Evaluating the enhancing potential of metal hydride in high explosives using a simulation approach.

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Abstract

Modelling and simulation in energetic materials (EM) is a well-known field and it keeps on growing and improving. Being able to simulate the EM before doing synthesis or formulation in the laboratory is a safe route. By using the right simulation tools, the performance parameters such as enthalpy of formation, detonation pressure, detonation velocity and sensitivity can be estimated. Metals are known as enhancing additives to energetic materials and are used to make enhanced explosive composites. Metal hydrides are derived from pure metals or metalloids which can be covalently or ionically bonded to hydrogen. Metal hydrides have also been used to enhance the EM performance parameters such as specific impulses for solid propellant. In this work theoretical formulation optimization was done for 2,4,6-trinitrotoluene (TNT), 1,3,5-Trinitroperhydro-1,3,5-triazine (RDX), 2,2-Bis[(nitroxyl)methyl]propane-1,3-diyl dinitrate (PETN) and composition B with Alane (AlH_3), magnesium hydride (MgH_2), titanium hydride (TiH_2), Zirconium hydride (ZrH_2), lithium aluminium hydride ($LiAlH_4$) and sodium aluminium hydride (NaAlH4). The theoretical density and detonation properties of the formulations were estimated with EXPLO5. The densities of the formulations were observed to be affected by the addition of metal hydrides. Where the metal hydrides are made from heavy metals, formulation density increased with increasing metal hydride quantities and the lighter metal hydrides did the opposite. Despite the observed increase in density for some formulations, this did not translate into more increased detonation pressure except for the TNT formulation with ZrH_2. AlH_3 performed well for all the explosives, including PETN formulation.

Keywords—Metal hydrides, Simulation, Performance parameters, energetic materials, EXPLO5

Introduction

The use of energetic materials classified as explosives, propellants and pyrotechnics has been increasing over the years both in military and civilian applications. These materials are made from organic and inorganic molecules. When initiated these materials can either detonate or deflagrate, hence they are called energetic materials [1]. To achieve desired physical properties for these, energetic materials are formulated or blended with other molecules. Some of the important properties are detonation performance, thermal properties, water resistance processibility and shelf life. These properties are sometimes achieved through the synthesis and formulation of energetic materials [2]. To enhance the performance of energetic materials, energetic or fuel components are added as part of the formulation. Aluminium (Al) is an example of such a fuel component, and it has been introduced to improve energetic materials' performance [3]. The use of Al as a metal additive in energetic materials has been widely applied because of its high calorific value, which can increase reaction temperature, blast, and incendiary effects [4]. In explosives, Al has shown the ability to improve air blasts and raise reaction temperatures while in propellants it has shown the ability to increase the specific impulse and flame temperature [5]. Al supersedes other metals like Boron which have even higher calorific value, but its application is limited by difficulties in ignition due to high melting and boiling temperatures (2 177 and 3 658 °C respectively) [4]. Despite the enhanced performance obtained from using Al as an additive, the high density of Al (2.7 g/cm3) when compared to metal hydrides, e.g., AlH3 (1.477 g/cm3) results in increased volumetric loading of the resulting propellants [6].

Studies have shifted into exploring metal hydrides (MH) as additives in energetic materials. Metal hydrides are conventionally used in hydrogen (H_2) storage, H_2 generation, and fuel cells and recently have been studied for application in energetic materials [7-9]. Other metals like magnesium (Mg), Boron (B) and their alloys have also been explored as fuel sources for propellants [10]. However, metal hydrides seem to be a more promising candidate as they possess higher combustion heat than the corresponding metals due to the introduction of “hydrogen energy” [11]. Besides the energy released from metal oxidation, the H_2 combustion also contributes to the overall released energy during the combustion processes [6]. Their chemical activity, high heat of combustion and generation of low molecular weight decomposition/combustion products also puts them in a better position to be used in energetic materials [12].

In this work, energetic materials formulated with metal hydrides were simulated to study the potential of these materials to enhance detonation performance.

