A Parametric Study of Cohesive Zone Modeling Applied to Interfaces Under High Impact Velocity Collisions

Tamanna Tasnim
Marquette University

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A PARAMETRIC STUDY OF COHESIVE ZONE MODELING APPLIED TO INTERFACES UNDER HIGH IMPACT VELOCITY COLLISIONS

by

Tamanna Tasnim

A Thesis submitted to the Faculty of the Graduate School,
Marquette University,
in Partial Fulfillment of the Requirements for
the Degree of Master of Science

Milwaukee, Wisconsin
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ABSTRACT
A PARAMETRIC STUDY OF COHESIVE ZONE MODELING APPLIED TO INTERFACES UNDER HIGH IMPACT VELOCITY COLLISIONS

Tamanna Tasnim
Marquette University, 2020

Understanding the response of energetic materials to dynamic loading is critical for the design and safety of energetic systems. Energetic materials may contain heterogeneous microstructures, and hotspots can form at microstructural interfaces. The hotspots in these microstructures can determine if a material is safe to use. This study presents an analysis of the effect of material interfaces on the dynamic behavior of a heterogeneous sandwich structure subjected to high-velocity impacts using the cohesive zone model. The current work explores the sensitivity of a sugar-PMMA heterogeneous system to interface properties like stiffness, strength, and fracture energy both for normal and oblique impacts. Cohesive zone modeling is common for quasi-static fracture problems but is less common for modeling interfaces in dynamics problems. The dynamic impact simulation is carried out using a three-dimensional finite element framework using the finite element software ABAQUS. These results show that the stiffness of the cohesive zone element significantly affects the reflection of the normal waves at the material interfaces. Furthermore, for both normal and oblique impacts, interface properties are found to have a first-order effect on velocity response. It is also found that the velocity response is more sensitive to the interface strength (normal strength/ shear strength) than fracture energy under high impact dynamic loading.
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Tamanna Tasnim

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1. Introduction

1.1. Motivation

Energetic materials (i.e. explosives, propellants, and pyrotechnics) are extensively used for military, mining, welding and, other commercial applications. Energetic materials may contain heterogeneous microstructures. Sometimes, in crystalline structures of energetic materials, the localized area is found which may have different properties than the rest of the material and shows temperature spikes, which are known as hotspots [1]. These hotspots in the microstructures can determine if a material is safe to use. Nowadays, due to the variety and number of high energy materials for numerous applications, information about chemistry, synthesis, properties, and salient features for these materials are available in the literature.

Explosives under rapid loading conditions can produce high-pressure gases. There are two common types of explosives-low and high explosives [2], [3]. In low explosives, a fast but subsonic wave can be generated from chemical reactions. For an intense reaction to occur, a high degree of confinement is needed, either in the form of casing or “self-confinement” due to a large number of low explosives surrounding the reaction site. On the other hand, in high explosives, the chemical reactions can build up into a supersonic detonation wave without any instant confinement. Based on the length scale, some properties of the material may become more important to study than the others. The mesoscale can be defined as the length scale between the continuum scale (where microstructure can be neglected) and the atomic scale. Mesoscale dimensions are typically ~0.1 µm to 1mm in explosives. One example of homogeneous explosives is liquid
nitromethane refined by diethylene-triamine (DETA). Although it may comprise of a mixture of chemicals, the physical structure of the liquid mixture often contains very few imperfections at the mesoscale level[4]. On the other hand, heterogeneous explosives at the mesoscale levels, for example, the polymer-bonded explosives have density discontinuities (specifically between the polymer and the explosive crystals) due to the transition to different material and defects (i.e. pores and cracks). Polymer bonded explosives include energetic crystals coated in a polymer binder, which essentially separates the crystals and thus, makes it safer to handle and easier to machine. These energetic crystals often have a size-distribution specially designed to facilitate a packing density of more than 90%[4]

Some extensively used heterogeneous energetic systems are hexahydro-1,3,5-trinitro-1,3,5-triazine (RDX) [5], octahydro-1,3,5,7-tetranitro-1,3,5,7-tetrazocine (HMX) [6] and 2,4,6-trinitrotoluene (TNT)[7] with molecular formulae C₃H₆N₆O₆, C₄H₈N₈O₈ and C₆H₂(CH₃)(NO₂)₃ respectively, which have many microstructural interfaces that affect the dynamic response of the material. These energetic crystals consist of both fuel and oxidizer constituents within their molecules. When decomposition triggers, it takes as small as a fraction of a microsecond to produce hot, high-pressure gases like CO₂, H₂O, and N₂, along with tiny solid carbon particles. Most polymer-bonded explosives are slightly porous in nature. Since, there is a reasonable range of maximum densities that can be achieved while manufacturing, this porous structure ensures their sensitivity for reliable initiation in their intended use. For these conventional high explosive detonations, chemical reactions are the fastest. In addition, they have the smallest variation in detonation velocity with explosive charge size [8]. Since their behavior is close to the classic theories of detonation, these
conventional explosives are usually referred to as “ideal” explosives [4]. These high explosives which were thought to be used universally for all weapon applications suffered from lack of consistency during ignition. This happened due to inadvertent ignition by impact or shock [9]. Higher performance has always been a principal criterion in the field of research. The energy released during the decomposition reactions, the number of moles and molecular weight of the gaseous products resulting from the combustion process, and density of the material are some critical factors to define the performance of explosives [10]. As a result, search for safer, more powerful, and stable explosive has been a constant quest for the scientists. Therefore, it is necessary to look for an alternative solution for energetic materials because the existing materials sometimes fail to meet the user demand, increased performance with reduced vulnerability, and low cost.

Due to the shock wave initiation under extreme loading conditions, material deformation and consequent chemical reactions make the dynamic response of energetic materials an extremely complicated process. This complex process involves a variety of length scales ranging from atomic (molecular) dimensions up to continuum (macroscale) levels [11]. As we consider the mesoscopic scales (grain size dimensions range from a few micrometers to a few hundred micrometers in crystalline solids or pressings of granular materials), the shock behavior of heterogeneous systems becomes complex. The shock response includes multiple waves that result in a complicated interaction with material heterogeneities or internal boundaries [12]. This mesoscopic scale has a dominating effect on shock response [13]. Studies show that the shock response of energetic materials also depends on the grain or crystal characteristics of the materials [14]. Crystal pressings
and/or binder materials in heterogeneous explosives can cause variation of the thermodynamics fields resulting in localization of energy to trigger the reaction.

Therefore, to characterize the dynamic response of energetic materials, low-density pressings of granular crystal sugar (sucrose) with polymers can be a critical field of research. Sugar can be used as an inert substitute for HMX and RDX due to its mechanically similar but non-explosive behavior. This low-density, porous granular sugar illustrates mesoscopic scale mechanical effects in the absence of rapid reactions which are illuminated in different literature. An array of magnetic gauge studies are available on low-density sugar, performed by Sheffield et al. [6], [15]. Several studies have been done on shock-loaded sugar which is elaborated in the literature[16]–[18].

Polymer materials have numerous applications in commercial, civil, and military fields. A polymer as adhesives, from basic glues to high strength epoxies, has applications in both the commercial and industrial sectors [26]. In the development of additive manufacturing field, these polymers have become particularly important, serving as a printable media [28]. Furthermore, they serve as binders for energetic composites [27]. For instance, polymer-bonded explosives as mentioned earlier is one potential example of sandwich structure energetic material. To define the sandwich structure, it basically comprised of face materials on two sides of a different core material in the middle. For the sandwich structure studied here, the face material is PMMA and the core material is sugar. The face/core interfaces make the dynamic behavior of this structure complex under high impact loading.

To predict, analyze, and design the applicability of the experimental results on energetic systems, many analysis codes such as CTH from Sandia National Lab [19], [20],
THOR codes [21], CHEETAH [22] (uses thermochemical computer codes), LOTUSES [23] and EDPHT [24], (based on empirical models), etc. are used to model energetic materials. CTH is an Eulerian hydrocode to solve the second-order explicit differential equations essentially developed for wave dynamics and shock-physics. As the term hydrocode implies, it was developed for fluid mechanics and thus, neglects these interfaces and contact models. In the Eulerian method, the computational cell or elements do not move with the material motion. However, using the finite element method with a Lagrangian description[25], the mesh moves with the material, and interfaces are maintained. Therefore, considering these two types of meshes, the Lagrangian approach can track the interfaces and geometry more naturally than the Eulerian mesh. Eulerian methods work much better for large deformations. Lagrangian methods have lots of mesh distortion with large deformation which makes them inaccurate. While Lagrangian methods allow the mesh to move with the materials, the mesh also moves with the interface, and thus does not loose interface details. Therefore, Lagrangian meshes might be a more accurate approach to model the interfaces.

