \overline{T} \), and temperature deviation \( \tilde{T} \) are estimated by

\[
\overline{T} = \frac{1}{n} \sum_i T_i
\]

(2.28)

\[
\tilde{T} = \left( \frac{1}{n-1} \sum_i (T_i - \overline{T})^2 \right)^{1/2}
\]

(2.29)

where \( n \) is the number of pixels contained in a hot-spot.

Hot-spot size and perimeter are proportional to the number of pixels contained within
the hot-spot, \( n \), and the number of boundary pixels, \( n_B \), possessed by that hot-spot, illus-
trated in Fig. 2.8. Each of these properties, along with hot-spot eccentricity \( \epsilon \), can be found
using the function \texttt{regionprops} in the \textit{Image Processing Toolbox}. The values returned by
this function are multiplied by a length scale, \( d \), given by

\[
d = \frac{\text{width of image in meters}}{\text{width of image in pixels}}
\]

(2.30)

The area and perimeter of a hot-spot is thus given by \( \tilde{A} = nd \) and \( \Gamma = n_Bd \), respectively.
Figure 2.8: A single digitized hot-spot with inner pixels colored green and boundary pixels in black.

Computation of the Surface-Surface and Point-Surface Nearest Neighbor functions for a digitized image is fairly straightforward. Each hot-spot surface (i.e., boundary) is comprised of a set of pixels, $n_B$, with locations $(x_i)$, with the full set of boundary pixels in the image given by $n_B = \{n_B^1(x_1), n_B^2(x_2), ..., n_B^n(x_n)\}$. For a given hot-spot, $p$, the Surface-Surface Nearest Neighbor distance is found by computing the distances between its boundary pixels and the boundary pixels of all other hot-spots in the domain and selecting the minimum value.

To compute the Point-Surface Nearest Neighbor distance, a set of random pixel locations is first generated from a uniform distribution over the range of the image domain. Any pixel locations which correspond to hot-spot material are discarded, and new pixel locations are selected. Once an appropriate pixel location has been determined, its Point-Surface Nearest Neighbor distance is found by computing the minimum distance between it and the set of hot-spot boundary pixels. This process is performed thousands of times to get a reasonable approximation of the true distribution. The computational overhead of computing these functions can be improved by organizing the set of hot-spot boundary pixel locations into a $kd$-tree data structure, which is a generalization of a binary search tree to higher dimensions.

The image analysis used in this study is only an approximation technique and the accuracy of this process depends on the resolution of the image, which must strike a balance between minimizing error and maximizing computational efficiency. Estimates for the error

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in hot-spot intensity and size are addressed in Chapter 3. In principle, hot-spot morphology could be determined directly from the finite element data; however, image analysis tools are efficient, and provide significant flexibility in characterizing hot-spot temperature fields.
Chapter 3
Analysis of Hot-Spot Statistics

In this chapter, the methods developed in Chapter 2 are used to characterize the distribution of hot-spots behind uniaxial deformation waves in granular HMX. In Section 3.3, marginal distributions of hot-spot intensity, size, and shape are presented for meso-structures with initial solid volume fractions of \( \phi_{s,0} = 0.577, 0.678, 0.768, \) and 0.835 using a threshold temperature \( T_{th} = 500 \) K, and fits are established for each of these PDFs. The significance of the fits and the sensitivity of the marginal distributions to material meso-structure and \( T_{th} \) is examined. In Section 3.4, joint distributions of hot-spot intensity and size are presented and an approach to estimate joint distributions from copulas parameterized to microstructural features is illustrated. Joint distributions of hot-spot intensity and size are important in establishing critical hot-spots, and the use of copulas to generate joint distributions may be a useful modeling tool for estimating hot-spot statistics. Hot-spot proximity and clustering is examined in Section 3.5 using nearest neighbor distribution functions, and the sensitivity of the integrated quantities of hot-spot number density, volume fraction, and specific surface area to piston speed and meso-structure is determined. The integrated quantities describe the aggregate heating response of a material to impact, and can be used to establish values for macro-scale model parameters. In Section 3.6, critical hot-spots are identified by combining hot-spot statistical information with the thermal explosion analysis of Tarver et al. [39], and estimates are presented for the fraction of reacted mass as a function of meso-structure and piston speed. Lastly, ignition time distributions are approximated for the fraction of reacted mass using an ignition law for HMX-based PBXs formulated by Henson, et al. [16]. Information about the distribution of ignition times represents an important first step in establishing the ignition probability of a material [40], and may be used to further development of a statistical theory for impact induced ignition.
3.1 Material Meso-Structures

In order to study the effects of particle packing density, particle shape, and wave strength on hot-spot formation, we numerically simulate inert impact of the materials shown in Fig. 3.1, and summarized in Table 3.1. The materials consist of hexagonally and/or circularly shaped, randomly packed, HMX particles having diameters of either 40 \(\mu m\), 60 \(\mu m\), or 80 \(\mu m\). In this study, the terms initial packing density and initial solid volume fraction are used interchangeably to mean the fraction of the total volume occupied by the explosive. The term initial porosity, also sometimes used, refers to the fraction of the total volume occupied by void space. For clarity, we use the monikers A, B, C, and D, arranged in Table 3.1 in terms of increasing initial particle packing density, to identify each meso-structure from this point forward. The average initial solid volume fraction, \(\bar{\phi}_{s,0}\), ranges from 0.584 to 0.835; however, variations in local porosity in each of the meso-structures exist. Distributions of local solid volume fraction for each meso-structure are shown in Fig. 3.2. The local solid volume fraction of meso-structure A exhibits significant fluctuations, with a standard deviation of 0.035, while the local \(\bar{\phi}_{s,0}\) of meso-structure D

<table>
<thead>
<tr>
<th>Meso-Structure Structure</th>
<th>(\bar{\phi}_{s,0})</th>
<th>Particle Shape</th>
<th>Average Size ((\mu m))</th>
<th>Particle Size Distribution ((\mu m))</th>
</tr>
</thead>
<tbody>
<tr>
<td>A</td>
<td>0.584</td>
<td>Hexagonal: Circular</td>
<td>60</td>
<td>40-60-80 (33.33% each)</td>
</tr>
<tr>
<td>B</td>
<td>0.678</td>
<td>Hexagonal: Circular</td>
<td>60</td>
<td>40-60-80 (33.33% each)</td>
</tr>
<tr>
<td>C</td>
<td>0.768</td>
<td>Hexagonal: Circular</td>
<td>60</td>
<td>40-60-80 (33.33% each)</td>
</tr>
<tr>
<td>D</td>
<td>0.835</td>
<td>Circular</td>
<td>60</td>
<td>40-60-80 (33.33% each)</td>
</tr>
</tbody>
</table>
Figure 3.1: Initial meso-structures generated for this study, with average initial solid volume fractions of (a) $\bar{\phi}_{s,0} = 0.584$, (b) $\bar{\phi}_{s,0} = 0.678$, (c) $\bar{\phi}_{s,0} = 0.768$, and (d) $\bar{\phi}_{s,0} = 0.835$.

is more uniform over the computational domain, with a standard deviation of only 0.005. Though variations in the internal meso-structure of a material will result in statistically inhomogeneous hot-spot fields, the spatial variation in hot-spot statistics is not considered in this study.

Simulations were performed for piston impact speeds of 300 m/s, 400 m/s, and 500 m/s, which are representative of speeds experimentally observed to cause weak initiation
Figure 3.2: Histograms of local solid volume fraction corresponding to (a) meso-structure \( A \), (b) meso-structure \( B \), (c) meso-structure \( C \), and (d) meso-structure \( D \).

of DDT in certain confinement conditions ([29],[37]). The computational domain is sufficiently long to enable quasi-steady waves to develop long before they reach the far-end boundary. Hot-spot fields were analyzed using deformed material in the quasi-steady region behind the wave. Figure 3.3(a) illustrates the development and quasi-steady wave regions, as well as the entropy layer near the piston surface resulting from an impedance mismatch at the piston-explosive interface. Note that the regions in Fig. 3.3(a) are for illustration, and are not to scale. The point at which the quasi-steady region begins is determined from plots wave speed versus position, as illustrated in Fig. 3.3(b). In this case, a quasi-steady wave is
achieved in less than 0.4 mm, and the development region accounts for approximately 4% of the total domain length. As mentioned, the hot-spot field is assumed to be statistically homogeneous, isotropic, and temporally invariant behind the wave, enabling the material in the quasi-steady region to be collectively analyzed.

### 3.2 Probability Density Functions - Properties

A key goal of this study is to obtain hot-spot statistics and to investigate how they are influenced by wave strength, initial packing density, and particle shape. To that end, fits are established for the marginal PDFs of hot-spot intensity, size, perimeter, shape, and proximity and the significance of those fits is examined. Parameter estimates are computed using MATLAB’s *Statistics Toolbox* [28], which computes maximum likelihood estimates and 95% confidence intervals for the parameters based on the sample data. In this section, the distribution functions chosen to describe hot-spot statistics are given and their parametric dependencies are illustrated.

#### 3.2.1 Generalized Pareto Distribution

A generalized Pareto distribution (GPD) reasonably describes the marginal PDFs of hot-spot intensity, size, perimeter, and eccentricity. The probability density function for
Figure 3.4: (a) The GPD parameter $k$ influences the shape of the distribution. Values of $k < 0$, $k = 0$, and $k > 0$ correspond to limiting forms of the GPD. (b) GPD constructed by varying the value of $\sigma$ while holding $k$ and $\theta$ constant. (c) GPD constructed by varying the value of $\theta$ while holding $k$ and $\sigma$ constant.

