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### Biocidal effectiveness of combustion products of iodine-bearing reactive materials against aerosolized bacterial spores

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### Abstract

Mechanochemically prepared metal-based iodine bearing reactive materials (RMs), generate  $I_2$ gas among other combustion products, and are therefore of interest as biocidal additives in agent defeat applications. In order to facilitate future use of these RMs, a phenomenological model is proposed that describes biocidal effectiveness of ternary Al·B·I<sub>2</sub> composites against aerosolized spores of Bacillus thuringiensis (Btk), a Bacillus anthracis surrogate. The model is based on experiments, in which aerosolized spores passed through an enclosed flow system, where on a sub-second time scale they were exposed to elevated temperatures and combustion products of different RM powders injected in an air-acetylene flame. Temperature distribution, and flow conditions in the exposure chamber were varied to achieve different temperature, iodine concentration profiles, and exposure times. The exposure effect was quantified experimentally via an inactivation factor IF, defined as the inverse fraction of microorganisms surviving the exposure. The process observed in the experiments was described using computational fluid dynamics (CFD) modeling, treating the bacterial spores as 1-µm unit-density particles injected in the airflow, and assuming continuous iodine release during RM particle combustion. То quantify the biocidal effect for each spore, an integral exposure function was introduced consisting of two Arrhenius terms corresponding to pure thermal and iodine-related inactivation. The corresponding activation energies were found as  $E_1 = 5$  kJ/mol, and  $E_2 = 10$  kJ/mol, respectively. The rate constant for the iodine-concentration dependent term was found as 32.3  $m^{3}$ /mol multiplied by the iodine concentration in mol/m<sup>3</sup>. A critical total exposure threshold was identified. Since the model proposed here depends only on thermal exposure and on iodine, it may be valid for a wider range of iodine bearing RMs.

**Keywords:** Biological aerosols; Agent defeat; Reactive materials

#### 1. Introduction

Stockpiles of biological weapons represent significant danger (Bleek, Kane, & Pollack, 2016); they may be targeted by advanced munitions designed to inactivate the highly pathogenic microorganisms (Baker, Gotzmer, Gill, Kim, & Blachek, 2009; Tan et al., 2006). Upon target blast, stress-resistant bio-agents, such as bacterial spores, can be aerosolized. While many microorganisms will likely be inactivated (killed), some may survive escaping the harsh condition of the explosion and fire. Release of a viable pathogenic bioaerosol in the atmosphere represents a significant health risk. To address this problem, recent research efforts focused on the development of iodine-bearing reactive materials (RMs) (A. Abraham, Obamedo, Schoenitz,

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