Reaction Engineering International

Advanced Computer Simulations Of Military Incinerators

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Outline

- Technical objectives of SBIR project
- Chemical kinetic mechanism development for agent destruction
- Equipment model development
- Applications of models

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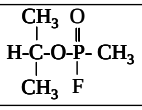
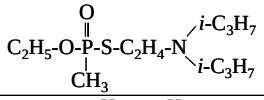
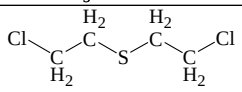
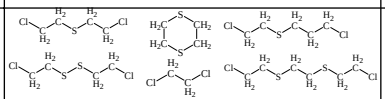
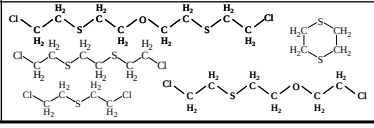
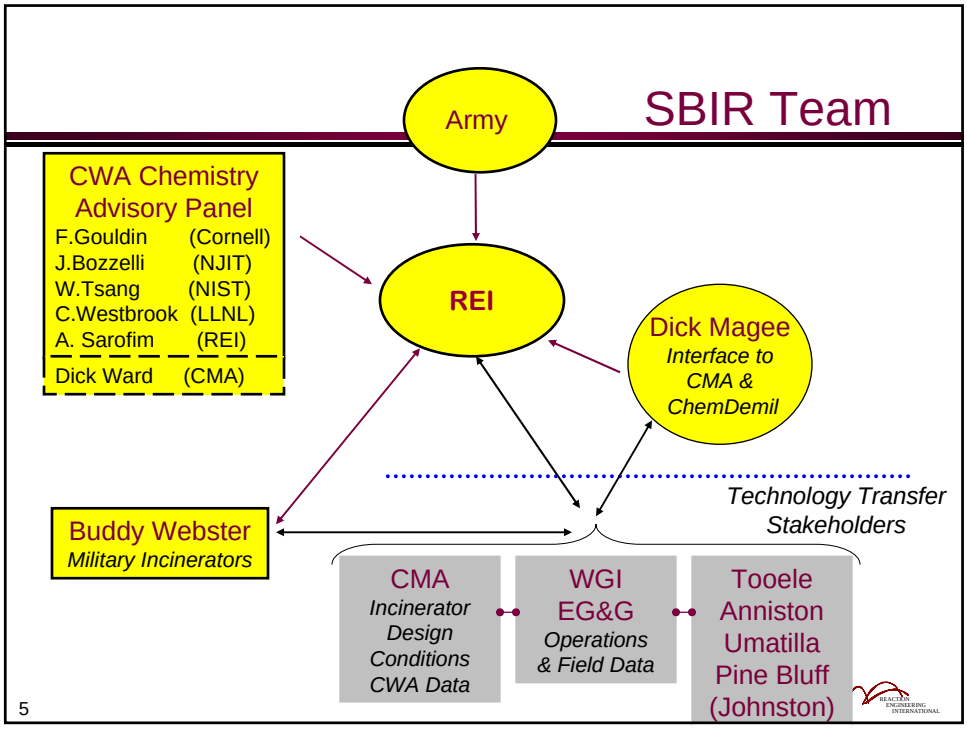
SBIR Phase II Technical Tasks

- Develop Chemistry Models for CWA
  - effort guided by Advisory Panel
  - use computational chemistry methods
  - simulants & agents
  - detailed chemical kinetic mechanisms
    - complete description of CWA decomposition
    - include PICs, NOx
    - use relevant, publicly available data
- Develop Furnace / Equipment Models
  - Incinerators: furnaces + afterburners
  - Pollution Abatement System (PAS)
  - benchmark with available data
- Develop Incinerator Simulator Tool Software

Chemistry Models for CWA's

Agent	Structure	Mechanism
GB		LLNL w/ Bozzelli-REI GB rate + P & F
VX		Bozzelli-REI
HD		Bozzelli-REI
H		Bozzelli-REI
HT		Bozzelli-REI