The GDP with shape parameter $k \neq 0$, scale parameter $\sigma$, and threshold parameter $\theta$, is given by

$$f(x) = \left( \frac{1}{\sigma} \right) \left( 1 + k \frac{x - \theta}{\sigma} \right)^{-1 - \frac{1}{k}} \quad (3.1)$$

where $\theta < x$ for $k > 0$ and $\theta < x < \sigma/k$ for $k < 0$. Here, $x$ represents the hot-spot feature of interest. If $k = 0$ and $\theta = 0$, the generalized Pareto distribution reduces to the exponential distribution. If $k > 0$ and $\theta = \sigma/k$, the GPD reduces to the classical Pareto distribution. The GPD is often used to model the distribution of exceedances over a threshold, also called extreme values. Hot-spots are often described as being at the tail of...
the temperature distribution, and therefore may be interpreted as exceedances. The GPD was chosen as a model for hot-spot intensity, area, perimeter, and eccentricity because it allows a continuous range of possible shapes and allows more control over the weight of the tail of the distribution. The significance of the shape, scale, and threshold parameters will now be discussed.

Table 3.2: Values of $\theta$ used in this study to fit the marginal distributions of hot-spot intensity, size, perimeter, and eccentricity.

<table>
<thead>
<tr>
<th>Marginal Distribution</th>
<th>$\theta$</th>
</tr>
</thead>
<tbody>
<tr>
<td>$h_T$</td>
<td>500 K</td>
</tr>
<tr>
<td>$h_{\tilde{T}}$</td>
<td>500 K</td>
</tr>
<tr>
<td>$h_{\tilde{A}}$</td>
<td>0 K</td>
</tr>
<tr>
<td>$h_{\tilde{A}}$</td>
<td>2.8 $\mu m^2$</td>
</tr>
<tr>
<td>$h_{\Gamma}$</td>
<td>7 $\mu m$</td>
</tr>
<tr>
<td>$h_{\epsilon}$</td>
<td>0</td>
</tr>
</tbody>
</table>

The GPD has three basic forms, determined by the value of $k$, and illustrated in Fig. 3.4(a), which was constructed by varying $k$ while holding all other parameters fixed. A value of $k = 0$ is used to model distributions whose tails decrease exponentially, such as a normal distribution. Distributions whose tails decrease as a polynomial, such as Student’s $t$, lead to $k > 0$. Distributions with finite tails, such as the beta, lead to $k < 0$. Changes in the scale parameter $\sigma$, are shown in Fig. 3.4(b), which was generated by varying $\sigma$ while holding $k$ and $\theta$ fixed. Increasing or decreasing $\sigma$ broadens or steepens the distribution, respectively, without changing its shape. Changes to the threshold parameter $\theta$ translate the distribution without altering the shape or scale. This is illustrated in Fig. 3.4(c).

The difficulty in using the GPD often centers around specifying its minimum threshold, which is unknown in many instances. In this study, the value of $\theta$ is chosen based on the resolution limitations (size and perimeter of a single finite element) of the simulation, and the choice of $T_{th}$. A summary of the GPD threshold values used in this study are given in Table 3.2
Figure 3.5: (a) GEV distributions generated by varying $k$ while holding $\sigma$ and $\mu$ fixed. (b) GEV distributions generated by varying $\sigma$ while holding $k$ and $\mu$ fixed. (c) GEV distributions generated by varying $\mu$ while holding $k$ and $\sigma$ fixed.

3.2.2 Generalized Extreme Value Distribution

Like the GPD, the Generalized Extreme Value (GEV) distribution is used in Extreme Value Theory to model exceedances, and is a generalization of type I, type II, and type III extreme value distributions. The GEV is used in this study to model the distribution of hot-spot area-to-perimeter ratio, which is important in determining the critical conditions for hot-spot ignition. The probability density function of the GEV, with location and scale parameters, $\mu$ and $\sigma$, and a shape parameter, $k$, is given by

$$f(x) = \frac{1}{\sigma} \exp\left(-\left(1 + k \frac{(x - \mu)}{\sigma}\right)^{-\frac{1}{k}}\right) \left(1 + k \frac{(x - \mu)}{\sigma}\right)^{-\frac{1}{k}},$$

(3.2)
Figure 3.6: (a) WBL distributions constructed by varying $A$ and holding $B$ fixed. (b) WBL distributions constructed by varying $B$ and holding $A$ fixed.

for

$$1 + k \frac{x - \mu}{\sigma} > 0.$$  \hspace{1cm} (3.3)

When $k < 0$, the GEV is equivalent to the type III extreme value. When $k > 0$, the GEV is equivalent to the type II. In the limit as $k \to 0$, the GEV becomes the type I. Figure 3.5(a) illustrates these cases by holding $\mu$ and $\sigma$ fixed and varying $k$. The same has been done for the scale and location parameters $\sigma$ and $\mu$, illustrated in Figs. 3.5(b) and (c). Like the scale parameter of the GPD, $\sigma$ steepens or broadens the distribution without altering the underlying shape, while the location parameter translates the distribution.

### 3.2.3 Weibull Distribution

The Weibull (WBL) distribution is used to describe the distribution of Nearest Neighbor distances which characterizes hot-spot proximity in this study. In this section, the PDF of the Weibull distribution is presented, and the reasons for its selection are provided.

The Weibull distribution was originally introduced by Waloddi Weibull to model the breaking strength of materials. Currently the WBL distribution is used in reliability and lifetime models. The probability density function for the Weibull distribution, with scale
parameter $A$ and shape parameter $B$, is given by

\[ f(x) = \frac{B}{A} \left( \frac{x}{A} \right)^{B-1} e^{-\left(\frac{x}{A}\right)^B}, \quad (3.4) \]

for $x \geq 0$. Figure 3.6 shows the sensitivity of the WBL distribution to different values of $A$ and $B$, where the shape and scale parameters have the same interpretation $\sigma$ and $k$ in the GPD and GEV. The Weibull distribution is often used in place of an exponential distribution to model the lifetimes of objects because it allows for a variable hazard rate (the hazard rate of an exponential distribution is a constant).

If the discussion is confined to the growth and coalescence stage of impact induced initiation, the coalescence of two hot-spots can be thought of as a “death” event in the sense that two individual hot-spots no longer exist. Consider, then, a distribution of hot-spots burning outward at a rate given by $\dot{r} = aP(t)^n$, which is typically observed in strand burner experiments, where $a$ is the burn rate coefficient and $n$ is the pressure coefficient.

The distribution of coalescence times, $t_f$, will be a function of the distribution of hot-spot proximities. The instantaneous rate of hot-spot coalescence (i.e. the hazard rate) will vary with time, as product gases pressurize the domain. Recognizing that the hazard rate will vary in the growth and coalescence process suggests that the Weibull distribution is an appropriate model to describe the hot-spot proximity distributions.

### 3.3 Hot-Spot Morphology - Marginal Distributions

In this section, error estimates in hot-spot size and temperature are provided to verify the accuracy of the image processing techniques used in this study, and predictions for the marginal distributions of hot-spot intensity, size, perimeter, and shape are presented and discussed.

#### 3.3.1 Error Estimates

Error estimates in hot-spot temperature and size were determined by generating a test hot-spot field which contained 100 isolated finite elements at different temperatures using
the visualization software Tecplot 360®, which is capable of quickly rendering temperature contours from numerical simulation data. The test field was exported from Tecplot as a Portable Network Graphics (PNG) file, which is a bitmapped image format that employs lossless data compression. The resolution of the digitized test field was 0.0306 $\mu$m$^2$/pixel ($\sim$ 80-100 pixels per finite element), and is approximately equivalent to the resolution of the hot-spot fields analyzed in this study. The test field was processed using the image analysis tools described in Chapter 2 and the results were compared to the actual area and temperature values of those elements.

The estimated finite element areas are within 0.04% of the actual finite element area and the estimated finite element temperatures are within 0.2% of the actual temperature. Increasing the resolution of the image will lower the error, but it is not likely to influence the distribution of hot-spot sizes significantly. The resolution of the digitized hot-spot fields analyzed in this study ranged from 0.0306-0.0352 $\mu$m$^2$/pixel due to matrix size limitations in MATLAB®. It should be noted that the finite element temperature data predicted by the meso-scale simulation is cell-centered; however, Tecplot automatically interpolates the cell-centered data to generate smoother temperature contours, resulting in temperature fluctuations within a finite element which are unresolved by the meso-scale simulations.

3.3.2 Hot-Spot Intensity

As mentioned in Chapter 2, hot-spot intensity is characterized by its mean temperature, peak temperature, and a temperature deviation about the mean, referred to as the hot-spot temperature deviation. Together, these quantities describe the leading order features of the fluctuating temperature field present within a hot-spot. Knowledge about the distribution of hot-spot intensities within a material can be used with statistical reactive flow models to better predict DDT in solid explosives.

Distributions of mean hot-spot temperature are shown in Fig. 3.7 for each meso-structure. Little variation in the mean hot-spot temperature distribution is observed with either piston speed or meso-structure. In meso-structures A-C, lower values of $U_p$ correlate
Figure 3.7: Predictions of hot-spot mean temperature distribution for piston speeds of 300 m/s, 400 m/s, and 500 m/s for (a) meso-structure A, (b) meso-structure B, (c) meso-structure C, and (d) meso-structure D with a slightly higher mean $\bar{T}$, while lower values of $\bar{\phi}_{s,0}$ correspond to slightly higher mean $\bar{T}$ at a given piston speed. At higher piston speeds, more material is heated to a temperature just above $T_{th}$ while the peak temperatures remain relatively unchanged, resulting in a mean hot-spot temperature which is more strongly biased towards $T_{th}$. Figure 3.8 and Table 3.3 summarizes the mean and standard deviation in $\bar{T}$ determined from the data at each piston speed for meso-structures A-D.
Table 3.3: Sample means and standard deviations for $\bar{T}$ determined from hot-spot data.