Methods

EXPLO5

The use of EXPLO5, a thermochemical computer code, for the calculation of detonation parameters of energetic materials including high explosives has been demonstrated by several researchers [13-16]. This code is based on the chemical-equilibrium steady-state model of detonation [17]. It uses the Becker-Kistiakowsky-Wilson (BKW) equation of state (EOS) for gaseous detonation products, the ideal gas and the Murnaghan equation of states for condensed products [18-21]. The detonation product composition in the code is calculated by applying the Gibbs energy minimisation method and is designed so that the users can choose between the explosive types of constants in the BKW-EOS [22].

The simulation was done for the explosives containing TNT, RDX, PETN and Comp B. A similar initial temperature of 3 383 °C was used. BKW-EOS with Becker-Kistiakowsky-Wilson (BKWN) set of constants were used for the calculations. Shock adiabats of products at a maximum pressure of 41 GPa and density of 1.025 g/ml were calculated. Expansion isentropes of products using a density decrease ratio of 1.25 g/ml and freeze temperature of 1 527 °C were calculated.

Formulation of the metal hydride composite explosives

The formulations consist of the commonly used explosives with metal hydrides as listed in Table I. The percentage of the metal hydride in the formulation varies from 5 - 25 %. These were added to EXLO5 to determine the effect of metal hydrides on the performance of the explosive materials.

TABLE I: FORMULATION OPTIMISATION OF SOME EXPLOSIVES WITH METAL HYDRIDE

Explosive charge	**Percentage composition Explosive to AlH_3 (EX: AlH_3)**				
TNT	95:5	90:10	85:15	80:20	75:25
RDX	95:5	90:10	85:15	80:20	75:25
PETN	95:5	90:10	85:15	80:20	75:25
Composition B (RDX 60 %: TNT 40%)	57:38:5	54:36:10	51:34:15	48:32:20	45:30:25
Percentage composition Explosive to MgH_2 (EX: MgH_2)					
TNT	95:5	90:10	85:15	80:20	75:25
RDX	95:5	90:10	85:15	80:20	75:25
PETN	95:5	90:10	85:15	80:20	75:25
Composition B (RDX 60 %: TNT 40%)	57:38:5	54:36:10	51:34:15	48:32:20	45:30:25
Percentage composition Explosive to TiH2 (EX: TiH2)					

TNT	95:5	90:10	85:15	80:20	75:25
RDX	95:5	90:10	85:15	80:20	75:25
PETN	95:5	90:10	85:15	80:20	75:25
Composition B (RDX 60 %: TNT 40%)	57:38:5	54:36:10	51:34:15	48:32:20	45:30:25
Percentage composition Explosive to ZrH_2 (EX: ZrH_2)					
TNT	95:5	90:10	85:15	80:20	75:25
RDX	95:5	90:10	85:15	80:20	75:25
PETN	95:5	90:10	85:15	80:20	75:25
Composition B (RDX 60 %: TNT 40%)	57:38:5	54:36:10	51:34:15	48:32:20	45:30:25
Percentage composition Explosive to $LiAlH_4$ (EX: $LiAlH_4$)					
TNT	95:5	90:10	85:15	80:20	75:25
RDX	95:5	90:10	85:15	80:20	75:25
PETN	95:5	90:10	85:15	80:20	75:25
Composition B (RDX 60 %: TNT 40%)	57:38:5	54:36:10	51:34:15	48:32:20	45:30:25
Percentage composition Explosive to $NaAlH_4$ (EX: $NaAlH_4$)					
TNT	95:5	90:10	85:15	80:20	75:25
RDX	95:5	90:10	85:15	80:20	75:25
PETN	95:5	90:10	85:15	80:20	75:25
Composition B (RDX 60 %: TNT 40%)	57:38:5	54:36:10	51:34:15	48:32:20	45:30:25

Results

EXPLO5 software packages were used to apply to predict the performance of energetic materials containing metal hydrides. The potential of metal hydrides to enhance high explosives materials was investigated using TNT, RDX, PETN and composition B explosive materials. These explosives are mostly applied in military space.

