High School: Capital High School
Area: Modeling (Chemistry)
Title: Exploring the Science Behind High Explosives

Definition of the problem:

Since the 1950s there have been numerous accidents involving modern high explosives. They can of course be quite dangerous, but at the same time they are central in various industrial applications, such as creating controlled explosions for mining and refineries or constructing underground tunnels. Military applications naturally come into play as well. HMX is one widely adopted, ringed nitramine that we take here as an example. Otherwise known as octagen or by its detailed organic formula, this highly energetic compound was developed during the Second World War primarily for military purposes and it is a key ingredient in modern nuclear weapons. Stability is crucial to the maintenance of safety when materials such as HMX must be stored and then called upon to function properly.

Solution:

The goal of our project is to understand ways of creating a safer explosive structure, one that would be compressed so that catalytic openings in the crystal are smaller. Since nitramines such as HMX contain very closely packed carbon, nitrogen, and oxygen atoms, their degradation chemistry can become very intense, releasing a tremendous amount of conventional energy. When properly harnessed this is advantageous, but avoiding accidents depends on subtle mechanistic details. We will simulate them here.

We will estimate the physics of heat transfer within the HMX crystal versus chemical energy release for internal openings of different sizes, so that the well-known energetic runaway or cascade can be calculated. Heat spilling from the degradation of a few HMX molecules either diffuses away through the solid itself, or else gets absorbed by neighboring molecules leading to a domino effect. We can use standard energy transport calculations to estimate both the time scale associated with heat loss and the amount that is ultimately generated. We plan to study the competition between heat dissipation and chemical evolution in order to decide how big or small crystalline defects need to be.

We are comparing chemistry and physics of the hotspot system to understand the safety aspect of high-explosive research. We will argue that a stable explosive is one in which larger voids are first compressed. By condensing an explosive one can make it safer. Effectively we would propose that manufacturing occur in such a way that the openings are smaller.

Progress to Date:

Recently, our team has been engaged in a series of productive lunchtime meetings here at Capital High. We've tackled numerous mathematical equations relating to hot spot thermochemical dynamics, and have started on development of related computer codes. In addition, we've been drafting text sections, ensuring that they are clear and concise. We've also established a detailed plan of action to guide our future work. We have decided to rely on Python as our programming platform -and the necessary code writing has already begun. Our

plan is to draw on the powerful Matplotlib library for data visualization. Currently, we're focusing on expanding these ideas so that we can present our work more comprehensively. We're anticipating the creation of models and output that will allow us to visually represent the heat energy and evolutionary kinetic results. Simulations will generate graphs that can serve as an explanation of the chemistry involved in explosive initiation.

Sources:

H. Eyring, R. Powell and C. Duffy (1949) The stability of detonation, Chemical Reviews 45(1), 69-181.

J. Ahkavan (2004) The Chemistry of High Explosives, Royal Society of Chemistry books.

M. Meyers and K. Chawla (2009) Mechanical Behavior of Materials, Cambridge University Press.

C. Handley, W. Lambourne and N. Whitworth (2018) Understanding the shock and detonation response of high explosives, Applied Physics Reviews, 5(011303).

https://www.pbs.org/wgbh/americanexperience/features/command-and-control-broken-arrows-how-many-nuclear-accidents-have-we-had/

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