Exploring the Science Behind

High Explosives

Santa Fe, New Mexico

Supercomputing Challenge

Final Report

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The Blast Masters - Team 2

Capital High School

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1. Executive Summary

Our project dives deep into the study of high explosive chemistry, particularly focusing on HMX, also known as Octogen. We've put a lot of time and effort into researching this powerful explosive, especially during school breaks and after-school sessions. Our main goal is to find ways to make HMX handling safer. Despite the complexity of its degradation, HMX must typically operate under extreme conditions, making it essential to comprehend the physical processes involved in decomposition. Such knowledge will help us uncover new ways to handle explosives more safely, and we have used Python programming to analyze data and create graphs and tables that show what we've learned. We hope to bring new insights to explosive materials science and improve safety standards, and we hope that our research can trigger significant steps forward in making high explosives safer to handle.

2. Description of the Problem

Since the 1950s, there have been numerous accidents involving modern high-explosives such as unexpected detonations occurring during manufacturing processes. While modern high-energy compounds are quite dangerous, they're also extremely important in various industrial applications -e.g. controlled explosions in mining, tunnel construction, and military uses including propellant production. HMX, known as octogen or else visually by its detailed organic formula, is a prime example. Originally developed during World War II, it is today a vital component in modern nuclear weapons. HMX is one kind of high explosive widely used around the world that is nominally stable but displays high detonation strength properties. Therefore, its manufacture and handling require the utmost in safety protocols and loss prevention. Stability is crucial when dealing with materials like HMX, in order to ensure permanence during storage and proper functioning when needed. Internal heat dissipation from hotspots has to outpace local microchemistry in order to avoid the explosive domino effect. It is this competition (tradeoff) that we investigate in the present report.

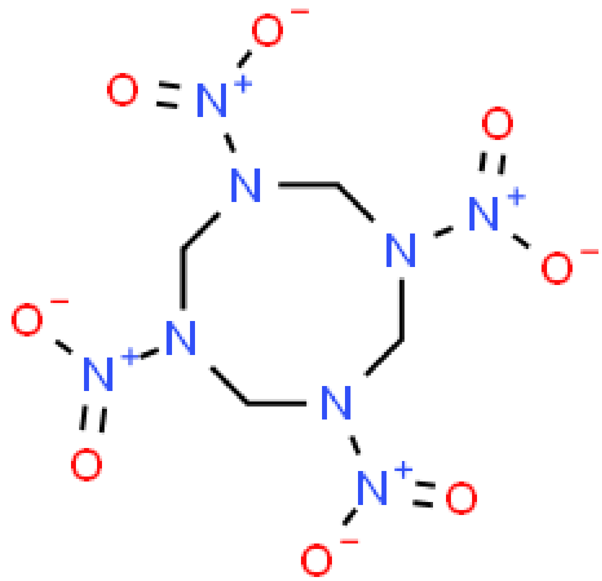
3. Solution

To address the safety problem at a computational (theoretical) level, our team developed several types of Python code -in order to analyze the heat dissipation from critical internal hot zones then compare time scales with the chemistry of initiation. We calculated the heat content of reactive microzones using a Python energy storage routine, by considering the specific heat of the explosive crystal harbored within hotspots and also factoring in heat conduction away from specific potential reaction zones. Corresponding chemical time scales for inception of the exothermic reaction set were estimated using basic statistical mechanics principles. Our Python scripts for the heat analysis and chemistry are included as appendices here for reference and convenience. Also appended is a time scale-comparison plotting routine which we developed in order to visualize our results.

4. What is HMX (Octogen)?

HMX stands for "High Melting Explosive" or “Her Majesty’s Explosive”. Also known as Cyclotetramethylenetetranitramine (Octogen), it is a powerful and stable high energy compounds used in military and industrial applications such as nuclear devices, plastic explosives, and rocket fuels. HMX is known for its high density, high detonation velocity, and high stability properties.