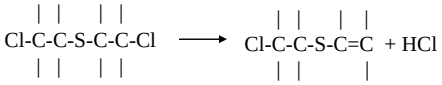
- Reliable test data not available
- Developed using computational chemistry methods
  - 100+ species
  - 500-1200 reactions
- Benchmarked with known rate constants for comparable molecules
- Reviewed by expert Advisory Panel



Chemical Kinetic Mechanism for H/HD/HT

- No test data available – rates from computational chemistry
- Kinetics for thickeners and impurities included
- HD detailed mechanism:
  - 109 species, 477 reactions
  - Couples to
    - Leeds sulfur mechanism
    - Cl chemistry of Procaccini, Ho, Bozzelli, et al
- H modeled by 6-specie blend
  - 5 species for impurities
  - Add-on to HD mechanism
  - 143 species, 548 reactions
- HT modeled by 5-specie blend
  - 4 species for impurities
  - Add-on to H/HD mechanism
  - 165 total species, 657 total reactions
- Improvements to S-H-O chemistry

Dominant destruction pathway:
HCl elimination from HD



$k = 1.85\times10^{13}e^{(-58.75/RT)}$ sec^{-1}

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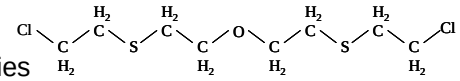
Thickeners & Impurities

- Kinetics for thickeners and impurities
- H modeled by 6-specie blend
- HT modeled by 5-specie blend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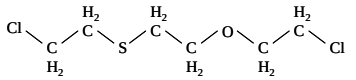
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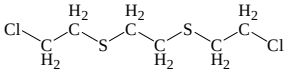
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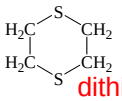
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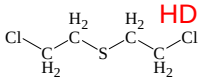
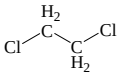
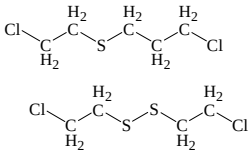

HD


1,2-dichloro-ethane



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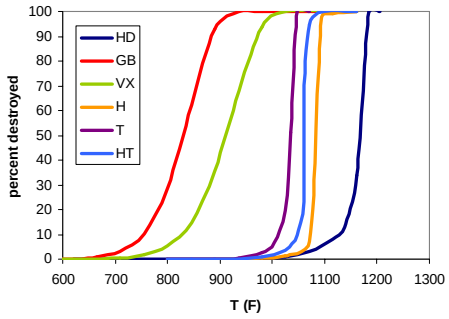
Calculated Incinerability Rankings

Approximation to UDRI Incinerability Ranking

(Temperature at which 99% of the compound is destroyed in 2 seconds)



Compound	T99(2)	Class
Benzene	1150 C	1
Toluene	895 C	2
Vinyl Chloride	770 C	3
Trichloroethane	635 C	4
HD	**628 C**	**4**
H	**603 C**	**4**
HT	**578 C**	**5**
T	**562 C**	**5**
Chloroform	545 C	5
VX	**541 C**	**5**
Hexachloropropene	505 C	5
GB	**491 C**	**5**
Strychnine	320 C	6

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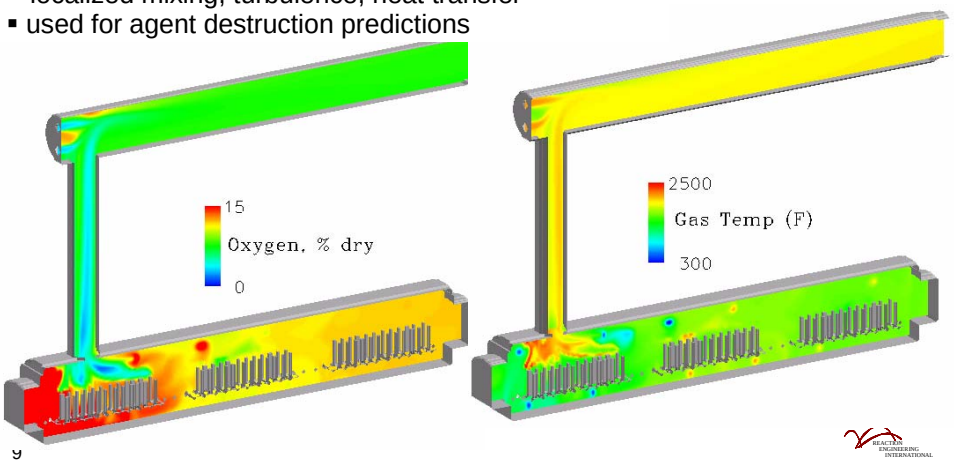
CFD Combustion