The density of the composite energetic materials

Formulating components of different densities might result in either higher density or lower density depending on the properties of each of the components. Density is an important property in energetic materials as the performance of the energetic materials is also a function of this parameter. Metals are known to have higher densities. High-density and high-enthalpy materials are known as high-energy-density materials. In formulations containing metals, an increase in density is expected and if the metal is energetic then this will result in improved performance. Metal hydrides have less density compared to their respective pure metals. An example of such is aluminium (2.70 g/ml) and aluminium hydride (1.477 g/ml). The density varies with the type of metal hydrides used as seen in **Fig. 1** to **Fig. 4**. Aluminium hydride and magnesium hydride have low density while titanium hydride and zirconium hydride show a very high density.

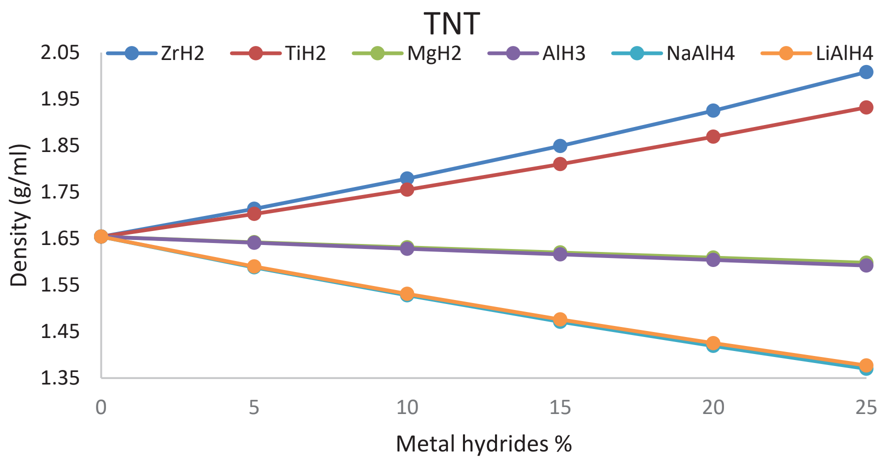

Fig. 1. Density of TNT and metal hydride formulations

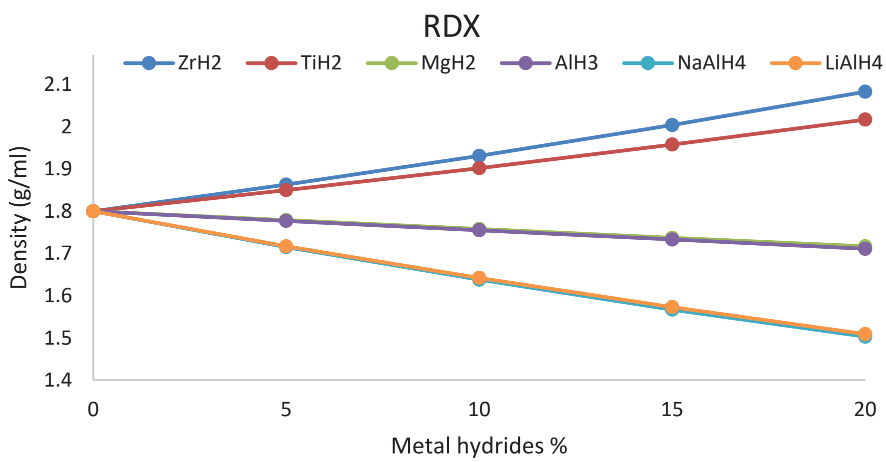

Fig. 2. Density of RDX and metal hydride formulations