<table>
<thead>
<tr>
<th>Meso-Structure</th>
<th>Piston Speed (m/s)</th>
<th>Mean (K)</th>
<th>Std. Dev. (K)</th>
</tr>
</thead>
<tbody>
<tr>
<td>A</td>
<td>300</td>
<td>539.57</td>
<td>37.27</td>
</tr>
<tr>
<td>A</td>
<td>400</td>
<td>538.08</td>
<td>37.34</td>
</tr>
<tr>
<td>A</td>
<td>500</td>
<td>536.29</td>
<td>29.92</td>
</tr>
<tr>
<td>B</td>
<td>300</td>
<td>537.91</td>
<td>34.12</td>
</tr>
<tr>
<td>B</td>
<td>400</td>
<td>535.09</td>
<td>33.73</td>
</tr>
<tr>
<td>B</td>
<td>500</td>
<td>532.97</td>
<td>29.06</td>
</tr>
<tr>
<td>C</td>
<td>300</td>
<td>533.26</td>
<td>31.52</td>
</tr>
<tr>
<td>C</td>
<td>400</td>
<td>530.31</td>
<td>33.43</td>
</tr>
<tr>
<td>C</td>
<td>500</td>
<td>527.33</td>
<td>24.10</td>
</tr>
<tr>
<td>D</td>
<td>300</td>
<td>540.43</td>
<td>33.75</td>
</tr>
<tr>
<td>D</td>
<td>400</td>
<td>535.19</td>
<td>34.36</td>
</tr>
<tr>
<td>D</td>
<td>500</td>
<td>538.77</td>
<td>33.75</td>
</tr>
</tbody>
</table>

Figure 3.8: Means and standard deviations for $\bar{T}$ plotted as a function of piston speed for each meso-structure.

Figures 3.9(a) and (b) show the dependence of the general Pareto parameters $k$ and $\sigma$ on piston speed and meso-structure. 95% confidence intervals for the parameter estimates are illustrated by error bars in Fig. 3.9. The uncertainty in $k$ and $\sigma$ is greatest at a piston speed of $U_p = 300$ m/s due to fewer number of hot-spots at that speed. At $U_p = 300$ m/s meso-structures $A$, $B$, $C$, and $D$ posses 25%, 25%, 9%, and 10%, respectively, of the total
number of hot-spot identified in those materials at $U_p = 500$ m/s. hot-spots The GPD shape parameter $k$ increases as piston speed is increased from 300 m/s to 400 m/s, then decreases as piston speed increases from 400 m/s to 500 m/s for all meso-structures. No clear correlation is predicted between $k$ and initial packing density. A negative value of $k$ is predicted in nearly all cases, except for meso-structure C at a $U_p = 400$ m/s. A negative value of $k$ is typically used to describe distributions with finite or truncated tails. In reality, conduction will cause the tail of the temperature distribution to be finite. A truncated Pareto distribution can be used to model distributions which have a finite upper bound, but it requires that an upper bound be defined. In this case, the negative values of $k$ may be numerical rather than physical, because the computing mean hot-spot temperatures averages out high temperature fluctuations within hot-spots. Estimates for $\sigma$ are relatively insensitive to changes in piston speed. Lower values of $\phi_{s,0}$ correlate with higher values of $\sigma$ for meso-structures A, B, and C, though the curves of A and B do intersect at $U_p = 300$ m/s; however, this not likely to be statistically significant. Estimates of $\sigma$ for meso-structure D are on the order of A and B which may indicate a particle shape effect. Larger values of $\sigma$ correlate with broader distributions and higher average $T$. 

Figure 3.9: Estimated GPD parameters, (a) $k$ and (b) $\sigma$, and 95% confidence bounds for hot-spot mean temperature as a function of piston speed for each meso-structure.
Figure 3.10: Predictions of hot-spot peak temperature distribution for piston speeds of 300 m/s, 400 m/s, and 500 m/s for (a) meso-structure A, (b) meso-structure B, (c) meso-structure C, and (d) meso-structure D.

Distributions of peak hot-spot temperature, shown in Fig. 3.10, are qualitatively similar to those observed for mean hot-spot temperature. Table 3.4 and Fig. 3.11 summarizes the results for sample means and standard deviations of peak temperature. Only minor variations (approximately Δ10 K) in the sample means are observed over the range of piston speeds considered. Lower values of $\bar{\phi}_{s,0}$ are associated with higher peak temperatures, on average, for meso-structures A-C. Again, particle shape effects may explain why the average peak temperature of meso-structure D is comparable to those of A and B. It may be that an abundance of hexagonal particles reduces the relative motion between explosive...
Table 3.4: Means and standard deviations for peak hot-spot temperature computed from the set of hot-spots found in each meso-structure.

<table>
<thead>
<tr>
<th>Meso-Structure</th>
<th>Piston Speed (m/s)</th>
<th>Mean (K)</th>
<th>Std. Dev. (K)</th>
</tr>
</thead>
<tbody>
<tr>
<td>A</td>
<td>300</td>
<td>563.14</td>
<td>85.49</td>
</tr>
<tr>
<td>A</td>
<td>400</td>
<td>567.77</td>
<td>89.56</td>
</tr>
<tr>
<td>A</td>
<td>500</td>
<td>573.61</td>
<td>89.69</td>
</tr>
<tr>
<td>B</td>
<td>300</td>
<td>561.45</td>
<td>68.11</td>
</tr>
<tr>
<td>B</td>
<td>400</td>
<td>561.67</td>
<td>81.23</td>
</tr>
<tr>
<td>B</td>
<td>500</td>
<td>566.16</td>
<td>78.33</td>
</tr>
<tr>
<td>C</td>
<td>300</td>
<td>550.36</td>
<td>54.29</td>
</tr>
<tr>
<td>C</td>
<td>400</td>
<td>552.11</td>
<td>85.23</td>
</tr>
<tr>
<td>C</td>
<td>500</td>
<td>549.77</td>
<td>58.62</td>
</tr>
<tr>
<td>D</td>
<td>300</td>
<td>565.78</td>
<td>60.38</td>
</tr>
<tr>
<td>D</td>
<td>400</td>
<td>559.97</td>
<td>65.30</td>
</tr>
<tr>
<td>D</td>
<td>500</td>
<td>571.17</td>
<td>78.07</td>
</tr>
</tbody>
</table>

Figure 3.11: Means and standard deviations for \( \hat{T} \) plotted as a function of piston speed for each meso-structure.
grains and minimizes frictional dissipation. Outliers in the high temperature tail of the peak temperature distribution observed in meso-structures $A$-$C$ are associated with energy localization concentrated at particle corners. It is important to note that the inclusion of sharp corners introduces numerical singularities at those locations, and so care must be taken when interpreting these results.

Figures 3.12(a) and (b) summarize the sensitivity of $k$ and $\sigma$ as a function of piston speed for the peak temperature distributions of each meso-structure. Trends in the sensitivity of $k$ and $\sigma$ to piston speed are qualitatively similar to the parameter estimates for mean temperature distribution. Estimates for $k$ are positive in all cases, with the exception of meso-structure $D$ at $U_p = 300$ m/s, which is different from the high frequency of negative $k$ observed for the mean temperature distributions.

Temperature fluctuations within a hot-spot are likely to influence its rate of reaction. As mentioned, the intensity of these fluctuations is characterized by a temperature deviation about the mean, referred to as hot-spot temperature deviations. The hot-spot temperature deviations are useful for placing confidence limits on estimated thermal explosion times of critical hot-spots.
Figure 3.13: Predictions of hot-spot temperature deviation distribution for piston speeds of 300 m/s, 400 m/s, and 500 m/s for (a) meso-structure A, (b) meso-structure B, (c) meso-structure C, and (d) meso-structure D

Hot-spot temperature deviations for each meso-structure are shown in Figure 3.13. Again, very little dependence on either piston speed or meso-structure is observed in these distributions. Variation in the sample means and standard deviations, summarized in Table 3.5 and Fig. 3.14, show no consistent trend with regard to piston speed. The temperature deviations are slightly higher, on average, for lower values of $\phi_{s,0}$, with the exception of meso-structure D, which has mean temperature distributions on the order of meso-structure A, though the reason for this is not entirely clear. Tarver et al. [39] have shown that the boundary temperature of a hot-spot must be raised or lowered several hundred degrees.
Table 3.5: Mean and standard deviations for hot-spot temperature deviations.