The molecular structure consists of an eight-membered ring of alternating carbon and nitrogen atoms, with a nitro group attached to each nitrogen atom.



5. Procedure

For this project, we followed a step-by-step procedure in order to dissect the timing of accidental detonation. First, we conducted thorough research to understand the properties and behaviors of HMX. Then, we created a report outlining our findings, which was presented to supercomputing judges recently at our local community college. After receiving input and refining our approach, we moved into the actual Python programming phase. Using the data gathered and the equations we adapted, we wrote several levels of coding to analyze the HMX Octogen and its heat conduction plus reactive chemical properties. The codes were utilized to create graphs and visual representations of our findings. Simple heat storage and transfer (loss) time equations will be evident in the attached Python segments, as well as the Boltzmann distribution-level chemical rate equations. In the former case, we assumed generic Cp and conductivity values. The chemistry of the energetic reactions was simulated as generic bulk and interfacial decomposition of the reactant itself, in the unimolecular sense. We took frequency and activation factors from the Atkins textbook series, for stretched and typical bond-breaking initiation steps. Our equations are implied in the appended coding, and the reader should note that we also include our plotting routines.

6. Results

The plots presented in this section place log10 values for the various timescales on the upward (y) axis versus log10 for the radius of the reaction zone along the horizontal (x). The geometries we assumed were consistent with experimental analyses dating back to the late nineteen forties and listed in the bibliography here. Horizontal lines correspond to weak and strong chemical bond breaking, or in other words, to surface-bound stretched bonds within the HMX melting zone versus those in bulk or condensed phases. We assume again following experiments described in our references that random microcompression, friction, and jetting events cause highly localized melting at and above about 1000 Kelvin, at sizes from one nanomater upward. By contrast with the horizontal chemistry results in the plot, the upward-sloping timescales represent conductive heat loss for reactive zones of various sizes. We assume that chemistry takes place at roughly a ten percent scale relative to simple spherical warming areas. It is clear from the crossovers in our plot that as zones become larger their ability to trap heat is enhanced and kinetic runaway becomes possible. Thus our main conclusion is that one path to safety is compression of open areas within the solid.

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this is ltdis -11.477121254719663
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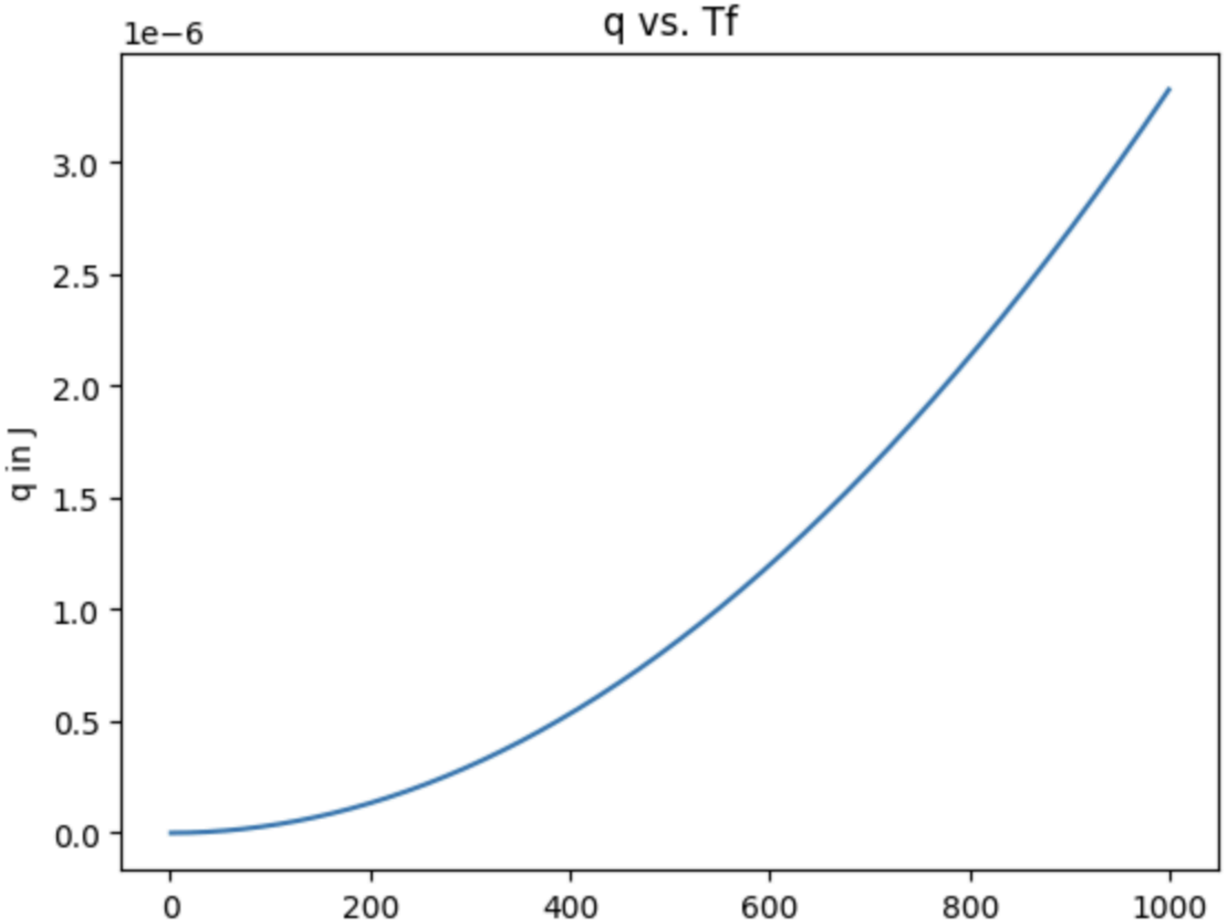