The impact behavior of a heterogeneous structure is influenced by several factors, not only the mechanical properties of the structure’s face components and core but also the parameters of the interfaces. The impact-loading can be divided into different categories depending on their velocity ranges, namely low velocity (applicable for large masses), intermediate velocity (medium masses), high/ ballistic velocity (focus on small mass), and hypervelocity impact (Meteorite craters, impacts by space debris)[26]. The high-velocity impact behavior varies from the low-velocity impact due to the significant changes in the energy transfer between the target and the projectile, energy dissipation, and damage
propagation mechanisms with the variation of velocity range of the projectile [27]. Therefore, the results drawn from the studies on low-velocity impacts do not generally apply to the high-velocity phenomenon. Any impact with velocity below 10 m/s can be considered as low-velocity impact, the intermediate impacts range from 10 m/s and 50 m/s, while the high velocity (ballistic) impacts have an array of velocity range from 50 m/s to 1000 m/s, and finally, hypervelocity impacts have the range of 2 km/s to 5 km/s [28]. A low-velocity impact is greatly affected by the boundary conditions defined in the system, on the other hand, a high-velocity impact can be defined as an event which is controlled by wave propagation, and is substantially independent of boundary conditions [29]. Most studies available on high-velocity impact behavior of heterogeneous structures are based on experimental tests [30], [31]. Although experimental studies provide information on the sandwich structure tested, to understand the impact phenomena of a heterogeneous sandwich structure accurately modeling of the interface can be a great tool. There are numerous mechanical parameters of the interfaces involved in the energetic systems which include stiffness, strength, and fracture energy of the interface. These mechanical parameters can be captured by the cohesive zone. And therefore, it is important to check how these parameters influence on ballistic behavior. This parametric study to check the sensitivity of the heterogeneous energetic system to interface properties requires a broad test program, which is time-consuming and expensive at the same time. To reduce the cost and time, it is useful to use numerical modeling of the interface.

1.2. Cohesive zone element approach

For finite element analysis, a cohesive zone element (CZE) is used to model the behavior of the interface. These cohesive zone elements are otherwise known as
“decohesion elements” and can be 1) point decohesion elements or discrete cohesive elements which are essentially three-dimensional non-linear springs and (2) continuous decohesion elements connecting line elements, 2D or 3D solid elements or plate or shell elements.

Cohesive zone modeling (CZM) is a suitable method in numerical simulations to model delamination, study the failure of bonded interfaces, analyze impacts on composite structures, and to predict the induced damage for its availability in widely-used finite element codes [32]. CZE is also used in fracture of homogeneous materials without bonded interfaces. The main advantage of CZM over element deletion is that they better model fracture because they naturally account for fracture energy, and do not lose mass like element deletion. Element deletion criteria can also account for fracture energy; however, it would need some extra caution to use. The element deletion is not quite sensitive to the size effect of strength and have far coarser mesh than preferred in any engineering application. Therefore, it is not possible to capture gradients adjacent to the crack tip and eventually overestimate the fracture energy[33]. Besides, CZM can be applied to general finite element codes since it is problem independent. These models are extensively used for matrix cracking and delamination to understand their connection to the fracture mechanics and predict the onset of delamination[32]. Furthermore, while considering the impact phenomenon, CZM provides the ability to anticipate the onset of the various damage modes and the growth of the damage as a result of the impact[32]. Therefore, these models are particularly used in a numerical progressive damage analysis that explains the event of damage development and the degradation of the properties of the plies and the interfaces[34]. While predicting impact damage, with CZMs, this damage propagation
process is based on fracture criterion defined in fracture mechanics. A primary advantage of considering the decohesion elements is the capability to predict both onset and propagation of delamination without prior knowledge of the crack location and propagation direction.

1.3. **Background study of cohesive zone modeling**

In 1987, Needleman[35] first introduced cohesive zone elements in finite element analysis, which is based on cohesive fracture formulations carried out by Dugdale 1960[36] and Barenblatt 1962 [37]. This irreversible cohesive zone elements for finite deformations were further developed by Ortiz and Pandolfi in 1999 [38]. Needleman reviewed the development of cohesive zone modeling in [39].

The behavior of cohesive zone elements can be described in terms of traction-separation law (TSLs) called the cohesive law. Based on the slope of the traction-separation curve, cohesive laws can be divided into two categories: (i) Intrinsic cohesive laws with an initial elastic slope; and (b) extrinsic cohesive laws which are initially rigid [40]

**1.3.1. Bilinear cohesive law**

Among classical energy-based cohesive laws, the bilinear cohesive law is most extensively used. It assumes initially a linear elastic traction-separation law [41][42] before damage and followed by damage initiation and damage evolution and failure of the elements is characterized by progressive degradation of the material stiffness which is illustrated in Figure 1.1.
To define the elastic behavior in the cohesive zone traction-separation law, an elastic stiffness matrix is assigned. This matrix relates the nominal stresses to the nominal strains. In the bi-linear traction-separation law in Figure 1.1, the nominal stress, $T$, increases linearly with the relative displacement $\delta$ until the onset of the decohesion process. When these two quantities, traction and separation reach the critical values, $T_{\text{ultimate}}$ and $\delta_0$, softening, or damage are observed as the relative displacement increases beyond $\delta_0$. Finally, failure of the interface occurs when the displacement reaches its final value $\delta_f$, and at this point traction, $T$ becomes 0. Damage evolution is defined by the fracture energy which is dissipated due to the damage process. The area under the traction-separation curve represents the fracture energy that must be equal to the critical energy release rate $G_C$ [43]. Furthermore, once the damage initiation criterion is met, material damage can occur according to a predefined damage evolution law which is linear in bi-linear cohesive law, where the slope of the damaged traction separation curve is governed by $G_C$. The damage
evolution law illustrates the rate at which the material stiffness is degraded once the corresponding initiation criterion is reached. Therefore, to simply describe the bilinear law:

\[ T_i = k_i \delta_i \]  

(1.1)

Where, \( k_i \) = Initial stiffness of the interface

If a three-dimensional system is considered, nominal stress vector, \( T_i \) comprises of three components one is the normal traction, \( T_n \) and the other two are shear tractions \( T_s \) and \( T_t \) respectively, and the corresponding separations are referred as \( \delta_n \), \( \delta_s \) and \( \delta_t \) respectively, which can be expressed as [43][44]:

\[ \delta_n = \frac{T_n}{K_{nn}} \]  

(1.2)

\[ \delta_s = \frac{T_s}{K_{ss}} \]  

(1.3)

\[ \delta_t = \frac{T_t}{K_{tt}} \]  

(1.4)

The area under the curves must be equal to the corresponding critical strain energy release rate. That is,

\[ G_C = \int_0^{\delta_f} T d\delta \]  

(1.5)

1.4. Arrangement of the thesis

Material presented in this thesis is divided into 5 chapters. This chapter, Chapter 1, provides the motivation of the study which includes background about energetic materials, impact behavior on heterogeneous materials, cohesive zone element approach, and a brief background about cohesive zone modeling. Chapter 2 provides a discussion of the physical system considered for the analysis, material properties (mechanical properties, equation of
state, thermal considerations), the key assumptions that will be used for the analysis of the
dynamic behavior of the heterogeneous system, and the physical basis for the model.
Chapter 3 presents a brief overview of ABAQUS/Explicit software and the models used in
this finite element software. In addition, a mesh convergence study and setting up the
proper time step are analyzed. Chapter 4 presents the analysis results of the dynamic
behavior of the sugar-PMMA heterogeneous system. Several analyses on the sensitivity of
interface properties (stiffness, normal and shear strength, fracture energy) in the sugar-
PMMA system are performed. Finally, this thesis finishes by providing a summary and
conclusions, and suggest future work and directions in Chapter 5.
2. Mechanical properties and physical basis

2.1. Overview

As discussed in chapter 1, the objective of this study is to perform a parametric study pertaining to interfaces in heterogeneous surrogate energetic systems under extreme loading conditions. To analyze the effect of interface parameters on the dynamic behavior of such a system, interface modeling is performed using cohesive zone finite elements. In this particular work, as part of determining the sensitivity of the heterogeneous system to interface conditions, a sugar-PMMA system is chosen for parametric analysis by numerical simulation. In this chapter, the physical models for sugar-PMMA, material properties (mechanical properties, thermal properties, and shock parameters), mechanical model, and the equation of state, etc. will be discussed.