<table>
<thead>
<tr>
<th>Material</th>
<th>Piston Speed (m/s)</th>
<th>Mean (K)</th>
<th>Std. Dev. (K)</th>
</tr>
</thead>
<tbody>
<tr>
<td>A</td>
<td>300</td>
<td>17.89</td>
<td>21.64</td>
</tr>
<tr>
<td>A</td>
<td>400</td>
<td>18.62</td>
<td>22.37</td>
</tr>
<tr>
<td>A</td>
<td>500</td>
<td>19.58</td>
<td>18.93</td>
</tr>
<tr>
<td>B</td>
<td>300</td>
<td>16.87</td>
<td>18.27</td>
</tr>
<tr>
<td>B</td>
<td>400</td>
<td>17.76</td>
<td>20.74</td>
</tr>
<tr>
<td>B</td>
<td>500</td>
<td>17.78</td>
<td>17.70</td>
</tr>
<tr>
<td>C</td>
<td>300</td>
<td>13.87</td>
<td>14.26</td>
</tr>
<tr>
<td>C</td>
<td>400</td>
<td>15.93</td>
<td>24.59</td>
</tr>
<tr>
<td>C</td>
<td>500</td>
<td>13.54</td>
<td>14.43</td>
</tr>
<tr>
<td>D</td>
<td>300</td>
<td>20.51</td>
<td>13.98</td>
</tr>
<tr>
<td>D</td>
<td>400</td>
<td>17.77</td>
<td>15.15</td>
</tr>
<tr>
<td>D</td>
<td>500</td>
<td>19.77</td>
<td>18.17</td>
</tr>
</tbody>
</table>

Figure 3.14: Means and standard deviations for $\tilde{T}$ plotted as a function of piston speed for each meso-structure.
to influence the critical temperature even slightly ($\sim 9 - 10$ K in HMX). The majority of hot-spots have temperature deviations of 100 K or below. Assuming a hot-spot is intense enough to react, this would suggest that reaction is largely determined by the hottest material in the hot-spot.

The GPD parameters for the hot-spot temperature deviations, which are summarized in Fig. 3.15, are insensitive to changes in piston speed or meso-structure. Meso-structure $D$ deviates from these trends, which may indicate a particle shape effect. Shape estimates for meso-structures $A$, $B$, and $C$ are nearly linear with piston speed and so any shift in the sign of $k$ is unlikely to be meaningful. Unlike meso-structures $A$-$C$, the shape and scale parameter estimates for meso-structure $D$ are sensitive to piston speed, though they approach those of the other meso-structures as piston speed is increased from 300 m/s to 500 m/s.

Overall, the distribution of hot-spot intensities appears largely insensitive to variations in $U_p$ or meso-structure over the range of impact speeds considered. Therefore, constant values of $k$ and $\sigma$ can be used to describe the temperature distributions. Table 3.6 summarizes these parameter estimates.
Table 3.6: Estimates for GPD parameters $k$ and $\sigma$ for mean, peak, and temperature deviation distributions.

<table>
<thead>
<tr>
<th>Distribution</th>
<th>$k$</th>
<th>$\sigma (K^{-1})$</th>
</tr>
</thead>
<tbody>
<tr>
<td>$h_T$</td>
<td>-0.06</td>
<td>39.74</td>
</tr>
<tr>
<td>$h_T$</td>
<td>0.06</td>
<td>55.98</td>
</tr>
<tr>
<td>$h_T$</td>
<td>0.24</td>
<td>0.10</td>
</tr>
</tbody>
</table>

Shock sensitivity studies of TATB-based explosives preheated to 523 K concluded that the increased amount of ignition measured during shock initiation was due primarily to higher initial porosity of the TATB charges and the formation of a greater number of hot spots during shock loading, and not due to chemical kinetics [43]. Though TATB is significantly different than granular HMX, the distribution of hot-spot intensities predicted in this study agree qualitatively with those findings, suggesting that the impact sensitivity of certain materials might be strongly influenced by hot-spot number density rather than increases in intensity.

### 3.3.3 Hot-Spot Size

Hot-spot size distributions and their sensitivity to piston speed and meso-structure are addressed in this section. Hot-spot size is computed as a volume per unit depth, which is equivalent to the area of the hot-spot. Figure 3.16 shows the PDFs of hot-spot size for each meso-structure at piston speeds of 300 m/s, 400 m/s, and 500 m/s.

Table 3.7 and Fig. 3.17 summarize means and standard deviations of hot-spot size for meso-structures $A-D$ obtained from image analysis. Higher values of $U_p$ yielded, on average, larger hot-spots and higher standard deviations for each meso-structure. The same effect is accomplished by decreasing the initial packing density of the material. This is qualitatively similar to experimental results of Sheffield, et al. [37], which demonstrated that more dense materials are less sensitive to shock initiation. Predicted hot-spot sizes for meso-structure $A$ and $B$ differ only slightly, which suggests there is a range of initial packing densities which does not influence sensitivity. This is consistent with the results of Czerski and
Proud [9] which showed that no significant changes in shock sensitivity occurred between samples with initial packing densities ranging between 32-49% of the theoretical maximum density (TMD).

Figures 3.18(a) and (b) show the variation and standard error in general Pareto parameters as a function of piston speed for each meso-structure. Higher error exists in $k$ and $\sigma$ at the lower piston speeds due to smaller number of hot-spots. Predictions for $\sigma$ increase monotonically with piston speed for all meso-structures and are sensitive to initial packing density. Lower values of $\bar{\theta}_{s,0}$ generally yielded higher values of $\sigma$, with the exception of

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Figure 3.16: Predictions of hot-spot size distribution for piston speeds of 300 m/s, 400 m/s, and 500 m/s for (a) meso-structure $A$, (b) meso-structure $B$, (c) meso-structure $C$, and (d) meso-structure $D$
Table 3.7: Means and standard deviations for hot-spot size computed from hot-spot sample.

<table>
<thead>
<tr>
<th>Meso-Structure</th>
<th>U_p (m/s)</th>
<th>Mean (µm²)</th>
<th>Std. Dev. (µm²)</th>
</tr>
</thead>
<tbody>
<tr>
<td>A</td>
<td>300</td>
<td>25.48</td>
<td>30.82</td>
</tr>
<tr>
<td>A</td>
<td>400</td>
<td>36.68</td>
<td>54.86</td>
</tr>
<tr>
<td>A</td>
<td>500</td>
<td>65.89</td>
<td>127.88</td>
</tr>
<tr>
<td>B</td>
<td>300</td>
<td>24.71</td>
<td>28.03</td>
</tr>
<tr>
<td>B</td>
<td>400</td>
<td>32.93</td>
<td>46.94</td>
</tr>
<tr>
<td>B</td>
<td>500</td>
<td>59.63</td>
<td>106.07</td>
</tr>
<tr>
<td>C</td>
<td>300</td>
<td>19.75</td>
<td>20.51</td>
</tr>
<tr>
<td>C</td>
<td>400</td>
<td>28.45</td>
<td>34.23</td>
</tr>
<tr>
<td>C</td>
<td>500</td>
<td>40.80</td>
<td>60.77</td>
</tr>
<tr>
<td>D</td>
<td>300</td>
<td>16.02</td>
<td>15.18</td>
</tr>
<tr>
<td>D</td>
<td>400</td>
<td>22.66</td>
<td>28.98</td>
</tr>
<tr>
<td>D</td>
<td>500</td>
<td>38.17</td>
<td>48.76</td>
</tr>
</tbody>
</table>

Figure 3.17: Means and standard deviations for hot-spot area plotted as a function of piston speed for each meso-structure.
Figure 3.18: Estimated GPD parameters, (a) $k$ and (b) $\sigma$, and 95% confidence bounds for hot-spot size as a function of piston speed for each meso-structure.

meso-structures $C$ and $D$ at a piston speed of 500 m/s. Results for $k$ are less conclusive; however, the sensitivity of $k$ to $U_p$ is qualitatively similar for meso-structures $A$, $B$, and $C$, which are primarily comprised of hexagonal particles. Meso-structure $D$ consists entirely of circular particles, and the qualitative differences observed in both $\sigma$ and $k$ between $A$-$C$ and $D$ may be a result of particle shape.

Table 3.8: Parameters for $A_1$, $A_o$.

<table>
<thead>
<tr>
<th>Coefficient</th>
<th>Value</th>
<th>Coefficient</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\alpha_o$</td>
<td>0.0010</td>
<td>$\beta_o$</td>
<td>1.7100</td>
</tr>
<tr>
<td>$\alpha_1$</td>
<td>0.0023</td>
<td>$\beta_1$</td>
<td>0.4630</td>
</tr>
</tbody>
</table>

It is possible to approximate the dependency of $\sigma$ on piston speed and initial packing density by $\sigma = A_1 U_p + A_o$, where $A_1 = \alpha_1 \phi_{s,0} + \alpha_o$ and $A_o = \beta_1 \phi_{s,0} + \beta_o$. Table 3.8 lists best fit values found for these parameters. The shape parameter $k$ is approximated as a linear function of piston speed, $k = A_1 U_p + A_o$, where $A_1 = 0.0016$ and $A_o = -0.3202$, which represents a least squares fit to the available data for materials $A$, $B$, and $C$. 
Figure 3.19: Predictions of hot-spot perimeter distribution for piston speeds of 300 m/s, 400 m/s, and 500 m/s for (a) meso-structure A, (b) meso-structure B, (c) meso-structure C, and (d) meso-structure D.

3.3.4 Hot-Spot Perimeter

Differences observed in run distances to detonation of coarse and fine granular explosive have been attributed to higher reactive surface areas present in the latter [37]. Therefore, knowledge about the distribution of hot-spot surface areas and their sensitivity to mesostructure may be potentially useful in furthering the development of improved DDT models. Figures 3.19(a)-(d) show the PDFs for hot-spot perimeter and their associated GPD fits.

The results are qualitatively similar to those obtained for hot-spot area. The average hot-spot perimeter ranges from approximately 29-49 μm. Lower initial solid volume
Table 3.9: Mean and standard deviations for hot-spot perimeter determined from sample data for each meso-structure.