- full 3D combustion flow field
  - gas velocity, composition, temperature
  - shell and wall heat transfer, temperature
- localized mixing, turbulence, heat transfer
- used for agent destruction predictions



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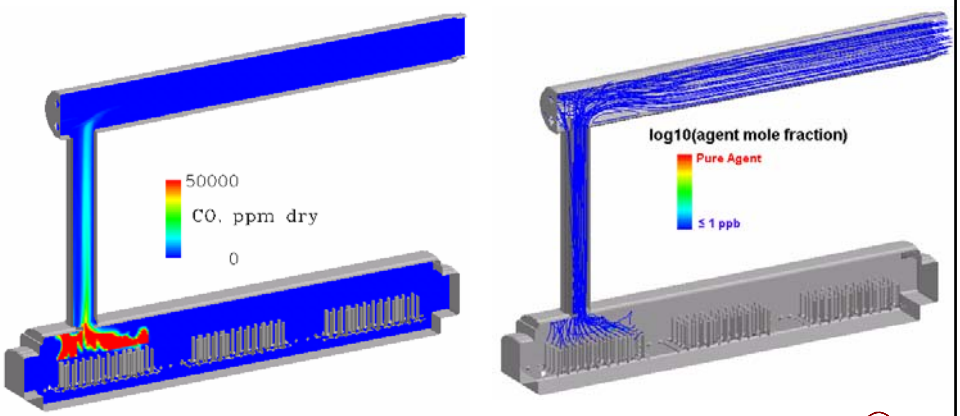
CFD Model Results & Agent Destruction

CFD Results provide details about
agent destruction along streamlines



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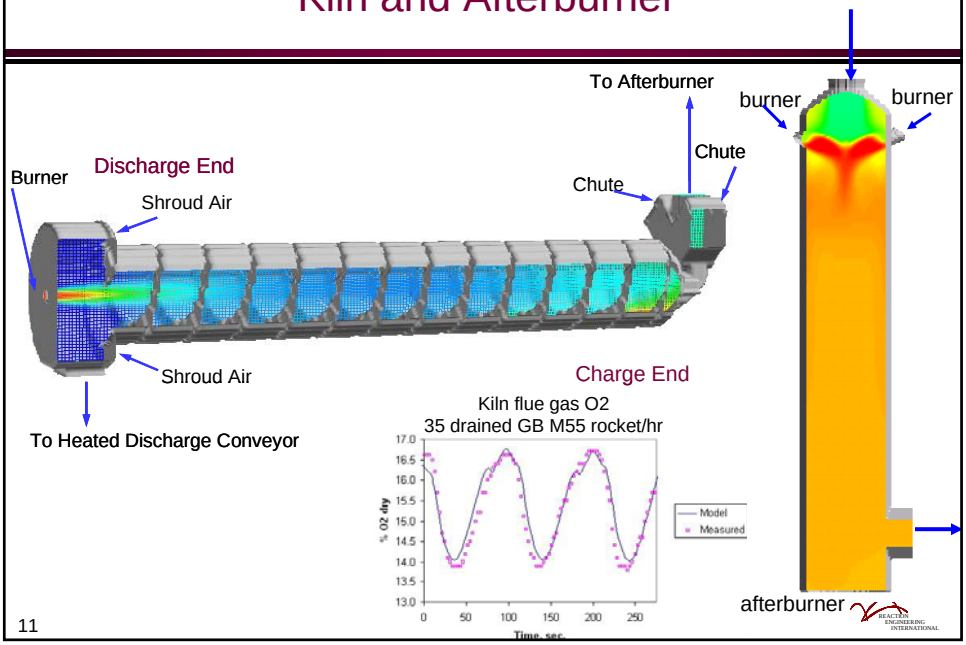
CO **Agent Destruction**