2.2. Physical system

A three-dimensional model of the sugar-PMMA system sandwich system is used for the simulations. This heterogeneous sandwich structure is comprised of face materials of PMMA on two sides of a sugar core material. To explore the dynamic response of the solid face/core interfaces accurately, the interaction between the sandwiched layers of solid sugar-PMMA is defined by cohesive zone finite (C-Z) elements. The computational domain consists of two components: the target (sugar-PMMA blocks with C-Z interfaces) and the impactor (aluminum flyer). This is shown schematically in Figure 2.1 The faces that are subjected to impact on both the impactor and the sandwich structure have an equal surface are

a. The flyer is a deformable solid block that moves at a high velocity.
Based on the relative angle of target and impactor, an impact can be classified into normal impact (uniaxial impact) and shear impact (non-uniaxial impact). Experimentally, a uniaxial flyer-plate impact or similar tests are conducted to study normal impact. In this test, a light gas-gun is used to shoot an impactor/sabot projectile into the target that generates one-dimensional longitudinal pressure wave (near-ideal) through the target and impactor[45]. This is a suitable approach to find out the effect of normal strength. But as the name suggests, this is limited by the flexibility of impact angle. Oblique impact tests [46] facilitate normal and shear impact using the same gas gun setup with a few modifications. This is done by performing the impact test in a slotted barrel with a keyed impactor. For oblique impact experiments on polymers specimens molded between metals, typical angles are used 15, 18, 20, 25 degrees, etc. [45] For this analysis, a 20-degree angle of obliquity is considered. This angle is with respect to the surface normal. The oblique-

Figure 2.1: Representation of physical model of heterogeneous sugar-PMMA system with cohesive zone interfaces
impact test is a perfect approach to find out the effect of shear strength. Figure 2.2 schematically presents the two types of impact, velocity considerations for each study, and the impact angle for the shear impact.

![Diagram of impact types](image)

**Figure 2.2**: Physical representation of normal impact and shear impact in sugar-PMMA system

Both the front and rear PMMA parts have a cross-section of 5cm×5cm. Although PMMA and sugar have equal cross-section areas, PMMA has a thickness of 5 times greater than the sugar block. Therefore, for this study, 5 mm thickness is set for PMMA while 1 mm is considered for the sugar. The aluminum flyer also has the same dimensions and cross-sectional area as the PMMA.

Table 2-1 represents the geometric parameters for the target-flyer system. Both the front and rear PMMA parts have equal cross-section. Although PMMA and sugar have an equal cross-section surface area, PMMA has a thickness of 5 times greater than the sugar
block. The aluminum flyer also has the same dimensions and cross-sectional area as the PMMA.

<table>
<thead>
<tr>
<th>Part name</th>
<th>Cross-section(cm)</th>
<th>Thickness, cm</th>
</tr>
</thead>
<tbody>
<tr>
<td>PMMA</td>
<td>5×5</td>
<td>0.5</td>
</tr>
<tr>
<td>sugar</td>
<td>5×5</td>
<td>0.1</td>
</tr>
<tr>
<td>Aluminum-flyer</td>
<td>5×5</td>
<td>0.5</td>
</tr>
</tbody>
</table>

2.3. Material Modeling

2.3.1. Overview

As part of the material modeling, a perfect plastic hardening model is applied for sugar while for PMMA the Johnson-Cook material model is used. The Mie-Grüneisen model, an equation of state for solids which obeys a linear relationship between shock and particle velocities, is considered for both the sugar and PMMA. In addition, the adiabatic heating effect is applied to the analysis model. To define the yield behavior, the von-Mises plasticity model is used, where the strength is considered pressure-independent.

2.3.2. Perfect plastic hardening model

A conventional elastoplastic theory is considered as the main basis for the plastic hardening model. It assumes that the elastic and plastic strains increments are additive [47] which can be expressed as follows:

$$\Delta \varepsilon_{ij} = \Delta \varepsilon_{ij}^e + \Delta \varepsilon_{ij}^p$$  \hspace{1cm} (2.1)
where $\Delta \varepsilon_{ij}$ is the total strain increment, $\Delta \varepsilon_{ij}^e$ is the elastic strain increment, and $\Delta \varepsilon_{ij}^p$ is the plastic strain increment. When plastic deformation and damage of the material are involved, plasticity can be defined by specifying yield stress ($Y$). For perfect plasticity, the yield stress remains constant and there is no hardening. In this work, the perfect plasticity model is only defined for sugar. In ABAQUS, there are options for the tabular inputs of two or more yield stresses and corresponding plastic strains. In this analysis, by setting up two constant values of yield strength with relevant plastic strain sugar is made perfect plastic.

### 2.3.3. Equations of state

A uniaxial flyer-impact test involves characterizing shock properties of the target by carrying out the impact test using a well-characterized impactor. The conservation of mass, momentum, and energy governs the relationship between the shocked and unshocked properties across the shock front for a constant cross-section. This relationship is known as the Rankine-Hugoniot jump conditions. If a steady wave propagation is considered, these can be expressed as:

\[
\frac{\rho_1}{\rho_0} = \frac{U_s - U_{p0}}{U_s - U_{p1}} \quad (2.2)
\]

\[
P_1 - P_0 = \rho_0 (U_{p1} - U_{p0})(U_s - U_{p0}) \quad (2.3)
\]

\[
e_1 - e_0 = \frac{P_1 U_{p1} - P_0 U_{p0}}{\rho_0(U_s - U_{p0})} - \frac{1}{2} \left( \frac{U_{p1}}{P_1} - \frac{U_{p0}}{P_0} \right)^2 \quad (2.4)
\]

where $\rho$ represents density, $U_s$ is shock wave speed, $U_{p}$ is particle velocity (prior to or after wave arrival), $P$ is pressure (compression is considered positive), and $e$ is internal
energy. Here, the subscript zero represents the properties of the uncompressed region while the subscript 1 represents the compressed material properties.

Many material Hugoniot often follows a linear relationship in respect to particle and shock velocity which can be expressed as:

\[ U_s = s U_p + C_0 \]  

(2.5)

where \( C_0 \) (intercept) denotes materials bulk sound speed and \( s \) represents the slope term between shock and particle velocity.

This linear relationship can, therefore, be used as a modified equation in conjunction with the conservation laws. In this regard, the parameters can be readily implemented into a Mie-Gruneisen EOS which can be expressed as:

\[ P = \rho_0 C_0^2 \chi \left[ 1 - \frac{\Gamma_0}{2} \chi \right] + \Gamma_0 \rho_0 c_v \Delta T \]  

(2.6)

where \( \chi = 1 - \frac{\rho_0}{\rho} \)

This is an analytic form of the equation of state for solids. Here, \( \chi \) denotes a compression term, while \( c_v \) represents content volume heat capacity and \( \Delta T \) is the temperature change. At the reference condition, \( \Gamma_0 \) represents the Grüneisen parameter [48], [49].

2.3.4. Johnson-Cook constitutive model

The Johnson-Cook (J-C) hardening model accounts for the effects of plastic strain, plastic strain rate, and temperature of the flow strength of a material[50]. It is extensively used for modeling where high loading rates and temperature are involved [51]. This is an effective model to predict the model parameters and simulating material behavior accurately [52]–[55].
The flow stress model can be expressed as:

\[
\sigma = (A + B (\varepsilon^{pl})^n) \left( 1 + C \ln \left( \frac{\dot{\varepsilon}^{pl}}{\dot{\varepsilon}_0} \right) \right) \left( 1 - T^* m \right)
\]  

(2.7)

Where, \( \sigma \) depicts flow stress, which is a function of equivalent plastic strain, \( (\varepsilon^{pl}) \),
equivalent plastic strain rate \( (\dot{\varepsilon}^{pl}) \), and homologous temperature, \( T^* \)
where, \( T \) represents the experimental temperature, \( T_{melt} \) is the melting temperature of the
material and \( T_{room} \) is the room/ reference temperature. The material constants are \( A, B, n, \)
\( C, \) and \( m \) which can be extracted from the experimental data. Among these values, \( A \) serves
as the yield stress of the material under reference conditions, while \( B \) is used as strain
hardening constant, \( n \) represents strain hardening coefficient, \( C \) is the strengthening
coefficient of strain rate, and \( m \) denotes thermal softening coefficient. The J-C constitutive
model is applied only for PMMA in this analysis.