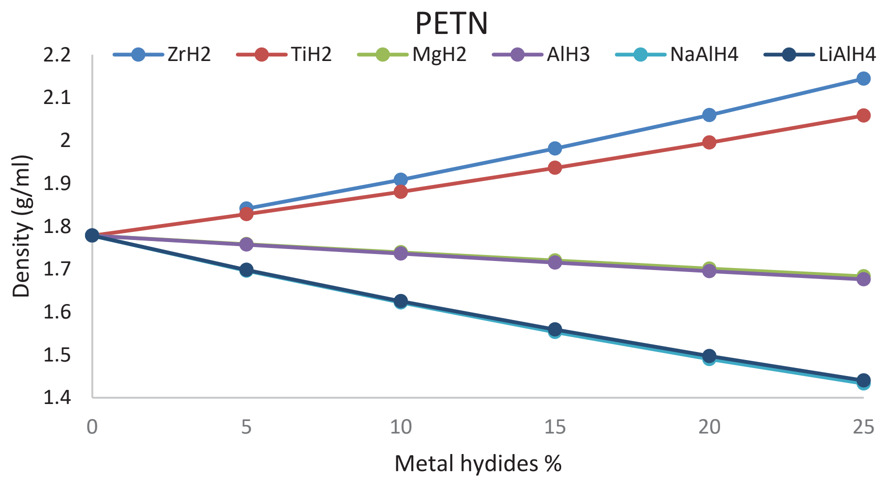

Fig. 3. Density of PETN and metal hydride formulations

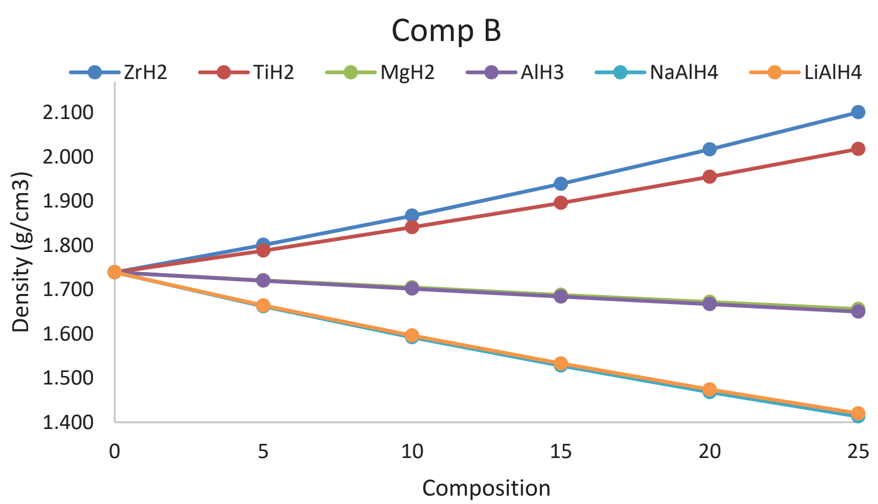

Fig. 4. Density of Comp B and metal hydride formulations

The graphs in **Fig. 1** and **Fig. 4** show the effect of the amount of metal hydrides on the density of explosive formulations. A similar trend is observed for all the explosives. ZrH_2 and TiH_2 are increasing the density of all the explosives. The density of these metal hydrides is high, hence there is an observed increase. For the rest of the metal hydrides, the more they have added to the formulation the lesser the density of the resulting formulation.

Detonation pressure of the formulated materials

A simulation of high explosives containing metal hydrides was completed to explore the potential of metal hydrides as enhancing additives. TNT, RDX, PETN and Comp B were used to study the potential of ZrH_2, MgH_2, TiH_2, $LiAlH_4$, $NaAlH_4$ and AlH_3. Detonation pressure and detonation velocity were obtained from EXPLO5. These are important in estimating the performance of energetic materials. **Fig. 5** to **Fig. 8** give a graphical representation of the data for all the explosives and their formulations.

