Applying Quantum Chemical Theory to the Fate of Chemical Warfare Agents

S&T CBIS Conference

Presented By

Tom J. Evans, Ph.D.
Tom Stark, Ph.D.
Cubic Applications, Inc.

26 October 2005

Agent Fate Program

- Five year DTO investigating the persistence and fate of chemical warfare agents (CWA)
- Major activity - generation and collection of accurate evaporation data derived from laboratory, bench scale experiments to open air field trials.
- Historically, data collection has consisted of factorial experiments to empirically measure the evaporation response.

Agent Fate Program

- Historical approach consisted of factorial-type experiments to collect data on agent persistency/behavior
  - Large number of potential factors
  - Many factor levels
- Even with statistical DOE techniques the number of permutations is very large.

Short Comings To Experimental Approach

- Impossible to do studies with **ALL** permutations of known/immerging threats and surfaces of interest
- Limited/no use of agents in the field
- Risk & cost associated with any agent work
- Rate of emerging threats is conceivably faster than rate of traditional approach to investigate

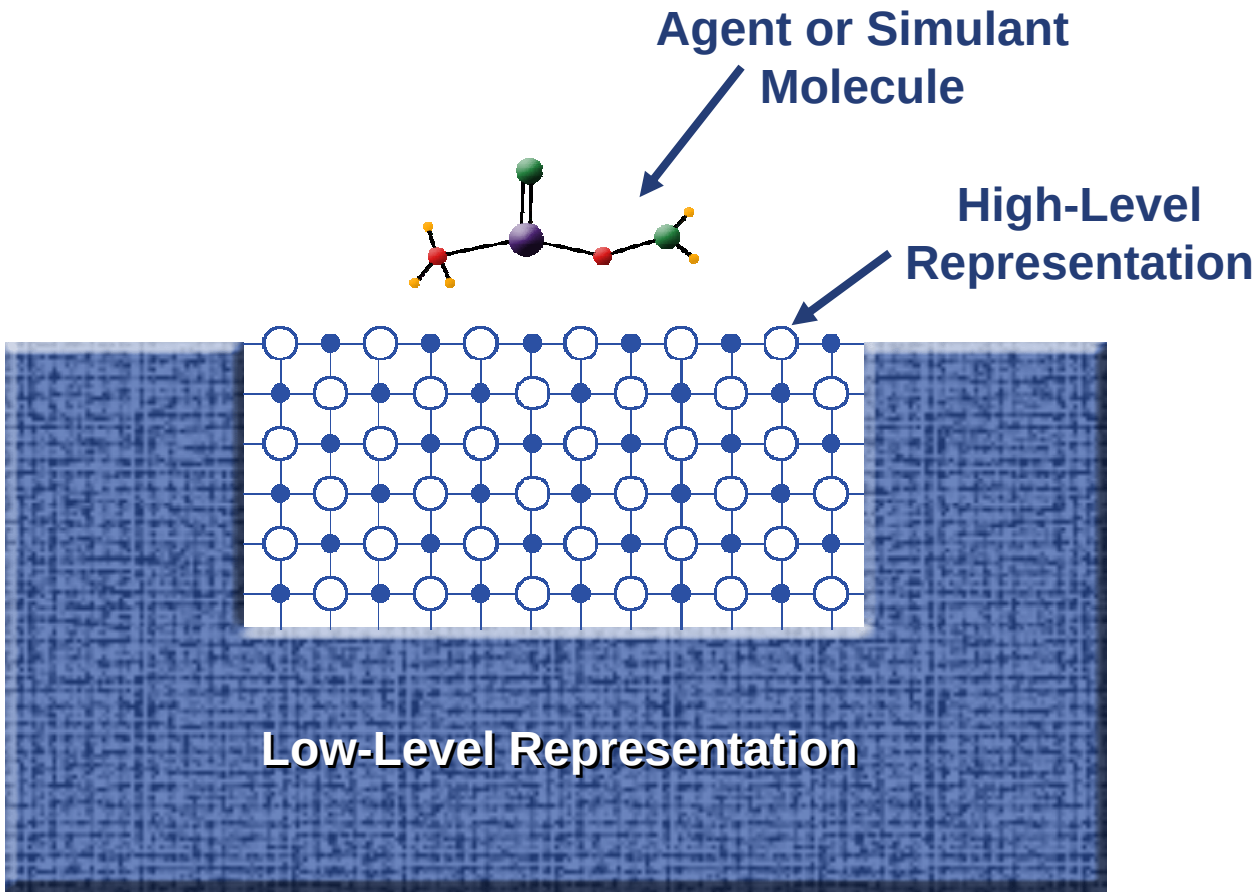
The Heart of the Problem

- Understanding fundamental principles
  - Streamlines current and future efforts
  - Directs experimental design on existing threats
  - Reduces the number of experiments for agent/substrate combinations
  - Focuses efforts as new threats immerge – helps deal with a “technical surprise”
- Much of experimental work is done with simulants
  - Need to determine reliability of simulant for representing agent
  - Data from agent/substrate and simulant/substrate can be compared side-by-side

Quantum Chemistry Calculations Important Points

- Quantum Chemical Theory (QCT) – Embedded Cluster
- QCT enhances but does not replace experimental efforts
- Surfaces of interest
  - Selected because they are well understood
  - Representative of more complex surfaces and materials
- Only recently have HPC capabilities (speed and memory) allowed for these types of approaches

Embedded Cluster



Advantages of Embedded Clusters

- Tool to investigate interactions at molecular level
- Limits prohibitive cost of all high-level QCT surface calculations
- Represents surface at realistic level of approximation
- Long range effects of surrounding cluster present

Conclusions

- Effort to incorporate QCT into Agent Fate Program signifies more than another tool
  - Recognition that shortcomings of purely experimental data can be overcome by modeling
  - Efforts to make the overwhelming fate of agent problem are moving to understanding fundamental principles
- QCT can be used to streamline programs efforts, while making contributions that move beyond Agent Fate

Questions?