**2.3.5. Adiabatic heating model**

Heat generation is a common phenomenon during high-speed deformation
materials (includes large amount of inelastic strain). This is called adiabatic heating where
the deformation time is so short that it does not allow for significant heat exchange with
the environment. However, this heat generation is an important effect in an analysis due to
temperature-dependent material properties are involved in the system.

In an adiabatic heating analysis, a heat flux per unit volume can be defined as:

\[
\dot{r}^{pl} = \eta \sigma \dot{\varepsilon}^{pl}
\]  

(2.8)

To keep balance in thermal energy, this heat flux is added into system. \( \eta \) is inelastic heat
fraction, \( \dot{\varepsilon}^{pl} \) is the equivalent plastic strain rate.
The heat equation that is solved at each integration point can be defined by, [56]

$$\rho c_v(T)\dot{T} = r^{pl}$$  \hspace{1cm} (2.9)

where, $\rho$ is the material density, and $c_v$ is a function of temperature. While modeling in ABAQUS, density, specific heat of the material, and inelastic heat fraction are the tabular input options to define the adiabatic heating model.

2.3.6. Elasticity model

In this work, the elastic model considered to analyze some specific study is the isotropic linear elastic model. The elastic coefficients in the isotropic model Hooke’s law are Young’s moduli, $E$ and Poisson Ratio, $\nu$. Hooke’s law shows a proportionality relationship to stress to the strain that holds for essentially elastic media[57]. While using the equation of state, there is another parameter named isotropic shear elasticity, $G$ [58] to describe the deviatoric response of materials. In this case, the material’s volumetric response is controlled by Mie-Gruneisen equation of state.

2.3.7. Von-Mises plasticity model

The von-Mises yield surface in this analysis, is used to define isotropic yielding. Von-Mises yield surface predicts that the yielding of the material is independent of the pressure. For von-Mises plasticity,

$$\sigma_{eff} - \sigma \leq 0$$  \hspace{1cm} (2.10)

where, $\sigma_{eff}$, von-Mises effective stress, and $\sigma$ defines yield strength or flow strength [59].

When the material is elastic, $\sigma_{eff} - \sigma < 0$ while the material is plastic, $\sigma_{eff} - \sigma = 0$. When perfect plasticity is considered for a material, yield strength is always constant (e.g. as considered for sugar). And, when considered otherwise, yield strength will not be
constant (e.g. J-C flow strength considered for PMMA). In ABAQUS, to define von-Mises plasticity, there are tabular options for the input of the uniaxial yield stress as a function of uniaxial equivalent plastic strain, temperature, and/or field variables.

In contrast to the von-Mises strength model, a Drucker-Prager criterion [60], [61], or Mohr-Coulomb material model shows pressure dependence.

### 2.4. Material Properties

The properties of materials required to run impact simulation in ABAQUS using the above-mentioned models are listed in the following tables. Table 2-2 through Table 2-4 list the corresponding properties of granular sugar, PMMA, and aluminum flyer respectively.

**Table 2-2: Granular Sugar mechanical properties, equation-of-state parameters, and thermal properties for ABAQUS analysis [62]**

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Crystal density ($\rho_o$)</td>
<td>1580.5 kg/m³</td>
</tr>
<tr>
<td>Young’s modulus</td>
<td>24.5 MPa</td>
</tr>
<tr>
<td>Poisson ratio ($\nu$)</td>
<td>0.25</td>
</tr>
<tr>
<td>Yield stress ($Y$)</td>
<td>110 MPa</td>
</tr>
<tr>
<td>Bulk sound speed ($C_o$)</td>
<td>3040 m/s</td>
</tr>
<tr>
<td>Slope of $U_s-U_p$ ($s$)</td>
<td>2.05</td>
</tr>
<tr>
<td>Grüneisen parameter ($\Gamma_o$)</td>
<td>1.04</td>
</tr>
<tr>
<td>Specific heat ($c_v$)</td>
<td>1318 J/kg-K</td>
</tr>
<tr>
<td>Inelastic heat faction ($\eta$)</td>
<td>0.9</td>
</tr>
<tr>
<td>Shear Modulus ($G$)</td>
<td>9.8 MPa</td>
</tr>
</tbody>
</table>
Table 2-3: Parameters for the PMMA mechanical, shock, and thermodynamic properties [63]

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Material density ($\rho_o$)</td>
<td>1190 kg/m$^3$</td>
</tr>
<tr>
<td>Young’s modulus</td>
<td>3 GPa</td>
</tr>
<tr>
<td>Poisson ratio ($\nu$)</td>
<td>0.45</td>
</tr>
<tr>
<td>Bulk sound speed ($C_o$)</td>
<td>2600 m/s</td>
</tr>
<tr>
<td>Slope of $U_s-U_p$ ($s$)</td>
<td>1.52</td>
</tr>
<tr>
<td>Grüneisen parameter ($\Gamma_o$)</td>
<td>1</td>
</tr>
<tr>
<td>Specific heat ($c_v$)</td>
<td>1200 J/kg-K</td>
</tr>
<tr>
<td>Inelastic heat fraction ($\eta$)</td>
<td>0.9</td>
</tr>
<tr>
<td>Shear Modulus ($G$)</td>
<td>1034.5 MPa</td>
</tr>
</tbody>
</table>

Table 2-4: Parameters for the aluminum mechanical, shock, and thermodynamic properties [63]

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Material density ($\rho_o$)</td>
<td>2700 kg/m$^3$</td>
</tr>
<tr>
<td>Young’s modulus</td>
<td>70 GPa</td>
</tr>
<tr>
<td>Poisson ratio ($\nu$)</td>
<td>0.32</td>
</tr>
<tr>
<td>Bulk sound speed ($C_o$)</td>
<td>5350 m/s</td>
</tr>
<tr>
<td>Slope of $U_s-U_p$ ($s$)</td>
<td>1.34</td>
</tr>
<tr>
<td>Grüneisen parameter ($\Gamma_o$)</td>
<td>2</td>
</tr>
<tr>
<td>Specific heat ($c_v$)</td>
<td>890 J/kg-K</td>
</tr>
<tr>
<td>Inelastic heat fraction ($\eta$)</td>
<td>0.9</td>
</tr>
<tr>
<td>Shear Modulus ($G$)</td>
<td>26.515 GPa</td>
</tr>
</tbody>
</table>

Table 2-5: Empirical parameters chosen for material strength models (PMMA and Al) Johnson-Cook material models [64]

<table>
<thead>
<tr>
<th>Material</th>
<th>Strength model</th>
<th>A (MPa)</th>
<th>B (MPa)</th>
<th>m</th>
<th>n</th>
<th>$T_m$(K)</th>
<th>$T_{room}$(K)</th>
</tr>
</thead>
<tbody>
<tr>
<td>PMMA</td>
<td>Johnson-Cook</td>
<td>10</td>
<td>11</td>
<td>1.2</td>
<td>0.65</td>
<td>433</td>
<td>293.15</td>
</tr>
<tr>
<td>Aluminum</td>
<td>Johnson-Cook</td>
<td>547.03</td>
<td>601.58</td>
<td>1.3</td>
<td>0.65</td>
<td>893.15</td>
<td>293.15</td>
</tr>
</tbody>
</table>
3. Modeling and finite element simulation for parametric study

3.1. Overview: Finite element modeling

As discussed in chapter 1, the prime motivation of this work is to investigate the dynamic response of energetic materials by modifying the interface properties in cohesive zone modeling. As part of this numerical study, an analysis of heterogeneous structure is performed using ABAQUS. In this research, analyses were conducted using ABAQUS Version 2018, following the instructions in ABAQUS Simulia User Assistance 2018. This particular chapter provides a brief overview of the ABAQUS program and the implementation of a heterogeneous model followed by a discussion about the key considerations for the model.

