



DIMP & Other Simulants Workshop

October 3 -5, 2023

Johns Hopkins University | Baltimore, MD

Tentative AgendaDay 1, Tuesday, October 3

Times include up to 5 min Q&A

Time	Title	Speaker
8:00 – 9:00	Registration and Continental Breakfast	

Setting the Stage		
9:00 – 9:15	Introductory comments	Eilers, Weihs, Davis
9:15 – 9:40	DTRA's interest	Lee Nelson (DTRA)
9:40 – 10:05	An Overview of the Agent Defeat Problem from an M&S Perspective	Raj Sinha (CRAFT Tech)

10:05 – 10:20 Coffee break

General Agent/Simulant Information		
10:20 – 10:40	Overview of agents and simulants	Mike Hunter (ARA)
10:40 – 11:15	Simulant use in three recent projects	Matthew Blais (SWRI)
11:15 – 11:50	Simulants: Use in Consequence Assessment Model Development and Testing	Michael Donovan (Leidos)

11:50 – 13:00 Lunch break

13:00 – 13:35	Chemical mechanisms deployed in UK and experiences in modeling simulant vs. agent	Aaron Longbottom (FGE, UK)
13:35 – 14:05	Overview of detailed thermal decomposition mechanisms developed for TEP, DIMP, DEMP, DMMP, etc.	Subith Vasu, Ramees Rahman (UCF)

Capabilities, Diagnostics, and Analysis for studying the defeat of agents/simulants		
14:05 – 14:30	Development of Computationally-Tractable Chemical Kinetics Models for CFD Simulations of Chemical Agent Defeat	Andrea Zambon (CRAFT Tech)
14:30 – 14:55	An Overview of Approaches to Accelerate Simulant Chemical Kinetics Evaluations in CFD Simulations of Chemical Agent Defeat	Andrea Zambon (CRAFT Tech)

14:55 – 15:10 Coffee break

15:10 – 16:00	Challenges/Needs for Optical Diagnostics	Keith Rein (Spectral Energies)
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Poster Session & Networking		
16:10 – 17:30	Poster Session & Networking	All

DIMP & Other Simulants Workshop

Day 2, Wednesday, October 4

Times include 5 min for Q&A

Time	Title	Speaker
8:00 – 9:00	Registration and Continental Breakfast	

Capabilities, Diagnostics, and Analysis for studying the defeat of agents/simulants		
9:00 – 9:05	Introductory comments	Hergen Eilers WSU)
9:05 – 9:30	Turbulence - Scales and mixing in detonation environments	Suresh Menon (GT)
9:30 – 9:55	Assessing Prompt Neutralization of DIMP via Reactive Materials	Tim Weihs (JHU)
9:55 – 10:20	Shocktube	Subith Vasu, Ramees Rahman (UCF)

10:20 – 10:35 Coffee break

10:35 – 11:00	Explosion chamber testing/Fast scanning LWIR absorption	Nick Glumac (UIUC)
11:00 – 11:25	Characterizing defeat of simulants via Pyroprobe/Brill cell, heated gas cell; and optical trapping of droplets	Hergen Eilers (WSU)
11:25 – 11:50	Characterization of Pyrotechnic Employment	Bruce King (CBC)

11:50 – 13:00 Lunch break

Decomposition of condensed-phase simulants		
13:00 – 13:25	Properties of liquid DIMP and other organophosphorus liquids	Ed Dreizin and Gennady Gor (NJIT)
13:25 – 14:00	Molecular dynamics prediction of DIMP and other organophosphorus liquids	Gennady Gor (NJIT)
14:00 – 14:35	On interaction of liquid DIMP with various oxides	Ed Dreizin (NJIT) and Lori Groven (SDSMT)

14:35 – 14:50 Coffee break

14:50 – 15:15	Bunker experiments with DIMP – experiments vs. simulations	Pierre Graumer and Antoine Osmont (French Commissariat à l’Energie Atomique (CEA))
15:15 – 15:40	Thermal decomposition of DIMP and its decomposition products under fast pyroprobe heating	Hergen Eilers (WSU)
15:40 – 16:15	Agent Reactivity on Zirconium Oxyhydroxide and Zr-based Metal-Organic Frameworks	Greg Peterson (CBC)
16:15 – 16:40	Tailoring Oxide Materials Properties Chemical Warfare Agent Degradation: Lessons Learned from DIMP	Kandis Leslie Abdul-Aziz (UCR)

16:40 – 16:50 Coffee break

16:50 – 18:00	Open discussion	All
<p>The role of interfaces in the decomposition of DIMP</p> <ul style="list-style-type: none"> • Experimental measurements show that the decomposition of DIMP appears to be impacted by various surfaces (e.g., stainless steel vs. brass; stainless steel vs. gold; ZnSe; quartz?) • How can we understand this behavior? • How can we account for it in our measurements? 		

DIMP & Other Simulants Workshop

Day 3, Thursday, October 5

Times include 5 min for Q&A

Time	Title	Speaker
8:00 – 9:00	Registration and Continental Breakfast	

Decomposition of gas-phase simulants		
9:00 – 9:05	Introductory comments	Hergen Eilers (WSU)
9:05 – 9:30	Gas-phase thermal decomposition of DIMP at temperatures below 350 °C (joint work with CRAFT Tech)	Ed Dreizin (NJIT)
9:30 – 9:55	Thermal decomposition of DIMP and its decomposition products in a heated gas cell	Hergen Eilers (WSU)
9:55 – 10:30	Theoretical investigation of the thermal decomposition of CWA surrogates	Pierre-Alexandre Glaude (University of Lorraine, France)

10:30 – 10:45 Coffee break

10:45 – 11:10	Reducing chemistry to the bare necessities (via video)	Pierre Boivin (University of Marseille, France) and Laurent Verdier (Ministere des Armees, France)
11:10 – 11:40	DIMP Decomposition Mechanisms on Metal Oxide Surfaces from Ab Initio Molecular Dynamics	Bryan Wong (UCR)
11:40 – 12:15	Dynamic measurements of DIMP decomposition in hydrogen/oxygen flames	Mark Phillips (UA)

12:15 – 13:30 Lunch break

13:30 – 15:00	Open discussion	All
Alternatives to DIMP / TEP <ul style="list-style-type: none"> • DIMP is expensive and large-scale production/consumption of DIMP is restricted by the chemical weapons convention. • What alternatives are available? • What properties do we need to simulate? 		
	Closing remarks	Hergen Eilers (WSU)
	Adjourn	