<table>
<thead>
<tr>
<th>Meso-Structure</th>
<th>Piston Speed (m/s)</th>
<th>Mean (µm)</th>
<th>Std. Dev. (µm)</th>
</tr>
</thead>
<tbody>
<tr>
<td>A</td>
<td>300</td>
<td>29.79</td>
<td>22.75</td>
</tr>
<tr>
<td>A</td>
<td>400</td>
<td>36.65</td>
<td>30.64</td>
</tr>
<tr>
<td>A</td>
<td>500</td>
<td>49.42</td>
<td>50.49</td>
</tr>
<tr>
<td>B</td>
<td>300</td>
<td>31.00</td>
<td>23.81</td>
</tr>
<tr>
<td>B</td>
<td>400</td>
<td>31.75</td>
<td>24.05</td>
</tr>
<tr>
<td>B</td>
<td>500</td>
<td>47.56</td>
<td>46.04</td>
</tr>
<tr>
<td>C</td>
<td>300</td>
<td>27.71</td>
<td>21.42</td>
</tr>
<tr>
<td>C</td>
<td>400</td>
<td>31.75</td>
<td>24.05</td>
</tr>
<tr>
<td>C</td>
<td>500</td>
<td>36.75</td>
<td>30.27</td>
</tr>
<tr>
<td>D</td>
<td>300</td>
<td>28.66</td>
<td>21.77</td>
</tr>
<tr>
<td>D</td>
<td>400</td>
<td>31.54</td>
<td>23.69</td>
</tr>
<tr>
<td>D</td>
<td>500</td>
<td>37.15</td>
<td>26.98</td>
</tr>
</tbody>
</table>

Figure 3.20: Means and standard deviations for $\Gamma$ plotted as a function of piston speed for each meso-structure.
fractions correlate with higher mean values of hot-spot perimeter and larger standard deviations, as well as longer “tails.” No substantial particle shape influence is predicted. Table 3.9 and Fig. 3.20 summarizes the mean and standard deviations of hot-spot surface area for each material and piston speed.

The variation in generalized Pareto parameters with piston speed for each meso-structure is shown in Figure 3.21(a) and (b). The shape parameter $k$ is linearly dependent on piston speed and changes slope as initial particle packing density is decreased. This change in slope is likely in response to the growth of the tail, which increases with decreasing initial particle packing density. Higher piston speeds correlate with higher values of $\sigma$.

The scale parameter $\sigma$ can be described by $\sigma = A_1 U_p + A_o$, where $A_1 = \alpha_2 \phi_{s,0}^2 + \alpha_1 \phi_{s,0} + \alpha_o$, and $A_o = \beta_1 \phi_{s,0} + \beta_o$. A least squares fit to the data yields the following values for these parameters: $\alpha_2 = 0.0096$, $\alpha_1 = -0.0104$, $\alpha_o = 0.0047$, $\beta_1 = -0.3164$, $\beta_o = 2.625$.

### 3.3.5 Hot-Spot Shape

In this section, the marginal distributions of hot-spot eccentricity and perimeter-to-area ratio are presented and discussed. As previously mentioned, hot-spot shape is characterized by an eccentricity, $\epsilon$, and a perimeter-to-area ratio, $L$. A change of variable is made, given
Figure 3.22: Predictions of hot-spot eccentricity distribution for piston speeds of 300 m/s, 400 m/s, and 500 m/s for (a) meso-structure A, (b) meso-structure B, (c) meso-structure C, and (d) meso-structure D circle. This is done in order to describe the distribution of hot-spot eccentricities with a GPD.

Figure 3.22 shows the PDFs for $\nu$, and their associated GDP fits, for each meso-structure. The distributions are similar for all meso-structures at every piston speed and indicate a majority of highly eccentric (planar) hot-spots. This correlates with observations made of the predicted temperature field which show the most intense heating occurs most
Table 3.10: Mean and standard deviations for hot-spot eccentricity, $\varepsilon$, determined from sample data for each meso-structure.

<table>
<thead>
<tr>
<th>Material</th>
<th>Piston Speed (m/s)</th>
<th>Mean</th>
<th>Std. Dev.</th>
</tr>
</thead>
<tbody>
<tr>
<td>A</td>
<td>300</td>
<td>0.8659</td>
<td>0.1401</td>
</tr>
<tr>
<td>A</td>
<td>400</td>
<td>0.8923</td>
<td>0.1214</td>
</tr>
<tr>
<td>A</td>
<td>500</td>
<td>0.8970</td>
<td>0.1126</td>
</tr>
<tr>
<td>B</td>
<td>300</td>
<td>0.8773</td>
<td>0.1438</td>
</tr>
<tr>
<td>B</td>
<td>400</td>
<td>0.8883</td>
<td>0.1295</td>
</tr>
<tr>
<td>B</td>
<td>500</td>
<td>0.8956</td>
<td>0.1127</td>
</tr>
<tr>
<td>C</td>
<td>300</td>
<td>0.8728</td>
<td>0.1445</td>
</tr>
<tr>
<td>C</td>
<td>400</td>
<td>0.8953</td>
<td>0.1122</td>
</tr>
<tr>
<td>C</td>
<td>500</td>
<td>0.8898</td>
<td>0.1067</td>
</tr>
<tr>
<td>D</td>
<td>300</td>
<td>0.8749</td>
<td>0.1554</td>
</tr>
<tr>
<td>D</td>
<td>400</td>
<td>0.8865</td>
<td>0.1272</td>
</tr>
<tr>
<td>D</td>
<td>500</td>
<td>0.8750</td>
<td>0.1279</td>
</tr>
</tbody>
</table>

Figure 3.23: Means and standard deviations for hot-spot eccentricity plotted as a function of piston speed for each meso-structure.
Figure 3.24: Estimated GPD parameters, (a) $k$ and (b) $\sigma$, and 95% confidence bounds for $\nu = 1 - \epsilon$ as a function of piston speed for each meso-structure.

frequently in the vicinity of interparticle contacts. A high concentration of planar hot-spots suggests dissipative heating due to surface phenomena is the most dominate hot-spot formation mechanism in these materials. Table 3.10 and Fig. 3.23 summarizes the means and standard deviations of hot-spot eccentricity.

Figure 3.24 shows the variation in GPD parameters for hot-spot eccentricity. In this case, $k$ and $\sigma$ are largely insensitive to variations in piston speed or meso-structure. The distributions of hot-spot eccentricity can thus be described with a single distribution, parameterized to best fit values of $k$ and $\sigma$, given by $k = 0.242$ and $\sigma = 0.0967$.

The second measure of hot-spot shape is given by its perimeter-to-area ratio, $\mathcal{L}$. Figure 3.25 shows the distribution of $\Gamma$ for 300 m/s, 400 m/s, and 500 m/s piston impact speeds of material $A$. These distributions were chosen to illustrate features which are representative of those seen in all meso-structures. There is evidence of at least two modes in these distributions, though the physical significance of these modes is unclear at this time. Describing these distributions would require a more complex distribution function. Instead, the reciprocal of $\mathcal{L}$ is considered, which is more “well-behaved” than $\mathcal{L}$. 

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Figures 3.26(a)-(d) show distributions of the reciprocal of $L$ and are reasonably described with a generalized extreme value distribution. Higher values of $U_p$ are associated with higher area-to-perimeter ratios, which correspond to larger hot-spots forming at higher piston speeds. The area-to-perimeter ratio is also sensitive to changes in initial solid volume fraction, with lower values of $\bar{\phi}_{s,0}$ correlating with higher area-to-perimeter ratios. Table 3.11 and Fig. 3.27 summarizes the means and standard deviations in area-to-perimeter ratio data for each meso-structure. Figure 3.28 shows the sensitivity of the GEV parameters to changes in piston speed and meso-structure. The shape parameter $k$:
Figure 3.26: Predictions of hot-spot area-to-perimeter distribution for piston speeds of 300 m/s, 400 m/s, and 500 m/s for (a) meso-structure A, (b) meso-structure B, (c) meso-structure C, and (d) meso-structure D

is linearly dependent on piston speed and there are only minor differences between meso-structures A, B, and C, while meso-structure D shows a marked difference in the value of $k$ which may be the result of particle shape. The scale parameter $\sigma$ shows a weak positive correlation with piston speed and weak negative correlation with initial particle packing density. The location parameter $\mu$ is also weakly correlated with piston speed and decreases monotonically with increasing initial packing density. The behavior of $k$ is approximated as a linear function of piston speed and is given by $k = a_1 U_p + a_0$ where
Table 3.11: Means and standard deviations of the hot-spot area-to-perimeter ratio determined from sample data for each meso-structure.

<table>
<thead>
<tr>
<th>Meso-Structure</th>
<th>Piston Speed (m/s)</th>
<th>Mean (µm)</th>
<th>Std. Dev. (µm)</th>
</tr>
</thead>
<tbody>
<tr>
<td>A</td>
<td>300</td>
<td>0.75</td>
<td>0.25</td>
</tr>
<tr>
<td>A</td>
<td>400</td>
<td>0.82</td>
<td>0.35</td>
</tr>
<tr>
<td>A</td>
<td>500</td>
<td>0.98</td>
<td>0.52</td>
</tr>
<tr>
<td>B</td>
<td>300</td>
<td>0.70</td>
<td>0.24</td>
</tr>
<tr>
<td>B</td>
<td>400</td>
<td>0.76</td>
<td>0.33</td>
</tr>
<tr>
<td>B</td>
<td>500</td>
<td>0.93</td>
<td>0.52</td>
</tr>
<tr>
<td>C</td>
<td>300</td>
<td>0.64</td>
<td>0.18</td>
</tr>
<tr>
<td>C</td>
<td>400</td>
<td>0.75</td>
<td>0.32</td>
</tr>
<tr>
<td>C</td>
<td>500</td>
<td>0.86</td>
<td>0.45</td>
</tr>
<tr>
<td>D</td>
<td>300</td>
<td>0.51</td>
<td>0.12</td>
</tr>
<tr>
<td>D</td>
<td>400</td>
<td>0.60</td>
<td>0.28</td>
</tr>
<tr>
<td>D</td>
<td>500</td>
<td>0.82</td>
<td>0.49</td>
</tr>
</tbody>
</table>

Figure 3.27: Means and standard deviations for area-to-perimeter ratio plotted as a function of piston speed for each meso-structure.
Figure 3.28: Estimated GEV parameters, (a) $k$, (b) $\sigma$, (c) $\mu$, and 95% confidence bounds for hot-spot area-to-perimeter ratio as a function of piston speed for each meso-structure.