3.1.1. ABAQUS/Explicit

ABAQUS is a general-purpose finite element analysis product, with a pre-processing and post-processing module as well as implicit and explicit time integration capabilities. In this work, for the dynamic analysis, ABAQUS/Explicit has been used. This specific dynamic finite element formulation can simulate the dynamic actions associated with large to small deformations, ballistic penetration, low and high-velocity impact, and wave propagation, etc.

Although, a complete ABAQUS simulation can be divided into three basic stages: preprocessing, simulation analysis, and postprocessing, for this specific analysis, more details have been added in a flowchart in Figure 3.1 to show what approaches were necessarily taken to solve the problem.
3.2. Modeling cohesive zone in ABAQUS

The cohesive layer is represented by a single layer of elements consistently distributed through the thickness of the layer, which is called a cohesive element. The cohesive zone has three possible configurations while modeling. It can either be considered as a finitely thick adhesive material where the macroscopic properties of the material are
preserved or an infinitesimally thin layer of adhesive where it is more practical to be defined by traction at the interface.

For the geometry of the cohesive layer, 1µm thin layer is chosen. As it has a finite thickness, this layer should have defined density. Hence, a density similar to that of PMMA is selected for cohesive elements. For this study, a bi-linear traction-separation cohesive law is used to model cohesive elements, for the elasticity definition uncoupled elastic behavior is chosen. In the material module, the elastic type defined is traction, which requires three elastic modulus inputs one in the normal direction and two in the transverse direction. To predict the damage process in cohesive elements, three nominal tractions one in the normal direction and two in the shear direction are defined. Finally, as the energy-based cohesive law is used, it requires the definition of the area under the curve of the traction-separation. This is the energy dissipated in the process that must be equal to the critical energy release rate $G_c$. To define the constitutive response of cohesive elements, the Traction Separation response is defined in the Cohesive Sections.

While connecting two components, the most appropriate method is to tie both faces of cohesive elements with the neighboring components. Although only one face of the cohesive element can be constrained to other components, the cohesive zone shows one or more singular modes of deformation [65]. One method to join cohesive elements to other components is by sharing nodes. Another method is to connect cohesive elements by using surface-based tie constraints to the elements of neighboring components, which is more appropriate if the neighboring parts do not have matched meshes. Hence, two cohesive layers are modeled in the system which is connected through tie-constraints with the
PMMA and sugar. Figure 3.2 shows a complete ABAQUS model of the sugar-PMMA system.

![Figure 3.2: Complete ABAQUS model of sugar-PMMA system](image)

### 3.3. Finite element boundary conditions

In ABAQUS, boundary conditions are set in the target-flyer system. As the boundary constraints, fixed displacements in the lateral direction are used which implies there will be no deformation along the y-axis and z-axis. To define the interactions between the flyer and front PMMA layer, the surface to surface contact is defined with tangential and normal interactions properties. In addition, pre-defined velocity is set in the flyer for which it will be moving at a higher velocity. As two impact tests are considered for the analysis, for the normal impact 120 m/s initial velocity is used while for the shear impact
200 m/s is used at an impact angle 20º. To set the initial temperature, room temperature (293 K) is considered for the whole system.

### 3.4. Mesh convergence study

While considering a finite element analysis, one of the prime factors on which the accuracy of a problem greatly depends on is mesh size. A refined mesh, in general, increases the accuracy of the model. However, it requires larger computational costs (i.e., computing resources and time). For the problem considered in this thesis, mesh size relates to the number of longitudinal and lateral direction elements used to model a single part. Two different types of impacts have been considered in the current study. In the normal impact, the number of elements in the parts is modified only in the longitudinal direction while the shear impact the number of elements is modified both in the lateral and the longitudinal directions. A mesh convergence study for the normal and shear impacts are performed separately. To determine the accurate dynamic response of a sugar-PMMA system computed by ABAQUS, three different mesh refinements are used. As discussed before, the part dimensions are different for PMMA and sugar, and hence, to have a uniform element size, the number of elements in PMMA and sugar must be different.

**Table 3-1: List of all types of meshes considered for the mesh convergence study**

<table>
<thead>
<tr>
<th>Mesh Type</th>
<th>Elements in the longitudinal direction</th>
<th>Elements in the lateral direction (y and z-axis)</th>
<th>Impact type</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>PMMA</td>
<td>Sugar</td>
<td>PMMA</td>
</tr>
<tr>
<td>Mesh 1</td>
<td>5</td>
<td>1</td>
<td>1</td>
</tr>
<tr>
<td>Mesh 2</td>
<td>50</td>
<td>10</td>
<td>1</td>
</tr>
<tr>
<td>Mesh 3</td>
<td>500</td>
<td>100</td>
<td>1</td>
</tr>
<tr>
<td>Mesh</td>
<td>PMMA Elements</td>
<td>Sugar Elements</td>
<td>PMMA Element Size</td>
</tr>
<tr>
<td>--------</td>
<td>---------------</td>
<td>----------------</td>
<td>-------------------</td>
</tr>
<tr>
<td>Mesh 4</td>
<td>600</td>
<td>120</td>
<td>1</td>
</tr>
<tr>
<td>Mesh 5</td>
<td>50</td>
<td>10</td>
<td>5</td>
</tr>
<tr>
<td>Mesh 6</td>
<td>50</td>
<td>10</td>
<td>50</td>
</tr>
<tr>
<td>Mesh 7</td>
<td>50</td>
<td>10</td>
<td>100</td>
</tr>
</tbody>
</table>

Figure 3.3: Mesh convergence study in sugar-PMMA system comparing velocity measured at the rear surface under normal impact.

Figure 3.3 represents the velocity response evaluated at the rear surface for the sugar-PMMA heterogeneous system subjected to normal impact. Hence, this plot corresponds to the three mesh types, Mesh 1, Mesh 2, and Mesh 3. In Mesh 1 type, there are 5 elements in the PMMA, and 1 element for sugar is defined through-thickness which is only in the longitudinal direction. While in Mesh 2, 50 elements in PMMA and 10 elements in sugar are assigned and lastly, in Mesh 3, 500 elements and 100 elements are set in PMMA and sugar respectively. From Figure 3.3 the velocity profile for Mesh 1 type,
does not agree with the other two mesh sizes defined. While for Mesh 2 and Mesh 3, the velocity profiles are similar.

Figure 3.4: Mesh convergence study in sugar-PMMA system comparing von-Mises stress measured at the rear surface under normal impact

An additional evaluation of von-Mises stress in the rear surface element projected onto rear surface nodes also been checked to figure out the effects of the mesh size. Figure 3.4 illustrates the plot for von-Mises stress in the sugar-PMMA system measured at the rear surface for Mesh 1, Mesh 2, Mesh 3, and Mesh 4 (an additional mesh type considering 600 elements in PMMA and 120 elements in sugar). Again, for Mesh 1, stress evolution profiles and magnitudes are noticeably different from the other three cases. While considering Mesh 2 and Mesh 3 types, stress amplitudes are different, but the profile fluctuation pattern is qualitatively similar. The result from Mesh 4 aligns with the stress
profile of Mesh 3. From the above results, it can be concluded that Mesh 2 and Mesh 3, both are reasonable mesh to use for study.

Accordingly, when the oblique impact is considered, three different types of meshes such as Mesh 5, Mesh 6, and Mesh 7 are chosen for the convergence study. For these three types, 50 elements in the longitudinal direction are kept fixed and 5, 50, and 100 elements are assigned in the lateral direction respectively. Since the sugar dimension is always similar, 10 elements are considered in the longitudinal direction, and the same variation is applied for the elements in the lateral direction as PMMA.

Figure 3.5: Mesh convergence study in sugar-PMMA system comparing velocity magnitude measured at the rear surface middle node under oblique impact with 20 degree angle
In Figure 3.5 and Figure 3.6, the plots represent the free surface velocities and von-Mises stress for the oblique impact wherein the flyer hits the target at a 20º angle. From the above plots, it can be decided that Mesh 6 and Mesh 7 (50 and 100 elements are defined in the lateral direction), reasonably agree with each other as compared to the Mesh 5 (5 elements defined in the lateral direction).