Deactivation Furnace System
Kiln and Afterburner



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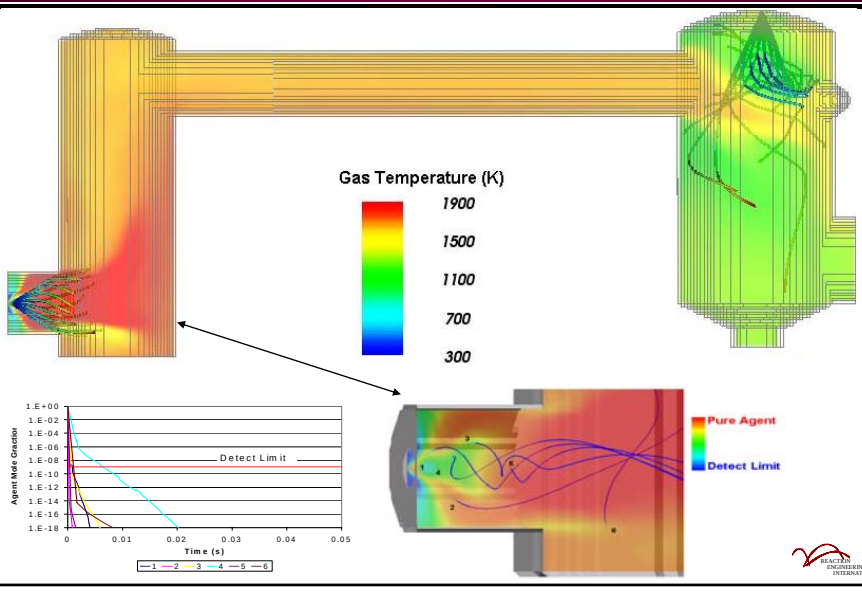
Liquid Incinerator Combustor



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Impact of SBIR Project on Chem Demil Program

- JACADS DAL VX event (RIM 57)
  - *Models* used to convince regulators to modify DAL clearance criterion
  - Resulted in significant cost savings
- Fate of phosphorus when processing organophosphorus agent
  - Analysis used in negotiations with regulators
    - Obtain "credit" for PFS emissions removal
    - Replace surrogate trial burn with agent trial burn
    - Eliminate requirement for high temperature test
- RIM-65 MPF evaluation for processing undrained mustard projectiles (with solid heels)
  - Analysis to assist TOCDF & ANCDF in negotiations with regulators to modify incinerator operation
- SBIR Phase II plus
  - HT mustard chemical kinetic mechanism
  - Improved understanding of mercury issues
  - HD TC processing
  - CMS burner evaluation
- Potentially ➔ extend models to non-incineration *thermal treatment*

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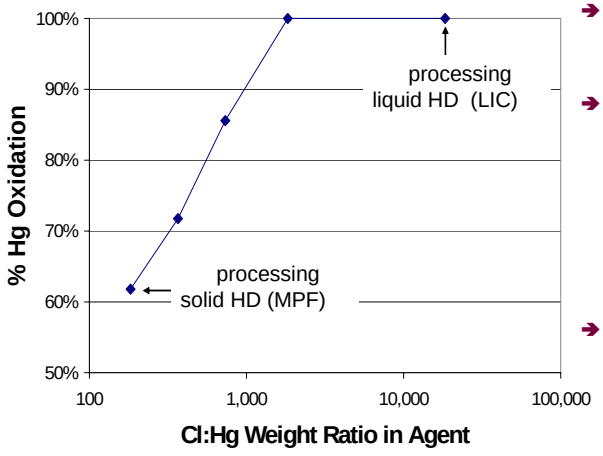
Model Results:
Effect of Agent Hg Content on Hg Oxidation