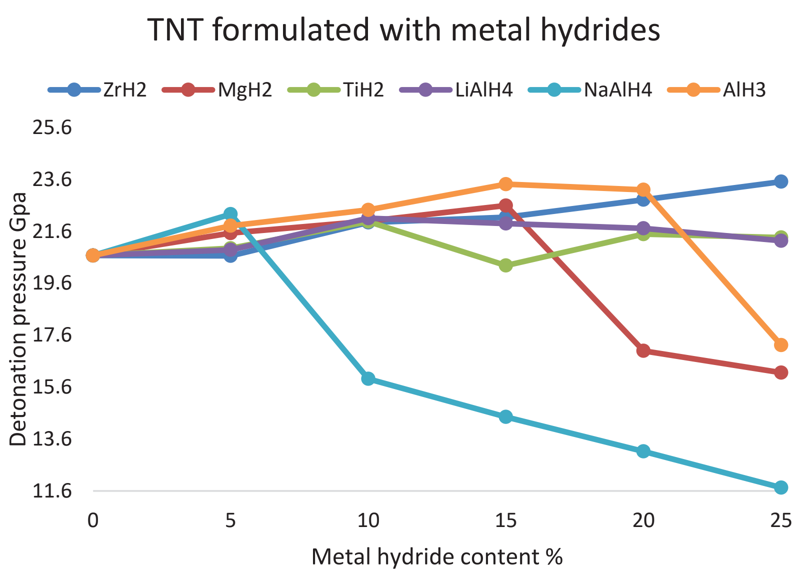

Fig. 5: Effect of metal hydrides quantities on detonation pressure of TNT formulations

It can be seen in Fig. 5 that for most formulations the detonation pressure increases with increasing % of metal hydride until an optimum is reached beyond which the detonation pressure starts to decrease. $NaAlH_4$ shows higher detonation pressure at 5% which then starts to decrease. AlH_3 shows higher detonation pressure between 5-20%. The same trend is observed with MgH_2, but the resulting detonation pressure is less, and it is between 5-15%. ZrH_2 show an increase and it is the highest at 25%. All the metal hydrides except $NaAlH_4$ show the potential to enhance the detonation pressure of the TNT between 5% to 20% of metal hydride in the formulations.

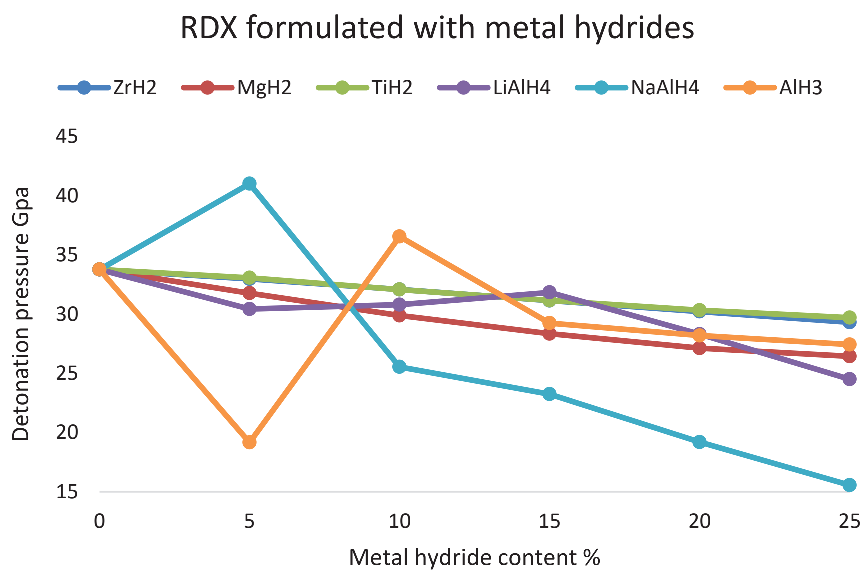

Fig. 6: Effect of metal hydrides quantities on detonation pressure of RDX formulations

In Fig. 6 formulations of RDX with metal, hydrides show a different trend. $NaAlH_4$ shows a higher detonation pressure of 5% and AlH_3 at 10% the rest of the formulations are showing a decrease in detonation pressure as metal hydride content is increased.

