Threat Agent Science Capability Area
Computational Chemistry Thrust Area

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Overview

• Organizational Overview
• New Computational Chemistry Thrust Area within the Threat Agent Science Capability Area Focus Areas
  • Potential applications
  • Current efforts
  • Planned thrusts
Objective

Develop and apply quantitative chemistry techniques and tools to provide accurate technical threat agent understanding and prediction

- Agent Fate on complex surfaces
  - i.e. concrete, asphalt, grass, sand, other operational surfaces
- Address emerging and new threat agents
- Agent/Simulant correlation and simulant design
- Application to agent toxicology and hazard
- Decrease dependence on empirical testing and infrastructure
Potential Applications of Computational Chemistry

- Assist in the Development of Accurate Models of Chemical Hazard Persistence and Risk Duration
- Chemical Agent Fate
  - Live Agent Tests are Expensive
  - Facilities Scarce
- Simulant Correlation
  - Design?
- Provide Insight into Chemical Agent Interaction with Surface Materials
  - What happens to the agent?
  - What “liberates” the agent from the substrate?
- Individual and Collective Protection
- Decontamination Issues
- Operational Considerations
- Toxicological Effects
Computational Chemistry
Thrust Area

• Two Focus Areas
  – Quantitative Structure Activity Relationships (QSAR)
  – Quantitative Chemical Theory (QCT)
  – Possible additional areas per proposal inputs

• QSAR
  – CBRTA Independent Assessment and Evaluation of QSAR in Predictive Modeling underway (Cipher Systems, SRC)
  – Results delivered

• QCT
  – FY06 New Start
  – Performers
    • Naval Research Laboratory (Dr. Bermudez)
    • AFRL (Mr. Kilpatrick, Dr. Evans)
Quantitative Structure Activity Relationships (QSAR)

• Problem
  – Efforts to “improve” simulants will result in more toxic simulants (Similar Property Principle)
  – Efforts to “improve” simulants still won’t accomplish the goal of the Thrust Area

• Emphasis should be on understanding correlation between simulant activity and agent activity, and using this understanding to make predictive statements about agent activity
• Use a combination of experimental and computational methods, in connection to QSAR
• Determine the correlation between agent/simulant structure and SPECIFIC activity
• Create mapping functions to map known simulant activity into set of unknown agent activities
QSAR
Understanding Agent and Simulant Activity

Experiment

Information used to create mapping function

QSAR

Computational
QSAR
Predicting Agent Activity

Known Agent or Simulant Activity

Mapping Function

Unknown Agent or Simulant Activity
Quantum Chemical Theory (QCT)

• Problem
  – Shortcomings of experimental approach to agent/surface interaction investigations
    ▪ Too many permutations
    ▪ Risk and cost associated with agent experimentation
    ▪ Rate of emerging threats faster than traditional empirical approach can accommodate
  – Extensive reliance on simulants to represent CWAs

• QCT is a readily available technology
  – First principles approach to understanding agent/surface interaction effects
  – Does not replace experimental efforts
  – Only possible given recent HPC improvements
    ▪ SGI Origin 3900 (128 MIPS R12000 CPUs, 256 Gb memory)
    ▪ Year 1 effort is ~ 50,000 CPU hours
Quantum Chemical Theory (QCT)

- QCT tools have been extensively developed and thoroughly tested by academia
  - No new software tools needed
  - Application to CWAs is direct extension of existing work
- New start effort
  - Joint AFRL and NRL project
  - Incremental approach to validate application of QCT modeling to agent fate and agent/simulant correlation
    - FY06: Validate quantitative reliability of QCT against simulant data
    - FY07: Evaluate extent of currently used simulants to reproduce properties of CWAs; begin calculations on agent surface interactions with solid oxide surfaces
    - FY08: Extend modeling of CWAs absorbed onto solid oxides to complex surfaces
  - Broad application to other areas within CB defense
Current Efforts

• Expansion of the Computational Chemistry Thrust Area
• Evaluation of Proposals for FY07 Start
  – Responses to JSTO Service Call
  – Responses to JSTO BAA For Industry
Questions?

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