

Abstract Submitted  
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**Modeling of TATB-Based HE Cook-off for Safety Analysis<sup>1</sup>**

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Lawrence Livermore Natl Lab — We investigate and model the cook-off behavior of LX-17 to understand the response of explosive systems in abnormal thermal environments. Decomposition has been explored via conventional ODTX (One-Dimensional Time-to-eXplosion), PODTX (ODTX with pressure-measurement), TGA, and DSC experiments under isothermal and ramped temperature profiles. The data were used to fit reaction rate parameters for proposed schemes in an ALE3D computational model. This model includes chemical reactions, thermo- and hydro-dynamics, and material properties, including thermal expansion, compressibility, and strength. These parameterizations were carried out utilizing a Python evolutionary optimization method on LLNL's high-performance computing clusters. Additional experiments will be conducted to further elucidate decomposition intermediates to improve the model. Once experimentally validated, this model will be scalable to several applications involving LX-17 and can be used to develop more sophisticated experimental methods. Furthermore, the optimization methodology developed herein should be applicable to other high explosive materials. LLNL-ABS-768048

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