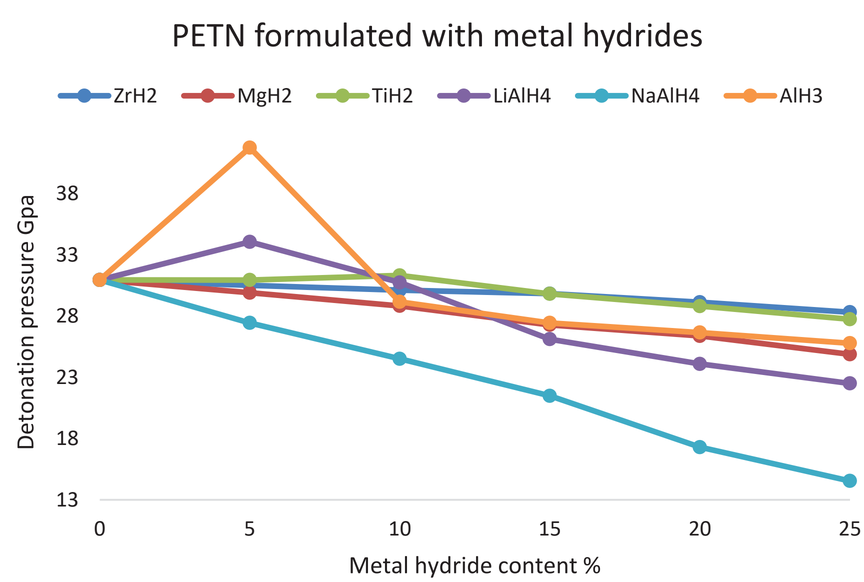

Fig. 7. Effect of metal hydrides quantities on detonation pressure of PETN formulations

Fig. 7 shows PETN formulations with the metal hydrides. AlH_3 shows the highest detonation pressure of 41.7 GPa at 5% followed by $LiaAlH_4$ also at 5%. TiH_2 shows a slight increase at 10%, and the rest of the formulations show a decrease in detonation pressure with increasing quantities of metal hydrides.

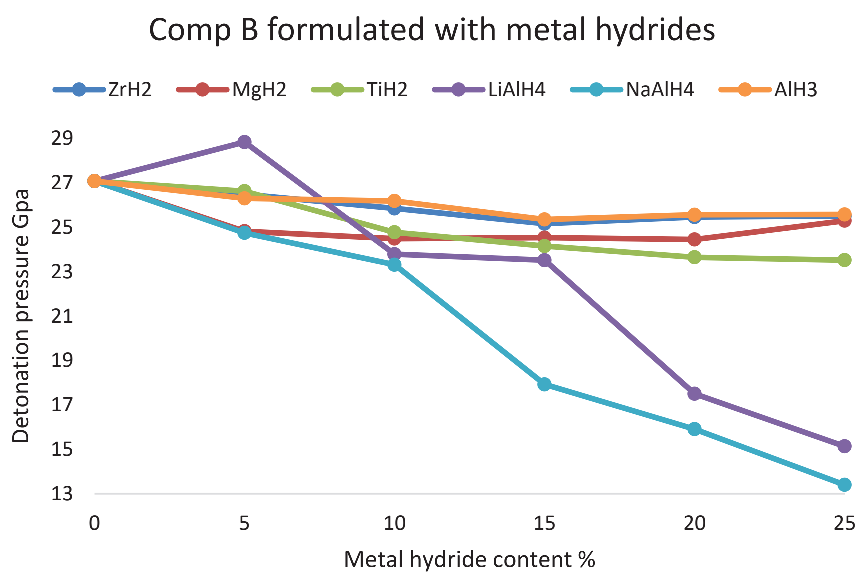

Fig. 8: Effect of metal hydrides quantities on detonation pressure of Comp B formulations

In Fig. 8, $LiaAlH_4$ formulation with Comp B is the only formulation that shows higher detonation pressure at 5%. All the other formulations, i.e., ZrH_2, MgH_2, TiH_2, $NaAlH_4$ and AlH_3, are showing a decrease.

