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from: Hobbs ML (1516, MS0836)

subject: Modeling cookoff of HMX based PBX explosives with inert binders (e.g. LX-07) *

Summary

We have previously developed a PBX 9501 cookoff model for the plastic bonded explosive PBX 9501 consisting of 95 wt% octahydro-1,3,5,7-tetranitro-1,3,5,7-tetrazoncine (HMX), 2.5 wt% Estane® 5703 (a polyurethane thermoplastic), and 2.5 wt% of a nitroplasticizer (NP): BDNPA/F, a 50/50 wt% eutectic mixture bis(2,2-dinitropropyl)-acetal (BDNPA) and bis(2,2-dinitropropyl)-formal (BDNPF). This five-step model includes desorption of water, decomposition of the NP to form NO_2, reaction of the NO_2 with Estane and HMX, and decomposition of HMX [1]. This model has been successfully validated with data from six laboratories with scales ranging from 2 g to more than 2.5 kg of explosive. We have determined, that the PBX 9501 model can be used to predict cookoff of other plastic bonded explosives containing HMX and an inert binder, such as LX-04 consisting of 85 wt% HMX and 15 wt% Viton A (vinylidine fluoride/hexafluoropropylene copolymer), LX-07 (90 wt% HMX and 10 wt% Viton A), LX-10-0 (95 wt% HMX and 5 wt% Viton A), and LX-14 consisting of 95.5 wt % HMX and 4.5 wt% Estane® 5702-F1 (a polyurethane thermoplastic).

Normally our cookoff models are verified using Sandia's Instrumented Thermal Initiation (SITI) experiment. However, SITI data for LX-04, LX-07, LX-10-0, and LX-14 are not available at pressed density; although, some molding powder SITI data on LX-10-0 and LX-14 exists. Tarver and Tran [2] provide some one-dimensional time-to-explosion (ODTX) data for these explosives. The applicability of the PBX 9501 model to LX-04, LX-07, LX-10-0, AND LX-14 was made using this ODTX data [2]. The PBX 9501 model is applied to these other explosives by accounting for the correct amount of HMX in the explosive and limiting the NP reaction. We have found the PBX 9501 model to be useful for predicting the response of these PBXs to abnormal thermal environments such as fire.

Parameters

Details of the model are presented in reference [1]. The energetic binder in the PBX 9501 model was changed to make the model suitable for PBXs with nonreactive binders. This was accomplished by setting the mass fraction of the Estane and NP to a small number, 0.00001, respectively. The mass fraction of HMX was then changed to be consistent with the specific PBX formulation. Details specific to LX-04, LX-07, LX-10-0, and LX-14 are presented in Table 1.

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Table 1. Composition of selected HMX-based explosives.

	Reactive components			Non-reactive components	
Explosive	wt% Estane	wt% BDNPA/F (NP)	wt% HMX[a]	Viton A	Estane 5702-F1
PBX 9501	2.5	2.5	95-0.5		
LX-04	0.001	0.001	85-0.5-0.001	15	
LX-07	0.001	0.001	90-0.5-0.001	10	
LX-10-0	0.001	0.001	95-0.5-0.001	5	
LX-14	0.001	0.001	95.5-0.5-0.001		4.5

[a] The moisture content (0.5 wt%) and trace amounts of Estane and NP are subtracted from the HMX composition.

Results

Figure 1 compares the model prediction (solid black line) with measured ODTX data (colored circles) from Ref. [2]. The good agreement is attributed to the ability of the PBX 9501 model to predict the effect of the HMX on ignition. As discussed in Ref. [1], the PBX 9501 simulation of the high density pressed ODTX was made by assuming no reaction of the nitroplasticizer. During decomposition of PBX 9501, the binder and plasticizer migrate and react near the edge of the aluminum confining anvil where the reaction energy is easily dissipated. The migration is caused by large differences in volumetric expansion characteristics of the binder/NP versus HMX. Furthermore, the small size and high density of the ODTX experiment favors this assumption. Favorable predictions of the other HMX based explosives were made using this same assumption.