$a_1 = 0.00133$ and $a_o = -0.257$. The scale parameter is described by $\sigma = b_2 U_p^2 + b_1 U_1 + b_o$, where $b_2 = \alpha_1 \overline{\phi}_{s,0} + \alpha_o$, $b_1 = \beta_1 \overline{\phi}_{s,0} + \beta_o$, and $b_o = \gamma_1 \overline{\phi}_{s,0} + \gamma_o$. Here $a_{0,1}$, $b_{0,1}$, and $\gamma_{0,1}$ are constants summarized in Table 3.12. The location parameter can be described by $\mu = c_1 U_p + c_o$, where $c_o = -0.914 \overline{\phi}_{s,0} + 1.1031$, and $c_1 = 0.0004$. 
Table 3.12: Quantities for area-to-perimeter GEV parameter estimates.

<table>
<thead>
<tr>
<th>Parameter</th>
<th>value</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\alpha_0 (s^2/m)$</td>
<td>$1.464 \times 10^{-5}$</td>
</tr>
<tr>
<td>$\alpha_1 (s^2/m)$</td>
<td>$-1.817 \times 10^{-5}$</td>
</tr>
<tr>
<td>$\beta_0 (s)$</td>
<td>$-0.012$</td>
</tr>
<tr>
<td>$\beta_1 (s)$</td>
<td>$0.015$</td>
</tr>
<tr>
<td>$\gamma_0 (\mu m)$</td>
<td>$2.671$</td>
</tr>
<tr>
<td>$\gamma_1 (\mu m)$</td>
<td>$-3.356$</td>
</tr>
</tbody>
</table>

3.3.6 Sensitivity Analysis

In this section we investigate the sensitivity of the marginal distributions to the choice of threshold temperature and discuss their implications. Hot-spot material in this study is selected by establishing a temperature threshold, $T_{th}$, where material having a temperature above $T_{th}$ is considered a hot-spot. However, there is no strict rule by which $T_{th}$ is selected. As $T_{th}$ is increased, a smaller fraction of explosive material will qualify as hot-spot material, which results in fewer hot-spots with higher mean temperatures and smaller sizes. This is illustrated in Figs. 3.29(a)-(d), which show the dependence of hot-spot intensity, size, and perimeter on the choice of $T_{th}$ for material $A$. These results are representative of the trends demonstrated by all meso-structures at all piston speeds.

Increasing the value of $T_{th}$ from 500 K to 800 K shifts the hot-spot intensity distributions by an equal amount along the abscissa and reduces the rate of decay of the tail, which is to say that hot-spots selected using a $T_{th} = 700$ K have a greater probability of having higher hot-spot intensities than those selected using a $T_{th} = 500$ K. This is true of both $h_T$ and $h_F$. Raising $T_{th}$ from 500 K to 700 K eliminates material below 700 K, increasing the mean temperature of a hot-spot by construction. In addition, the increase in $T_{th}$ significantly reduces the number of hot-spots in the domain, which changes the percentage of hot-spots with peak temperatures at or above 700 K. Therefore, changes in $h_T$ and $h_F$ are physical.
Figure 3.29: Distribution sensitivity to choice of $T_{th}$.

Hot-spot sizes and perimeters are smaller for larger values of $T_{th}$, which results in a steepening of $h_A$ and $h_l$ and an elimination of the tail observed at $T_{th} = 500$ K. The similarity of $h_A$ and $h_l$ at $T_{th} = 700$ K and 800 K suggests there exists a range of $T_{th}$ which will not influence hot-spot size and perimeter. The same does not hold true for $h_T$ and $h_F$.

The sensitivity of these distributions to the choice of $T_{th}$ raises questions about the flexibility of this approach. Comparisons between meso-structures can only be made between hot-spot distributions computed using the same value of $T_{th}$. The problem of threshold choice is often encountered in Peaks Over Threshold (POT) models used in Extreme Value Theory. [30].
It should be noted, however, that analyzing hot-spot temperature fields at several different levels of $T_{th}$ may be necessary to completely characterize hot-spots in these systems.

### 3.4 Hot-Spot Morphology - Joint Distributions

Marginal distributions are unable to provide information on the dependency structure between random variables. Joint distributions are able to provide this additional piece of information. In this study, we focus on joint distributions of hot-spot size and temperature because they play a fundamental role in identifying critical hot-spots. Figures 3.30(a)-(d) show the variations in the joint distribution of hot-spot size and peak temperature with piston speed for each meso-structure. A positive correlation exists between hot-spot size and peak temperature. Figures 3.31(a)-(c) show contours of probability for material $A$ at piston speeds of 300 m/s, 400 m/s, 500 m/s. These contours are representative of the probability contours for the remaining meso-structures. Only the contours for material $A$ are shown for the sake of brevity.

The dependency between univariate distributions may be parameterized using copulas [34]. A copula is a function that links univariate marginals to their full multivariate distribution, while preserving the original marginal distributions, by mapping the random variables of interest, in this case $\tilde{T}$ and $\tilde{A}$, into other variables that have “well-behaved” distributions and for which it is easy to define a correlation structure. Several parametric copulas exist, such as Gaussian and Student-t copulas, that can be used to describe the dependency structure between variables. It may be possible to correlate the parameters of the copula with microstructural features, such as initial particle packing density and particle shape, based on the marginal distributions obtained from a few “training meso-structures”. These correlations can then be used to generate predictive models that can estimate the distribution of hot-spots in a variety of materials without the need for computationally intensive meso-scale simulations.
To illustrate this idea, the marginal distributions of hot-spot peak temperature and size obtained for meso-structure A at 500 m/s were used to calculate the correlation for a Student-t copula, which is parameterized by its linear correlation matrix, $\rho$, and degrees of freedom, $\nu$. These parameters are determined using built-in MATLAB routines. A Monte Carlo simulation was used to generate hot-spot distributions with the same number density, marginal distributions, and dependency structure as meso-structure A using the copula correlation and the GPD fits to the original data. Figure 3.32(a) shows the joint distribution of hot-spot size and peak temperature resulting from a 500 m/s piston impact for material A computed directly from hot-spot temperature fields, while Figure 3.32(b)
Figure 3.31: Joint distribution of hot-spot area and peak temperatures showing contours of probability for piston speeds of (a) 300 m/s, (b) 400 m/s, (c) 500 m/s.

shows predictions for the same joint distribution using the copula technique. Though the results are preliminary, they suggest it may be possible to generate a set of copulas parameterized to features of the meso-structure which could then be used to estimate probable hot-spot distributions for a variety of materials without the need for computationally intensive simulations.
Figure 3.32: (a) Contours of probability for a 500 m/s piston impact computed from meso-scale data. (b) Predictions for probabilities of hot-spot size and temperature computed using copulas.

3.5 Hot-Spot Proximity and Integrated Quantities

3.5.1 Hot-Spot Proximity

Hot-spot proximity is characterized using two distribution functions: a surface-to-surface nearest neighbor function, and a point-to-surface nearest neighbor function. As discussed in Chapter 2, these distributions provide information about hot-spot proximity and clustering, which are important for hot-spot growth and coalescence. Figure 3.33 shows the results for the surface-to-surface function, and Table 3.13 and Fig. 3.34 summarizes the mean and standard deviations for these distributions.

The average distance between neighboring hot-spots is within the average particle size and ranges from approximately 12-56 µm. Because hot-spot number and size increase with initial porosity and piston speed the distance between hot-spots decreases making the likelihood of hot-spot coalescence, as well as the rate of hot-spot coalescence, increase. These distributions are reasonably described by a Weibull distribution and show a strong dependence between hot-spot proximity and both piston speed and initial porosity.
Figure 3.33: Variation in hot-spot surface-surface nearest neighbor distribution with piston speed for each meso-structure.

Figure 3.35(a) and (b) show how Weibull parameters $A$ and $B$ vary with piston speed and initial packing density. Similar results are evident in the point-to-surface distributions, which are shown in Figures 3.36(a)-(d).

Average point-surface distances range between 36-62 μm and indicate a sensitivity to piston speed and initial porosity. Table 3.14 and Fig. 3.37 summarizes the means and standard deviations in point-surface distance for each meso-structure.

In order to investigate the clustering of hot-spots, we compare the surface-surface and point-surface nearest neighbor distribution functions. For a system of uniformly distributed hot-spots, these distributions would lie roughly on top of one another, while clustering
Table 3.13: Mean and standard deviations for surface-surface distributions.