The detonation velocity of the formulated materials

Detonation velocity is the propagation velocity of the shock wave through a detonating energetic material. This is one of the parameters that determine the performance of the explosive material. The higher the detonation velocity the better is the performance of the explosive material.

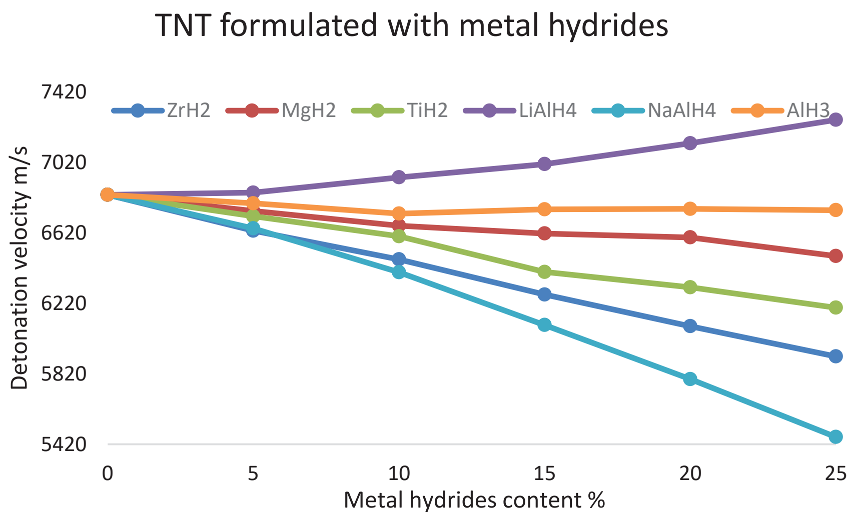

Fig. 9. Effect of metal hydrides quantities on detonation velocity of TNT formulations

Fig. 9 shows the formulations of the TNT with the metal hydrides, $LiAlH_4$ is the only one that shows an increase of detonation velocity with increasing % of $LiAlH_4$. All other metal hydrides decrease the performance of TNT.

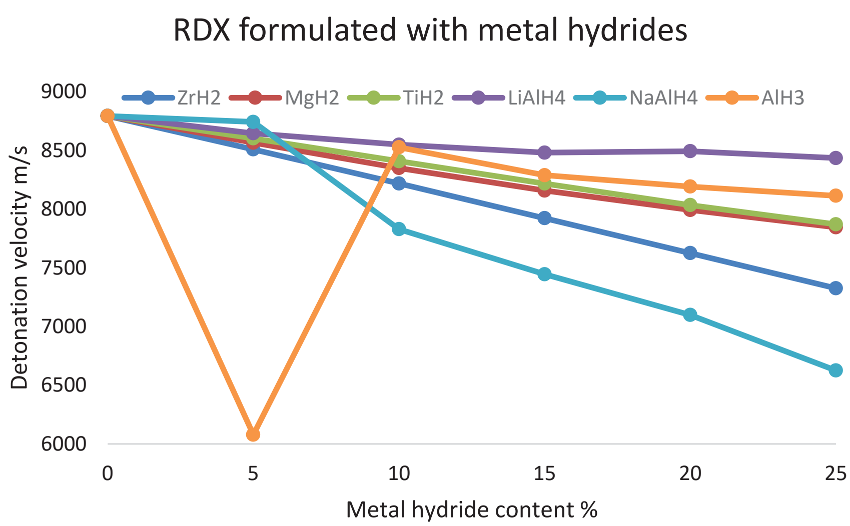

Fig. 10: Effect of metal hydrides quantities on detonation velocity of RDX formulations