7. Encountered Issues

Throughout our project, our team met with challenges that tested our skills and perseverance. Initially, we struggled to identify a real-world problem to address, especially since we didn't have many concrete examples to look at during the beginning of our project. This made it difficult to stay focused and motivated. Additionally, although we had previously taken both chemistry and physics courses, our understanding was limited for the equations relevant to the project. In the coding phase, we were forced to locate and fix numerous bugs that tended to cause delays and set us back. Finding real-world examples of accidents related to specifically

HMX was challenging, further complicating our research. However, despite these obstacles, we remained determined and worked together through weekly meetings to overcome them. With time and effort, we eventually learned and improved, and ultimately we were able to generate some very interesting results.

8. Additional Research

Although we spent many hours together researching and reading excerpts from college-level books; to further develop this project we did some additional research online regarding real accidents that have been caused by HMX. Surprisingly, after decades of manufacturing, some of these incidents are quite recent. Since the compound is central in nuclear weapons research and production, our assessment is that the work we have done is very relevant locally here to the technology sector of New Mexico.

- German investigators now believe that the explosive octogen was used to sabotage the Nord Stream gas pipelines. They concluded that it was brought to the site on a rented yacht named Andromeda. Traces of octogen were found on the yacht, indicating its involvement in the sabotage. The sabotage, which occurred on September 26, 2022, caused significant damage to the Nord Stream pipelines, leading to criminal charges of international terrorism.
- On June 1, 2009, at 7:00 am, an explosion occurred at the HMX Plant in Rafaela, Argentina, during the discharge of the ninth batch of HMX. This resulted in one operator being injured, along with damage to equipment. The most likely causes were friction and impact. To prevent recurrence the expected measures were taken, including studying the

process flow, replacing metal piping with reinforced plastic, and improving maintenance procedures.

- In 2012, there was an explosion in an HMX (octogen) plant located in New York, NY. The incident happened after the batch nitration of HMX, causing one operator to be injured and hospitalized. The plant sustained minor damage, leading to changes in its design before restarting operations.