<table>
<thead>
<tr>
<th>Meso-Structure</th>
<th>Piston Speed (m/s)</th>
<th>Mean (µm)</th>
<th>Std. Dev. (µm)</th>
</tr>
</thead>
<tbody>
<tr>
<td>A</td>
<td>300</td>
<td>32.78</td>
<td>32.01</td>
</tr>
<tr>
<td>A</td>
<td>400</td>
<td>20.54</td>
<td>17.61</td>
</tr>
<tr>
<td>A</td>
<td>500</td>
<td>12.43</td>
<td>10.53</td>
</tr>
<tr>
<td>B</td>
<td>300</td>
<td>32.07</td>
<td>33.50</td>
</tr>
<tr>
<td>B</td>
<td>400</td>
<td>21.17</td>
<td>19.31</td>
</tr>
<tr>
<td>B</td>
<td>500</td>
<td>12.52</td>
<td>10.51</td>
</tr>
<tr>
<td>C</td>
<td>300</td>
<td>50.56</td>
<td>52.24</td>
</tr>
<tr>
<td>C</td>
<td>400</td>
<td>32.34</td>
<td>27.78</td>
</tr>
<tr>
<td>C</td>
<td>500</td>
<td>17.37</td>
<td>14.11</td>
</tr>
<tr>
<td>D</td>
<td>300</td>
<td>55.63</td>
<td>88.81</td>
</tr>
<tr>
<td>D</td>
<td>400</td>
<td>36.40</td>
<td>46.72</td>
</tr>
<tr>
<td>D</td>
<td>500</td>
<td>22.86</td>
<td>19.55</td>
</tr>
</tbody>
</table>

Figure 3.34: Means and standard deviations for $r_{s,s}$ plotted as a function of piston speed for each meso-structure.
Figure 3.35: Variation in GP parameters for hot-spot mean temperature distribution with piston speed for each meso-structure.

Figure 3.36: Variation in hot-spot point-surface nearest neighbor distribution with piston speed for each meso-structure.
Table 3.14: Mean and standard deviations for the point-surface distributions.

<table>
<thead>
<tr>
<th>Meso-Structure</th>
<th>Piston Speed (m/s)</th>
<th>Mean (µm)</th>
<th>Std. Dev. (µm)</th>
</tr>
</thead>
<tbody>
<tr>
<td>A</td>
<td>300</td>
<td>61.70</td>
<td>45.59</td>
</tr>
<tr>
<td>A</td>
<td>400</td>
<td>31.82</td>
<td>22.66</td>
</tr>
<tr>
<td>A</td>
<td>500</td>
<td>19.97</td>
<td>16.78</td>
</tr>
<tr>
<td>B</td>
<td>300</td>
<td>72.55</td>
<td>57.40</td>
</tr>
<tr>
<td>B</td>
<td>400</td>
<td>34.22</td>
<td>23.62</td>
</tr>
<tr>
<td>B</td>
<td>500</td>
<td>18.41</td>
<td>12.96</td>
</tr>
<tr>
<td>C</td>
<td>300</td>
<td>106.92</td>
<td>76.04</td>
</tr>
<tr>
<td>C</td>
<td>400</td>
<td>49.01</td>
<td>31.15</td>
</tr>
<tr>
<td>C</td>
<td>500</td>
<td>23.24</td>
<td>14.91</td>
</tr>
<tr>
<td>D</td>
<td>300</td>
<td>229.17</td>
<td>196.67</td>
</tr>
<tr>
<td>D</td>
<td>400</td>
<td>119.67</td>
<td>96.15</td>
</tr>
<tr>
<td>D</td>
<td>500</td>
<td>35.62</td>
<td>22.39</td>
</tr>
</tbody>
</table>

Figure 3.37: Means and standard deviations for \( r_{p,s} \) plotted as a function of piston speed for each meso-structure.
Figure 3.38: Variation in Weibull parameters for hot-spot point-surface nearest neighbor distribution with piston speed for each meso-structure.

Figure 3.39: Comparison between nearest neighbor distributions with piston speed for each meso-structure.
Figure 3.40: Comparison between nearest neighbor distributions with material for each piston speed.

would yield a larger number of short distance hot-spot neighbors and tend to separate the two distributions. Figure 3.39 shows nearest neighbor cumulative distribution function comparisons across piston speeds for each material. There is clear evidence of hot-spot clustering in all materials at every piston speed, with the hot-spot clusters being more sparsely distributed at the lower piston speeds.

Figures 3.40(a)-(c), which show comparisons of the nearest neighbor functions with material for each piston speed, reveal several features of interest. Most notably, a shift in the degree of clustering is observed between the materials over the range of piston speeds simulated. At 300 m/s, material $D$ possess the most strongly clustered hot-spot
distribution; however, at 500 m/s, material A appears to be the most strongly clustered though the reason for this is not entirely clear. We note that material A, in addition to having the lowest packing density, also contains the largest deviations in packing density. It may be that, at higher piston speeds, the influence of deviations in initial porosity on hot-spot clustering is more pronounced than at the lower speeds, where substantially fewer hot-spots are formed.

### 3.5.2 Integrated Quantities

Figures 3.41(a)-(c) show the variation in hot-spot number density, volume fraction, and specific surface area with piston speed for each meso-structure. An exponential growth in each of these quantities is predicted over the narrow range of piston speeds considered. The integrated hot-spot quantities are sensitive to changes in initial particle packing densities ranging from 67%-83% TMD. No significant changes are observed in these quantities below an initial solid volume fraction of 67%. This is similar to observations seen in the hot-spot size distribution, and are qualitatively similar to the results of Czerski and Proud [9]. The effect of particle shape on these quantities appears to be minor. The slopes of the curves are similar for all materials except for hot-spot number density, in which the rate of increase of hot-spot number density is slightly lower for $\tilde{\phi}_x = 0.577$, and 0.678 due to the clustering of hot-spots in those materials at higher piston speeds. That is, two nearby hot-spots may become a single hot-spot if, at a higher impact speed, the material between them is heated above $T_{th}$.

These hot-spot properties can be approximately described by the general expression

$$\ln Y = A_1 U_p + A_o, \quad (3.5)$$

where $Y$ is the property of interest, and $A_1$ and $A_o$ are given by
Figure 3.41: Variation in hot-spot number density, volume fraction, and specific surface with piston speed for each meso-structure.

Table 3.15: Parameters for $A_1$ for each average quantity.

<table>
<thead>
<tr>
<th>Quantity</th>
<th>$\alpha_2$</th>
<th>$\alpha_1$</th>
<th>$\alpha_o$</th>
<th>$\beta_2$</th>
<th>$\beta_1$</th>
<th>$\beta_o$</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\rho_{HS}$</td>
<td>0.0000</td>
<td>0.0140</td>
<td>-0.0006</td>
<td>0.0000</td>
<td>-9.9290</td>
<td>8.1628</td>
</tr>
<tr>
<td>$\phi_{HS}$</td>
<td>0.0327</td>
<td>-0.0353</td>
<td>0.0216</td>
<td>-52.071</td>
<td>62.2190</td>
<td>-23.534</td>
</tr>
<tr>
<td>$s_{HS}$</td>
<td>0.0000</td>
<td>0.0085</td>
<td>0.0050</td>
<td>0.0000</td>
<td>-9.0609</td>
<td>3.6333</td>
</tr>
</tbody>
</table>


\[ A_1 = \alpha_2 \theta^2_{s,0} + \alpha_1 \bar{\theta}_{s,0} + \alpha_0 \]  
\[ A_0 = \beta_2 \bar{\theta}^2_{s,0} + \beta_1 \bar{\theta}_{s,0} + \beta_0 \]  

(3.6)  
(3.7)

Table 3.15 lists the values for \( \alpha \) and \( \beta \) used in this study.

3.6 Discussion and Combustion Implications

Analysis of inert temperature field predictions indicates that hot-spot intensity is unaffected by changes in piston speed, initial particle packing density, or particle shape over the ranges \( 300 \text{ m/s} \leq U_p \leq 500 \text{ m/s} \) and \( 0.57 \leq \bar{\theta}_{s,0} \leq 0.84 \). Significant changes in the hot-spot size and perimeter distributions, as well as the integrated quantities of hot-spot number density, volume fraction, and specific surface area are associated with changes in piston speed and meso-structure. This is best illustrated by considering the predicted temperature fields of meso-structure \( A \) and \( D \), shown in Fig. 3.42, which represent the maximum and minimum values of initial solid volume fraction.

![Figure 3.42: Predicted temperature field behind a uniaxial wave for \( U_p = 500 \text{ m/s} \) in (a) a small region in meso-structure \( A \), and (b) a small region in meso-structure \( D \).](image)

To investigate the ignition implications of these results, an ignition manifold is applied to the joint distributions of hot-spot size and peak temperature to identify critical hot-spots.
Figure 3.43: Critical hot-spots predicted in (a) Meso-Structure A, (b) Meso-Structure B, (c) Meso-Structure C, (d) Meso-Structure D.

Peak temperatures were used to identify critical hot-spots instead of mean temperatures because no critical hot-spots were predicted to occur when critical temperature was based on the mean temperature. The ignition manifold used in this study is based on the analysis by Tarver, et al. [39], for the critical size and temperature of cylindrical hot-spots. The ignition manifold is illustrated by the solid curve in Fig. 3.43. Hot-spots above this curve are identified as critical and assumed to locally experience thermal explosion. This manifold may be summarized by the following expression

$$T_{\text{crit}} = c_2 (\ln \hat{A}_{\text{crit}})^2 + c_1 \ln \hat{A}_{\text{crit}} + c_o,$$  \hspace{1cm} (3.8)
where $T_{\text{crit}}$ is the critical temperature, $\hat{A}_{\text{crit}}$ the critical size, and $c_o$, $c_1$, and $c_2$ are constants given by $c_o = 1.029 \times 10^3$, $c_1 = -34.083$, and $c_2 = 0.973$.