The plots in the above figures show that the accuracy of the ABAQUS model is highly dependent on mesh size for this problem and that a very fine mesh was needed to achieve convergence.

For the parametric study, a set of simulations are performed to determine the effect of different parameters in the interfaces. Hence, for the further study of normal impact cases, Mesh 2 (50 elements for PMMA and 10 elements for sugar in the longitudinal
direction) is considered. On the other hand, for shear impact cases, Mesh 6 (50 elements and 10 elements for PMMA and sugar in the longitudinal direction and 50 elements in the lateral direction for PMMA and sugar) are considered.

3.5. Choosing proper time-step

To accurately predict the response of the wave phenomenon stability of the numerical method is important. Courant–Friedrichs–Lewy or CFL condition, is a condition that provides the information on whether an explicit scheme is stable or not, and depends on velocity, size of a single element, and time step. According to Culbert B. Laney’s definition of the CFL condition [66], ‘the full numerical domain of dependence must contain the physical domain of dependence.’ To explain the CFL condition, it expresses information about how it passes the information through mesh elements. For any explicit linear/ non-linear problem, the Courant number (C) should be \( \leq 1 \) [67], which implies, information move from one cell to another cell within one time-step. When this \( C > 1 \), information moves through two or more cells at each time-step affecting convergence negatively. The Courant number can be expressed as follows:

\[
C = \frac{a \Delta t}{\Delta x}
\]

(3.1)

where \( a \) = velocity magnitude in the corresponding material

\( \Delta t \) = timestep

\( \Delta x \) = single mesh element length

For problems having stability issues in a transient simulation, choosing the right time-step is crucial. A value of \( 1 \times 10^{-9} \) s is chosen empirically for the timestep (\( \Delta t \)) considering the stability and computational cost. PMMA is considered for the study which has a single element size (\( \Delta x \)) of 0.1 mm. Velocity in the PMMA is calculated using \( a = C_o \).
=1588 m/s. Based on that, the courant number, $C$ is 0.01588 which is less than 1 satisfying the CFL condition. Depending on the Poisson ratio, the velocity in a medium changes which will be discussed further in the effect of Poisson ratio section.
4. Results and discussion

4.1. Overview: Parametric study

To explore the sensitivity of a sugar-PMMA heterogeneous system to the interface properties of strength, stiffness, and fracture toughness, a parametric study is performed. Two different impact types are applied (normal impact and oblique impacts) to the target system to investigate the dynamic response under high impact loading. By the modification of strength, stiffness, and fracture toughness, the sensitivity of the system to these properties is determined. In general, velocity magnitude profiles at the rear surface of the heterogeneous system are checked for variable stiffness, strength, and fracture toughness of the interfaces. In addition, under the normal and shear impact, the velocity responses are compared to check the effect of normal strength and shear strength in the interface. Similarly, the sensitivity of this sugar-PMMA system is checked by varying fracture toughness of the interface.

4.2. Sensitivity to stiffness

To explore the numerical effects of cohesive zone elements on wave propagation, a homogeneous system separated into three sections with cohesive zones and a homogeneous system without cohesive zones are studied. This homogeneous system without any interfaces will be referred to hereafter as a rigid connection model. To understand how the cohesive zone properties control wave propagation, the dynamic behavior of the system with interfaces is compared with a rigidly connected system. To begin the study, PMMA as a homogeneous system is considered to study the effect of the
cohesive zone. Hence, a pure PMMA system separated by cohesive zone interfaces will be compared with the rigid connection PMMA model. To observe this phenomenon, normal impact (no obliquity) is considered with 120 m/s impactor velocity. However, to predict the numerical effect accurately, it is essential to find out the proper range of stiffness for the interface that will reduce numerical error as compared to the rigid connection and reduce any reflective waves. Thus, at first PMMA system with interfaces is considered to find out the sensitivity of the stiffness as interface property. Velocity magnitudes at the rear surface are analyzed by varying elastic modulus (as a property to define stiffness) of the cohesive zone in both normal and shear direction.

Figure 4.1: Velocity (magnitude) profiles measured at the rear surface in sugar-PMMA (with cohesive zone interfaces) target impacted at 120 m/s (normal impact) varying CZ elastic modulus in normal and shear direction
Figure 4.1 shows velocity magnitude profiles in the rear surface with time for different values of stiffness ($K_{nn}$ defines stiffness in the normal direction and $K_{s}/K_{tt}$ stiffness in the shear/transverse direction). After a set wave travel time (~4 µs), there is an initial rise followed by several incremental steps toward a final state before a second rise. This indicates wave reverberation within the PMMA specimen with each step increasing the normal stress and pressure and also it indicates that the wave reaches the back surface of the system. The first stage of reverberation is particularly significant since it is equivalent to a uniaxial impact state. Under high-velocity impact, due to sudden action of compressive pressure wave, a shock wave generates in the system resulting in a higher velocity magnitude of around 200 m/s. As seen in Figure 4.1, with the increase of stiffness, the wave profile becomes similar, and not much significant change in magnitude and profile are noticed. Thus, interface with a very high stiffness is considered for further study.

Now, choosing this high stiffness interface can also be verified by comparing the velocity magnitude plot for a PMMA homogeneous system with a cohesive zone connection and rigid connection PMMA system. In this case, both the rigid connection system and system with interfaces have the same dimensions and same material properties and model parameters.
Figure 4.2: Comparison between velocity (magnitude) profiles in c-z PMMA and rigid connection PMMA measured at the rear surface ($K_{nn} = 46500$ MPa, $K_{ss}/K_{tt} = 23250$ MPa) target impacted at 120 m/s (normal impact)

Figure 4.2 presents the free surface velocity profile in the rear surface as a representative of the dynamic response to compare how the interface stiffness influences the system. The presented analysis is also conducted with a normal impact at a velocity of 120 m/s. When the contact adjacent faces of the cohesive zone elements are connected with neighboring components, the exchange of any information highly depends on the C-Z stiffness. It can be seen from the Figure 4.2, that there are some reflections of a purely numerical nature for the system with interfaces, but a stiff cohesive zone element is shown to minimize this reflection. Considering the wave profiles, these are similar both for the rigid connection and system with interfaces, but the wave hits the rear surface
approximately 0.2 µs earlier in the rigid connection than the system with interfaces. While there is some numerical error associated with C-Z elements, this error in phase and magnitude of the wave will be considered acceptable as compared to the phase and magnitude changes introduced by a heterogeneous system and changes in C-Z strength and toughness.

4.3. Effect of the heterogeneous material in wave propagation

A set of elastic properties values are used to predict a reasonable range for stiffness in the previous section. Further, this high value for stiffness is verified using the homogeneous rigid connection model and homogeneous system with c-z interfaces. A high value for interface stiffness ($K_{nn} = 46500$ MPa, $K_{ss}/K_{tt} = 23250$ MPa) is determined from the analysis. Subsequently, applying the same interface parameters, sugar as the core element with interfaces between PMMA is used. This will show how a different material as the core structure affects the shock profile. Thus, a comparison between a homogeneous system and a heterogeneous system with interfaces regarding wave profile will be established.
In Figure 4.3 the wave profiles and magnitudes look similar, however, the velocity amplitude for the sugar-PMMA system differs compared to the homogeneous PMMA model. The time the wave takes to reach the back surface is 4 µs for both systems. Then, the wave magnitude for the sugar-PMMA system is lower than the PMMA system until around 12 µs. After 12 µs, the sugar-PMMA system velocity magnitudes slightly exceed the magnitudes in the PMMA system.
4.4. Effect of Poisson ratio

To verify the wave arrival time on the back surface of the material model, a linear elastic system of PMMA is considered. A linear isotropic elastic model is characterized by defining two elastic parameters.