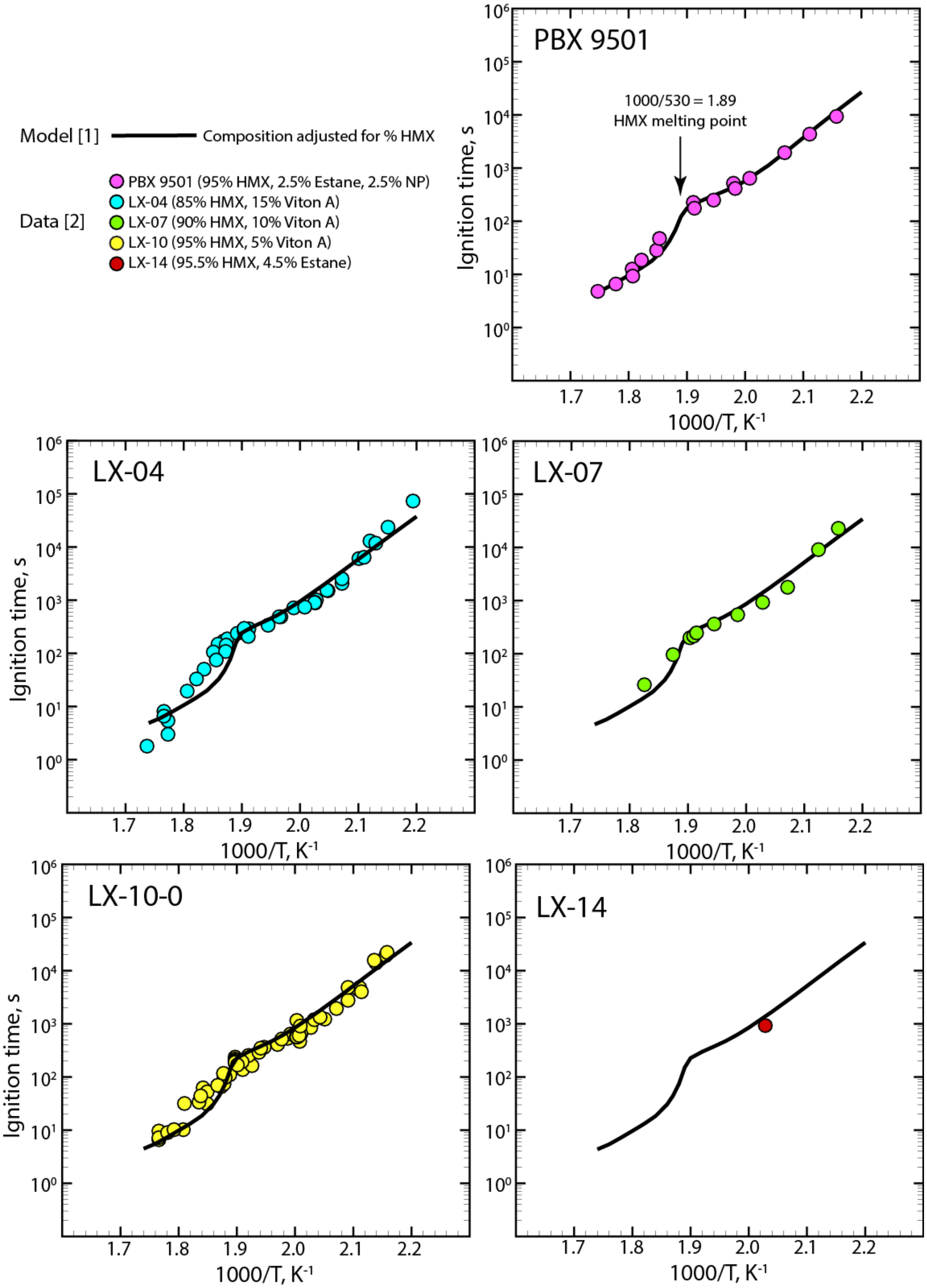
Conclusions and recommendations

This memo presented predictions from a recently developed PBX 9501 model [1] to ODTX data [2] for PBX 9501, LX-04, LX-7, LX-10, and LX-14. Successful predictions were made by turning off the nitroplasticizer chemistry. The NP chemistry was neutralized by setting the NP and Estane compositions to a small number (0.001 wt%). I recommend that the PBX 9501 model [1] be used for HMX-based plastic-bonded explosives with inert binders by setting the composition of the Estane® and NP to small amounts such as 0.001 wt% as was done in the current work. The model is pressure dependent and requires calculation of the thermodynamic pressure for sealed systems. For vented systems, the pressure exponents should be set to zero as discussed further in Ref. [1]. The model is unique in that it can predict thermal response for both sealed and vented systems. Further validation using Sandia's Instrumented Thermal Ignition (SITI) experiment should be considered for future work.

Bibliography

[1] M. L. Hobbs, M. J. Kaneshige and W. W. Erikson, "Modeling the measured effect of a nitroplasticizer (BDNPA/F) on cookoff of a plastic bonded explosive (PBX 9501)," *Combustion and Flame,* vol. 173, pp. 132-150, 2016.

[2] C. M. Tarver and T. D. Tran, "Thermal decomposition models for HMX-based plastic bonded explosives," *Combustion and Flame,* vol. 137, pp. 50-62, 2004.


Model [1]
Composition adjusted for % HMX
Data [2]
PBX 9501 (95% HMX, 2.5% Estane, 2.5% NP)
LX-04 (85% HMX, 15% Viton A)
LX-07 (90% HMX, 10% Viton A)
LX-10 (95% HMX, 5% Viton A)
LX-14 (95.5% HMX, 4.5% Estane)
PBX 9501
1000/530 = 1.89
HMX melting point
LX-04
LX-07
LX-10-0
LX-14
Ignition time, s
1000/T, K-1

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