Figure 3.44 shows reacted mass fractions, based on peak temperatures, for each material as a function of piston speed. There is an exponential growth in the fraction of reacted mass with piston speed for all meso-structures, which is qualitatively similar to the predictions for hot-spot number density, volume fraction, and specific surface area. No critical hot-spots are predicted to occur in meso-structure $D$ at 300 m/s. On average, lower values of $\bar{\phi}_{s,0}$ correlate with higher reacted mass fractions. The reacted mass fraction curves of meso-structures $A$ and $B$ are observed to intersect at $U_p = 300$ m/s, but this is most likely a numerical artifact. A single critical hot-spot accounts for the difference in reacted mass between those meso-structures at that speed, suggesting that the inconsistency is not statistically significant.

By combining inert hot-spot distribution predictions with thermal explosion data, it is possible to estimate the distribution of ignition times in the material. The probability of shock induced ignition in reactive gases has been related to the distribution of observed explosion times[40]. The ignition time distributions obtained in this study may provide
Figure 3.45: Estimated ignition times based on [16].

the foundation for future work into a similar theory for impact induced ignition in reactive solids by providing insight into the early time ignition behavior of the material [12].

Here, we use an expression for explosion times given by Henson, et al. [16], for HMX based materials:

\[
\tau(T) = \exp \left[ \ln \left( \frac{1}{B} \right) + \frac{E_r}{RT} \right]
\]

(3.9)

where \( B = 5.9 \times 10^{12} \text{s}^{-1} \), \( E_r = 148.9 \text{ kJ/mol} \), and \( R \) is the gas constant. It should be noted that no critical hot-spots were observed when mean hot-spot temperatures were used, and so the following analysis utilizes the peak hot-spot temperatures to illustrate the approach,
which will provide a lower limit on the estimated ignition time distributions. Figure 3.45 shows estimated ignition time distributions for each meso-structure for a piston impact speed of $U_p = 500$ m/s. A piston speed of 500 m/s was used for illustrative purposes. The limited number of critical hot-spots predicted at the lower speeds makes statistical characterization difficult. Similar local ignition times are predicted for all meso-structures, though meso-structures $A$ and $B$ are observed to have a number of critical hot-spots with substantially longer ($\sim 50-100$ $\mu$s) with cook-off times.

The most significant difference between the distributions is predicted in the number of critical hot-spots, though precisely how many critical hot-spots are necessary to transition from local ignition to global ignition is unknown. It may be that only a single critical hot-spot is needed to trigger global ignition. These results predict that local ignition will occur in all meso-structures on similar time scales. This prediction suggests that observable differences in impact sensitivity between these materials may be more closely tied to the growth and coalescence stage, which is likely to be sensitive to the number and size of hot-spots and not with hot-spot intensity, over the narrow range of piston speeds considered in this study.

To illustrate this, distributions of nearest neighbor distances are combined with experimentally observed burn rate data for HMX to estimate critical hot-spot coalescence times. The coalescence time between two critical hot-spots, initially separated by a distance $r_{s,s}$, and burning outward at a constant rate $\dot{r}$, is given by

$$
\tau_c = \frac{r_{s,s}}{2\dot{r}},
$$

(3.10)

where $\tau_c$ is the coalescence time associated with the surface-to-surface distance $r_{s,s}$, and $2\dot{r}$ represents the rate of closure between two burning hot-spots. Figure 3.46 shows the distribution of surface-to-surface distances between critical hot-spots in meso-structures $A$ and $D$ resulting from a 500 m/s piston impact. A similar range of $r_{s,s}$ distances are
Figure 3.46: (a) Surface-to-surface distances between critical hot-spots in meso-structures $A$. (b) Surface-to-surface distances between critical hot-spots in meso-structures $D$. (c) A comparison of the estimated coalescence times for critical hot-spots in meso-structures $A$ and $D$.

observed in both meso-structures, though meso-structure $A$ possesses a larger number of critical hot-spots (60) in comparison with meso-structure $D$, in which 18 critical hot-spots are observed.

Figure 3.46(c) shows the estimated coalescence times for the critical hot-spots of both meso-structures. Here, a constant burn rate of $\dot{r} = 10 \, \mu m/\mu s$ was chosen and is representative of experimentally observed burn rates in binderless HMX for pressures above 4 MPa [8], which is consistent with average pressure predictions from the meso-scale simu-
lations for piston speeds of 500 m/s. As with $r_{s,s}$ distances, the range of $\tau_c$ is similar for 99% of the critical hot-spots in both meso-structures, which suggests that the quantity of critical hot-spots plays a dominate role in establishing the impact and shock sensitivity.
Chapter 4
Conclusions and Recommendations

The primary objective of this study was to formulate a methodology for characterizing hot-spots that can be used to examine the influence of meso-structure on impact induced heating of solid high-explosive. To that end, a Peaks over Threshold approach is proposed to filter out cooler explosive material and generate hot-spot temperature fields from predicted, inert temperature fields formed behind quasi-steady uniaxial waves in granular explosive. Commonly used image processing algorithms can then applied to identify hot-spots and quantify their intensity, area, perimeter, and shape, which are collectively referred to as hot-spot morphology. The statistical nature of the hot-spots can then be characterized by a general multivariate probability density function. This study focuses primarily on the associated marginal distributions of hot-spot intensity, area, perimeter, and shape, as well as joint distributions of hot-spot area and temperature, as they are important in the early time ignition response of solid explosives. Additional integrated quantities, such as hot-spot number density and volume fraction, as well as hot-spot proximity and clustering information is also obtained which is important in the subsequent growth of reaction in these materials.

To illustrate how the approach can be applied, the inert impact of four meso-structures, composed of randomly packed hexagonal and/or circular shaped particles of granular HMX ($C_4H_8N_8O_8$) with average initial solid volume fractions, $\bar{\phi}_{s,0}$, in the range $0.57 \leq \bar{\phi}_{s,0} \leq 0.84$, was numerically simulated using a combined finite element-discrete element code developed by Panchadhara and Gonthier [32]. The influence of wave strength, initial particle packing density, and particle shape on the distribution of hot-spots formed behind quasi-steady compaction waves was determined by examining trends in the resulting marginal distributions, and correlations between piston speed and initial particle packing density were characterized by establishing parametric fits to the marginal distributions of hot-spot
intensity, area, perimeter, and shape. Predictions indicate that hot-spot temperature distributions are largely insensitive to changes in piston speed, $U_p$, or $\bar{\phi}_{s,0}$ over the ranges $300 \leq U_p \leq 500$ m/s and $0.57 \leq \bar{\phi}_{s,0} \leq 0.84$. Higher piston speeds and lower initial solid volume fractions correlated with larger hot-spot areas and larger hot-spot perimeters within these ranges. Distributions of hot-spot eccentricity, used in this study to characterize hot-spot shape, show a high concentration of planar hot-spots, which indicate dissipation in the vicinity of contact surfaces is the dominate hot-spot formation mechanism in these meso-structures. Changes in initial particle shape did not produce significant changes in the distribution of hot-spots. The most significant changes were observed in the hot-spot number density, volume fraction, and specific surface area, which were shown to be sensitive to changes in initial particle packing densities ranging from 67%-83% TMD, and are predicted to grow exponentially with piston speed over the ranges considered in this study. No significant changes are observed in these quantities below an initial solid volume fraction of 67%, which is qualitatively similar to the results of Czerski and Proud [9]. Overall, the results indicated that changes in piston speed or initial particle packing density primarily influence the number and size of hot-spot in the domain and not their intensity.

The combustion implications of this result were examined by combining inert heating predictions for uniaxial waves with thermal explosion data and analysis to identify critical hot-spots and compute the local fractions of ignited mass. Critical hot-spots were identified using an ignition manifold based on the analysis by Tarver, et al. [39], for the critical size and temperature of cylindrical hot-spots. Predictions for reacted mass fraction based on peak hot-spot temperature showed an exponential growth with piston speed for all meso-structures, which is qualitatively similar to the predictions for hot-spot number density, volume fraction, and specific surface area. On average, lower values of $\bar{\phi}_{s,0}$ correlated with higher reacted mass fractions. Predictions for the ignition time distribution, estimated using an expression for explosion times given by Henson, et al. [16], were found to be insensitive to changes in piston speed or meso-structure. Similar local ignition times are
predicted for all meso-structures, though the number of critical hot-spots predicted for each meso-structure varied significantly. Precisely how many critical hot-spots are necessary to transition from local ignition to global ignition is unknown and it may be that only a single critical hot-spot is needed to trigger global ignition. These predictions suggest that observable differences in impact sensitivity between these materials may be more closely tied to the growth and coalescence stage, which is likely to be sensitive to the number and size of hot-spots and not with hot-spot intensity, over the narrow range of piston speeds considered in this study.

Recommendations for future work include an examination of particle size effects on hot-spot formation and extending the analysis to metalized explosive systems. It is also suggested that a local analysis of the hot-spot fields be performed to investigate the influence of statistical anisotropy on the hot-spot distributions.
References


Vita

John N. Gilbert enrolled at Louisiana State University in 2008 in pursuit of a Bachelor of Science in mechanical engineering. In 2010, he accepted an invitation to the Accelerated Master’s Program offered by the Department of Mechanical Engineering. Gilbert earned his B.S. in 2011, and is a candidate for the Master of Science in Mechanical Engineering degree to be awarded in December 2012.