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Incorporation of a Chemical Kinetics Model for Composition B in a Parallel Finite-Element Algorithm ELIZABETH KALLMAN, DENISE PAULER, Ball Aerospace & Technologies Corp. — A thermal degradation model for Composition B (Comp B) explosive is being evaluated for incorporation into a finite-element algorithm [1]. The RDX component of Comp B dominates the thermal degradation since its decomposition process occurs at lower temperatures than TNT. The model assumes that solid and liquid RDX decompose by the same mechanisms, but along different reaction pathways [2, 3]. A steady-state approximation is applied to the gaseous intermediates and is compared to the full transient analysis for the entire reaction scheme. The parallel finite-element algorithm is used to predict the pressure increase on the interior of the metal casing of confined Comp B due to the production of gases during thermal decomposition.

References [1] E. M. Kallman, "Scalable Cluster-Based Galerkin Analysis for Kinetics Models of Energetic Materials," SIAM CSE, March 2-6, 2009. [2] D. K. Zerkle, "Composition B Decomposition and Ignition Model," 13th International Detonation Symposium, July 23-28, 2006. [3] J. M. Zucker, A. J. Barra, D. K. Zerkle, M. J. Kaneshige and P. M. Dickson, "Thermal Decomposition Models for High Explosive Compositions," 14th APS Topical Conference on Shock Compression of Condensed Matter, July 31-August 5, 2005.

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