![Diagram showing velocity magnitude profiles with different Poisson's ratios](image)

Figure 4.4: Velocity (magnitude) profiles measured at the rear surface of rigid connection PMMA target impacted at 120 m/s (normal impact) for different Poisson’s ratio

In Figure 4.4 velocity magnitudes in the rear surface for different Poisson’s ratio i.e. $\nu =0, 0.3, \text{ and } 0.45$ are observed. Note that, the expected arrival time for each wave in the rear surface appears to be slower than the analysis PMMA model with the Poisson’s
ratio 0.45. Expected times are calculated based on PMMA elastic wave speeds. From the equation of elastic wave propagation in the uniaxial system,

\[ C_0 = \sqrt{\frac{E}{\rho}} \]  

(4.1)

Where, \( C_0 \) elastic wave speed in a medium, \( E \) refers to the elastic modulus of the material, and \( \rho \) is the material density. However, this elastic (dilatational) wave propagation in an unbounded medium greatly depends on the Poisson’s ratio of a particular material., And, it travels at a velocity slightly higher than \( C_0 \). For instance, for a metal with a Poisson Ratio, \( \nu = 0.3 \), this wave velocity would be 1.2 \( C_0 \) instead of \( C_0 \) [63]. Therefore, considering Poisson ratio 0 and 0.3, time to travel matches with simulation results and thus, explains why the wave propagation in the PMMA system is with Poisson’s ratio is faster.

In addition, when the plastic hardening and equation of state are considered for the model, these models suggest that the speed of wave propagation will increase with pressure resulting in plastic shock-wave formation. In fact, normal stress alone can induce some plasticity in the system [68]. Large amounts of plasticity will reduce this effect that is due to boundary conditions, but this simulation shows why elastic wave speeds differ for polymer materials with high Poisson’s ratios.

4.5. Sensitivity to strength

In Figure 4.5, to understand the sensitivity to normal strength in the sugar-PMMA system, velocity responses are observed under normal impact for a wide range of normal strength values. From the plot, a spike in the velocity magnitudes (~200m/s) due to the shock wave is found (just around 4 \( \mu s \)), which means the wave arrives at the rear surface
at this time. As this is a normal impact, hence the velocity magnitude involves only the normal velocity.

![Velocity Profiles](image)

**Figure 4.5:** Normal velocity profiles measured at the rear surface of the sugar-PMMA system for variable normal strength. Target impacted at 120 m/s (normal impact)

The study to understand the sensitivity of normal strength of the interfaces involves the same interface stiffness discussed before and a medium-range for fracture energy (50 mjoule/mm²) is chosen. Initially, velocity profiles are similar up to 8 µs, and the first wave is always the same because it is compressive. However, after a certain time, significant fluctuations in velocity magnitude are noticed.

For the lower range of strength, these magnitude fluctuations in the rear surface are prominent. Due to constantly passing compressive waves in the system, degradation in the
interface occurs. When degradation occurs in the interface, C-Z elements fail in the system which results in losing the interaction between the neighboring components.

Now, to explore the sensitivity of shear strength in the sugar-PMMA system, the same geometry is considered for the analysis under the oblique impact. Pre-defined velocity is set as an initial condition in both the $x$ and $y$-axis to simulate the transverse velocity with components dictated by impact velocity and oblique angle. For instance, a 200 m/s impact velocity hitting at $20^\circ$ angle will introduce flyer velocity components of $\sim 188$ m/s in the $x$-direction and $\sim 66$ m/s in the $y$-direction. And, the mesh contains, 50 elements for PMMA and 10 elements for sugar in the longitudinal direction (through the thickness of the component) and 50 elements in the lateral direction are defined for the oblique impact simulation.

![Figure 4.6: Velocity magnitude profiles measured at the rear surface of sugar-PMMA. Target impacted at 200 m/s (Oblique impact 20º with 188 m/s along the normal direction and 66 m/s along the shear direction) for variable shear strength](image)
Figure 4.6 represents the velocity magnitudes measured at the rear surface of the sugar-PMMA heterogeneous model. For this work, a comparatively high value \((10^{10} \text{ MPa})\) of normal strength \((T_n)\) at the interface is taken into consideration and then, the value for the shear strength \((T_s / T_t)\) is varied for a small to a high range to show the effect of the C-Z shear strength under an angled impact of 20°. A similar phenomenon compared to the test for normal strength can be noticed in these results as well, which is for a very high range of strength at the interface, the velocity magnitudes profile and the fluctuations get similar. When the interface is strong, a full wave can pass through the interface while with a weak interface, the wave breaks up due to the degradation resulting in more frequencies in the wave profile. Note that, even after the degradation occurs in the interfaces the information can still pass through the cohesive zone to the rear surface. Hence, it is important to understand if the CZ strength (normal/shear) affects the first compressive wave or if it affects the second tensile wave (as the first wave is always compression).

Cohesive element modeling is important for bonding two different components. The degradation of the cohesive element depends on the type of loading. Cohesive elements, in general, do not incur damage in compressive loading. This characteristic is used in modeling some specific types of contact and handled by the cohesive element itself. As the C-Z element do not degrade in compression even if they have already failed in tensile or shear loading, the two components connected by a stiff cohesive element avoid interpenetration [69]. This method is best suited for modeling where the deformation in cohesive elements involves small sliding. As the wave propagating in the system is a compressive wave, cohesive elements can retain their resistance due to this specific type of contact resulting in passing information through the interface.
4.6. Normal and transverse wave

Figure 4.7 (a) and (b), represents the normal and transverse velocity profile for the oblique impact. Impactor hitting the target at 20° angle with 200 m/s velocity (188 m/s along the impact direction and 66 m/s in the transverse direction). For this analysis, high normal strength (10^{10} MPa) and a low shear strength value (0.05 MPa), and 50 mj/ mm^2 fracture energy value are chosen.

Figure 4.7: (a) Longitudinal surface velocity (b) Transverse velocity- measured at the rear surface in the sugar-PMMA system. Target impacted at 200 m/s (with 20° angle,188 m/s along the normal direction and 66 m/s along the shear direction)
Figure 4.7 (a) the longitudinal (normal) velocity profile, whose arrival time to hit the rear surface is around 5 µs. The impact interface between the sugar and PMMA immediately experiences both normal and shear stress loading, however, the normal stress wave (traveling faster) arrives first at the rear surface. The shear wave is seen to arrive approximately 2 µs later.

4.7. Sensitivity to fracture energy

From the previous studies about the effect of stiffness and strength, a reasonable stiff interface ($K_{nn}=46500$ MPa, $K_{ns}/K_{tt}=23250$ MPa) and normal strength value (100 MPa) are chosen for the fracture toughness study for normal impact.

![Figure 4.8: Normal velocity magnitude measured at the rear surface of the sugar-PMMA system. Target impacted at 120 m/s (normal impact) for variable fracture energy](image)
From Figure 4.8 it can be noticed that for a lower range of fracture energy velocity magnitudes, seem to be reflecting more. In contrast, for the fracture energy ≥500 mj/mm², it becomes effectively infinite and thus, minimum damage occurs in the interface. In addition, a similar phenomenon is observed compared to the study of strength, which is a velocity spike of 200 m/s is noticed at around 4µs time, up to 8 µs the profile looks similar for the low to the high value of fracture energy. Depending on the fracture energy range of 0.05 mj/mm² to 5000 mj/mm², the velocity magnitude fluctuates from 200 m/s to around 40 m/s.

Now, to explore the sensitivity of fracture energy in the sugar-PMMA system under the shear impact, the same geometry, initial velocity, impact angle, and same element numbers are considered for the analysis.

Figure 4.9: Velocity magnitude profile measure at the rear surface middle node in sugar-PMMA system for variable fracture energy
Figure 4.9 illustrates velocity magnitudes at the rear surface based on a wide range of fracture energy of the interfaces under shear loading. For this study, the same stiff property (46500 MPa) along with a normal strength of $10^{10}$ MPa and shear strength 0.5 MPa is chosen. Again, it can be noticed that for a lower range of fracture energy, velocity magnitudes noticeably fluctuating more. Moreover, for the fracture energy $\geq 10000$ mj/mm$^2$, minimum damage occurs in the interface due to nearly infinite fracture toughness. Additionally, velocity spikes of 300 m/s are noticed at around 4µs time, also up to 8 µs, the profile looks similar for the low to the high value of fracture energy. Depending on the fracture energy range of 0.01 mj/mm$^2$ to 100000 mj/mm$^2$, the velocity magnitude fluctuates from 300 m/s to around 150 m/s.

4.8. Qualitative validation with experimental results

To compare numerical predictions of the analysis model with experimental results, a new heterogeneous structure of epoxy molded in between aluminum is modeled in ABAQUS by following the experimental work of Peter Sable [68].