9. Conclusions

Our project dives deep into a study of high explosive chemistry, focusing particularly on HMX, also known as Octogen. We've dedicated a lot of time and effort to this research, often working during school breaks and after school. Our main goal is to make handling HMX safer. HMX is a widely used high explosive known for its stability and powerful detonation properties. We used Python programming to analyze data and create graphs and tables to understand its reactive behavior. The fundamental result is that larger reaction microzones retain heat due to surface/volume effects thereby allowing chemical domino effects to initiate accidental detonation. We conclude that minimization of hot spot volumes is critical to safety. In elucidating the competing physical and chemical processes involved in decomposition, we aim to bring new insights to explosive materials science. Through comparisons such as this it may be possible to improve safety standards, ultimately making high explosives easier to handle. Additionally, incidents involving HMX, such as the Argentina commercial explosion in 2009 or its alleged use in sabotaging the Nord Stream pipelines, all underscore the need for superior safety measures in handling such powerful explosives.

10. Achievements

Throughout this project, we have learned and gained a variety of new skills. We have learned how to schedule meetings; and be prompt and prepared so that we can conduct successful weekly gatherings. We have learned how to communicate effectively with one another and to implement new ideas into a technical project (fold in changes, roll with the punches). We have learned how to discuss and debate scientific concepts among ourselves, and how to sit down and work efficiently with one another. We have learned how to apply our research, programming, and computer science skills to a very important and relevant modern chemistry problem. Additionally, we are exposed directly to the world of professionalism since we are required stand in front of a group of judges and present our project!

Not only have we applied knowledge from previous science and programming classes to this project, but we have also gained professional/social skills that we know will be extremely valuable and beneficial. As high school students soon going on to seek higher education, we are proud of these achievements and will continue to apply them towards our future careers!

11. Furthering our Project

Although we succeeded in documenting realistic and important results, there are still a few things that we would like to do to further our work. First of all, we would like to finish the graphing and visualization process, since we encountered a variety of errors that delayed our progress significantly. We would like to dive deeper into data analysis and into the graphs and tables that we've created by analyzing trends or patterns to uncover insights that could lead to greater improvements in explosive safety. Additionally, we believe that it would be a wonderful idea to be able to share what we have learned with classmates and even younger students; educational outreach aimed at a variety of different age groups would allow our project to further expand. We would have the advantage of receiving additional feedback from those around us.

12. Acknowledgements

Scott Elliott - Thank you for your tireless support, guidance, and time. You have been an incredible mentor, we appreciate the countless hours that you put into allowing us to express our ideas and craft them together leading to wonderful outcomes. Thank you for your patience, and thank you so much for motivating us to do our absolute best. We have learned countless new things from you, and we hope to work alongside you again in the future!

Irina Cislaru - Thank you for your continuous motivation throughout the year and for allowing us to complete this project! We have learned so much from you, and owing to your remarkable teaching experience we have been able to apply previous knowledge and skills successfully.

Barbara Teteycz - Thank you for encouraging us to take on this project, since it has permitted us to extend our computing skills tremendously.

The Supercomputing Challenge - Thank you so much for providing students of New Mexico with this wonderful opportunity. Throughout the year, we have been able to successfully work with our mentor, and gain new skills, while applying prior and newly attained knowledge. We have truly learned how to work as a technical team, and this has given us a glimpse of the world of professional scientific computing.

13. Works We Relied On in Our Research

P. Atkins

Physical Chemistry

W.H. Freeman, New York, 1999

R. Wolfson

University Physics

Addison Wesley, New York, 2007

J. Akhavan

Chemistry of Explosives

Royal Society of Chemistry, London, 2004

C. Handley, B. Lambourn, H. James, and W. Belfield

Understanding the Shock and Detonation Response of High Explosives at the mesoscale

Applied Physics Reviews 5, 011308, 2018

H. Eyring, R. Powell, G. Duffy, and R. Parlin

The Stability of Detonation

Chemical Reviews 45 pages 69-181, 1949

Austin Powder International

(104l) Explosions In HMX (Octogen) Plants

APPENDICES: OUR CODES