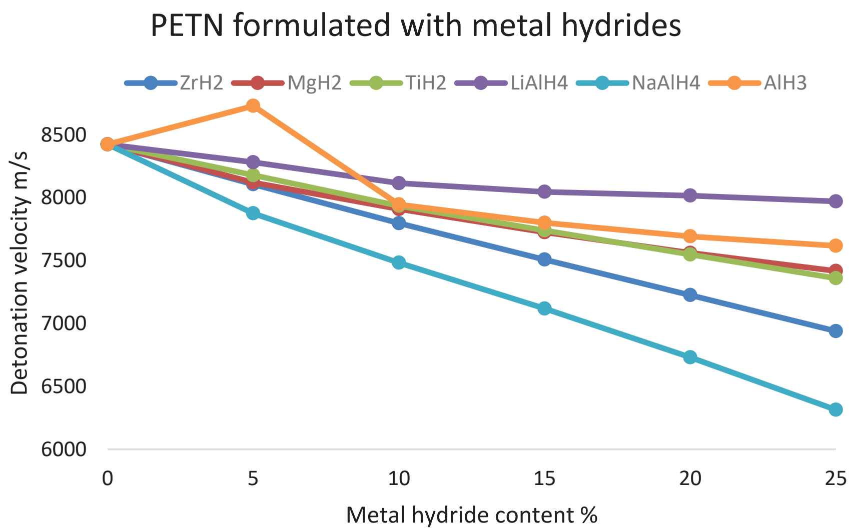

Fig. 11: Effect of metal hydrides quantities on detonation velocity of PETN formulations

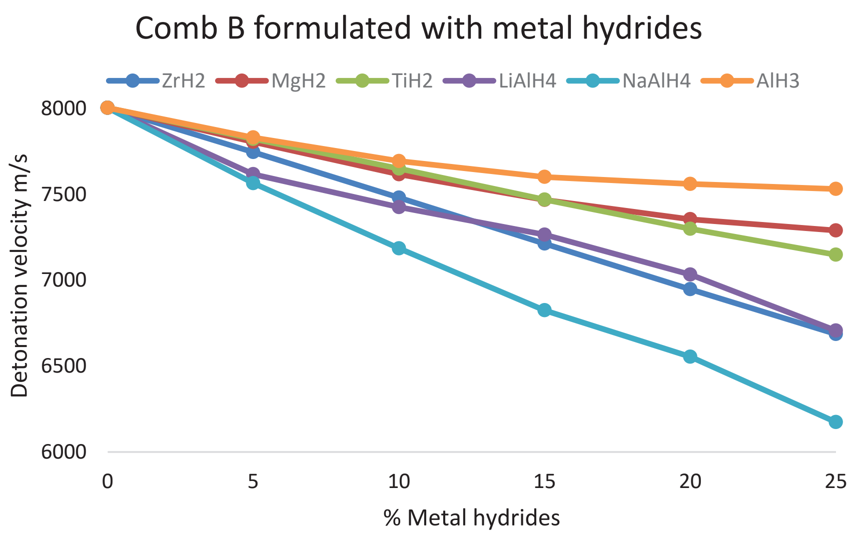

Fig. 12: Effect of metal hydrides quantities on detonation velocity of Comp B formulations

RDX formulations in Fig. 10 show no enhancement for all the metal hydrides. AlH_3 containing formulation in Fig. 11 shows an increased detonation velocity of 8700 m/s at 5% metal hydride with the rest of the other formulations showing no enhancement. Comp B consists of 60% RDX and 40% TNT, containing more RDX and that might be the reason that there is no observed enhancement.

Conclusion

The EXPLO5 simulations of the energetic materials containing metal hydride were done successfully. The densities of the formulations were observed to be affected by the addition of metal hydrides where the metal hydrides made from heavy metals increased the formulation densities and the lighter metal hydrides decreased the density. Despite the observed increase in density for some formulations, this did not translate into more increased detonation pressure except for the TNT formulation with ZrH_2. AlH_3 seems to be performing well for all the explosives, including PETN formulation. $LiAlH_4$ and $NaAlH_4$ are shown to be effective at a low percentage (5%) for some of the explosive materials. The metal hydride additives show no considerable effect on the detonation velocity only TNT formulation with $LiAlH_4$ and PETN formulation with AlH_3.

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