Table 4-1 represents the geometric parameters for the cylindrical Epoxy-Aluminum target and aluminum flyer system. The front anvil, rear anvil, and the flyer are of the same material which is aluminum. To define the geometry, different thicknesses are applied for the impactor, front anvil, epoxy, and rear anvil. The impactor was given initial velocity in both the x and y-axis to simulate transverse velocity under the oblique impact. The oblique angle is set 20º which implies a 96.7 m/s shot velocity experimented at 20º would have imposed impactor velocity components of 90.9 m/s in the normal direction and 33.1 m/s in
the transverse direction. The impactor diameter is used as 5 cm and a consistent target diameter is set at 7 cm and the target-impactor sets are concentric to one another. Figure 4.10 shows the heterogeneous model of Epoxy-Aluminum in ABAQUS.

Table 4-1: Geometric parameters considered to model the Epoxy-Al system

<table>
<thead>
<tr>
<th>Part name</th>
<th>Diameter (cm)</th>
<th>Thickness, cm</th>
</tr>
</thead>
<tbody>
<tr>
<td>Epoxy</td>
<td>7</td>
<td>0.05</td>
</tr>
<tr>
<td>Front Aluminum anvil</td>
<td>7</td>
<td>0.4</td>
</tr>
<tr>
<td>Rear Aluminum anvil</td>
<td>7</td>
<td>0.7</td>
</tr>
<tr>
<td>Aluminum impactor</td>
<td>5</td>
<td>1.0</td>
</tr>
</tbody>
</table>

Figure 4.10: Abaqus model of Epoxy-Aluminum system
As part of the material modeling, the Johnson-Cook constitutive model is used for epoxy, anvil materials, and aluminum flyer. The Mie-Grüneisen equation of state is also applied for both the materials. Finally, the adiabatic heating model is applied to this analysis model. To define the yield behavior, the von-Mises pressure-independent plasticity model is used.

Table 4-2 presents the mechanical properties, equation of state parameters, and thermodynamic parameters for epoxy. Table 4-3 presents the empirical parameters chosen for the Johnson-Cook material strength model of epoxy. For anvil materials, and the flyer the same mechanical, thermal properties, shock properties, and Johnson-Cook material parameters are considered as mentioned in the earlier study for aluminum in the sugar-PMMA system in Table 2-4 and Table 2-5. Then, Table 4-4 presents the empirically chosen values for the c-z interface properties.

Table 4-2: Parameters for the Epoxy mechanical, shock, and thermodynamic properties[70]

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Material density ($\rho_o$)</td>
<td>1140 kg/m³</td>
</tr>
<tr>
<td>Young’s modulus</td>
<td>3.76 GPa</td>
</tr>
<tr>
<td>Poisson ratio ($\nu$)</td>
<td>0.39</td>
</tr>
<tr>
<td>Bulk sound speed ($C_o$)</td>
<td>2690 m/s</td>
</tr>
<tr>
<td>Slope of $U_s-U_p$ ($s$)</td>
<td>1.51</td>
</tr>
<tr>
<td>Grüneisen parameter ($\Gamma_o$)</td>
<td>1.2</td>
</tr>
<tr>
<td>Specific heat ($c_i$)</td>
<td>1000 J/kg-K</td>
</tr>
<tr>
<td>Inelastic heat faction ($\eta$)</td>
<td>0.9</td>
</tr>
<tr>
<td>Shear Modulus ($G$)</td>
<td>1352.5 MPa</td>
</tr>
</tbody>
</table>
Table 4-3: Empirical parameters chosen for Johnson-Cook material strength models of Epoxy [70]

<table>
<thead>
<tr>
<th>Material</th>
<th>Strength model</th>
<th>A (MPa)</th>
<th>B (MPa)</th>
<th>m</th>
<th>n</th>
<th>Tm (K)</th>
<th>Tr (K)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Epoxy</td>
<td>Johnson-Cook</td>
<td>84</td>
<td>15</td>
<td>0.53</td>
<td>0.2</td>
<td>350</td>
<td>293.15</td>
</tr>
</tbody>
</table>

Table 4-4: Empirically chosen parameters used for cohesive-zone interface

<table>
<thead>
<tr>
<th>Properties</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Elastic Properties (MPa)</td>
<td>$K_{mn} = 46500 \text{ MPa}$, $K_{ss} = K_{tt} = 23250 \text{ MPa}$</td>
</tr>
<tr>
<td>Strength (MPa)</td>
<td>$T_n = 10^{10} \text{ MPa}$, $T_n / T_n = 500 \text{ MPa}$</td>
</tr>
<tr>
<td>Fracture Energy (mJoule/mm$^2$)</td>
<td>100 mj/ mm$^2$</td>
</tr>
</tbody>
</table>

To define the mesh, an eight noded element with a hexahedral shape with linear order is chosen. For the epoxy layer, front anvil and rear anvil 1331 elements, 2662 elements, and 5324 elements are defined respectively. While there are two CZE layers each consists of 1331 elements and 2662 elements in total. Finally, 3680 elements are defined in the impactor geometry. The total number of elements is 15659, the total number of nodes is 18532 in the whole assembly which includes cohesive elements.
4.8.1. Compare normal and transverse velocity with experimental results

Figure 4.11: A comparison of experimental and simulated rear surface velocities conducted on the epoxy-Al system. Impact velocity of 96.7 m/s at a 20 angle of obliquity.

Figure 4.11 represents the comparison between simulated results and experimental results. Here, the normal velocity magnitude from simulation seems to match reasonably well with the velocity profile and amplitude of the experimental results. While the transverse velocity magnitude seems quantitively different compared to experimental transverse velocity with respect to amplitude and frequencies. There are some reasons that might be responsible for this discrepancy. For the numerical simulation, the material modeling used is very simplified compared to the complexity of the materials used experimentally. Additionally, a finer mesh may be needed.
5. Summary and Conclusions

5.1. Summary and Conclusion

In this thesis, an investigation of the effect of material interfaces on the dynamic behavior of a heterogeneous sandwich structure subjected to a high impact is presented. The major goal of this work is to analyze the sensitivity of sugar-PMMA system to interface parameters such as stiffness, strength (normal and shear strength), and fracture energy under normal and oblique impact by cohesive zone modeling. To this end, the finite element method is used to perform the dynamic simulation by using ABAQUS. A perfect plastic hardening model and the Johnson-Cook constitutive model are considered for sugar and PMMA respectively. The Mie-Grüneisen model, an equation of state is considered for both the sugar and PMMA. The adiabatic heating effect is also applied to this high deformation analysis model.

Analyzing the results, it can be concluded that the effect of a stiff cohesive zone is significant as it reduces greatly the reflections of the normal waves. Moreover, both for the normal and shear impact, the dynamic response of heterogeneous system seems more sensitive to interface strength (normal strength/shear strength) than fracture energy.

In addition, this numerical analysis results show that a simple standard cohesive zone model can capture some qualitative trends as experiment results of the epoxy-Al system. By comparing results, the normal velocity amplitude from simulation has a good agreement with experimental velocity amplitude. The transverse velocity, on the other hand, shows a similar trend in velocity profile though amplitudes are quantitively different.
5.2. Recommendation for future study

In this work, the dynamic impact test of a heterogeneous sugar-PMMA system is simulated using material models implemented in finite element software ABAQUS. Although with the material parameters and material model assumptions, it is shown that the strength, stiffness, and fracture energy have a large or first-order effect on the results, this work can be extended in several ways. The following are some directions for future work, some of them are already in the process:

I. Some material properties can only be determined from experiments. Hence, due to a lack of proper experimental data, some parameters are empirically chosen for the analysis. Therefore, collaborating with experimental works and using experimentally obtained parameters as inputs would improve the accuracy of the numerical model.

II. In this analysis, the von-Mises model is used as the yield criteria which is not pressure-dependent. However, in oblique impact test material plasticity depends on both shear (deviatoric) stress and pressure (volumetric) stress. This behavior can be described by the Mohr-Coulomb or Drucker-Prager model which is pressure-dependent. One of the future studies could be to model with the Drucker-Prager model.

III. Polymers are known to be viscoelastic in nature [71], [72] but in this model, it is not accounted for here. Hence, considering a viscoelastic model could change some of the frequency response of the heterogeneous system.
Bibliography