- Shown is calculated Hg oxidation at different ratios of Cl:Hg in feed
- TOCDF HD TCs:
  - Liquid HD
    Hg ~ 10's ppm
    Cl:Hg ~ O(10,000)
  - Solid agent
    Hg ~ 100's -1000's ppm
    Cl:Hg ~ O(100)
- Cl:Hg >2000 results in complete oxidation of Hg in quench tower

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Ramifications of Hg Removal Modeling

- Predicts increased Hg capture when:
  - increase Cl/Hg ratio in munitions
  - decrease cooling rate in PAS
- Hg^0 capture in PAS can be increased by
  - Increasing Cl/Hg ratio
    - » e.g. add chlorocarbons used in trial burns
  - Decreasing cooling rate in quench tower
    - » control of quench flow rate or droplet size
- Control of mercury removal in PAS influences waste handling strategies
  - High Hg removal efficiency
    - ➔ waste stream contaminated by Hg^0 is restricted to brine wastes
  - Low Hg removal efficiency
    - ➔ carbon in the PFS is also contaminated by Hg^0.

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Processing Partially Drained TCs in MPF

- Motivation:
  - Many mustard ton containers can not be fully drained
  - What level of solid heel in ton containers can be processed in MPF in a “reasonable time” ?
  - Use wash-out process or incineration ?

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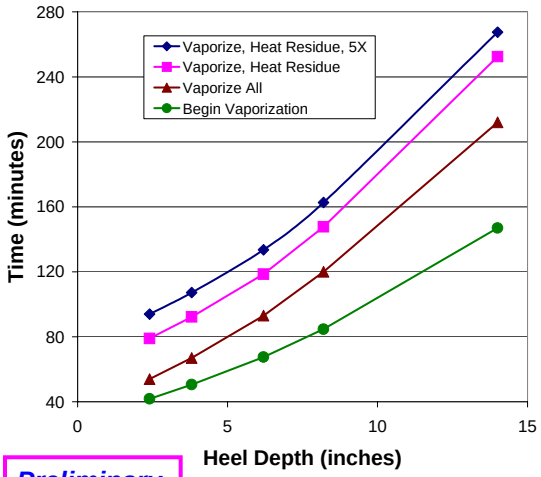
Feed Cycle (Process) Time
Partially Drained Ton Container With Solid Heel



Preliminary Results

- Peak Vaporization Rate
  - 2. 5" heel < 600 lb/hr
  - 14" heel < 1100 lb/hr
- If all processing in Zone 1 (no overlap) will have long furnace residence time
- *Opportunity to increase throughput* if overlap zone 1 & 2 processing

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CMS Burner
Recommendations From Previous Work

- ➔ Higher temperature alumina-based refractory
- ➔ Lower and/or consistent feed rates
- ➔ Controls improvements
- ➔ Burner modifications

Partial listing of issues raised in one or more of the following studies:

- MicroEnergy Systems, July, 2000
- CR&E, May, 2002
- WDC, May, 2004

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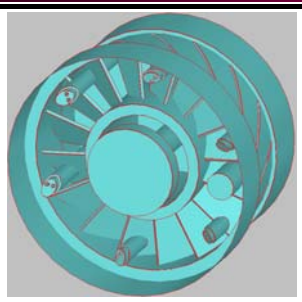
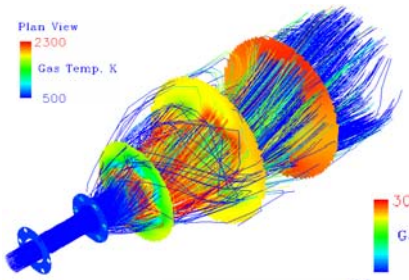
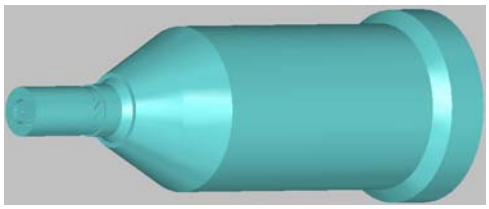
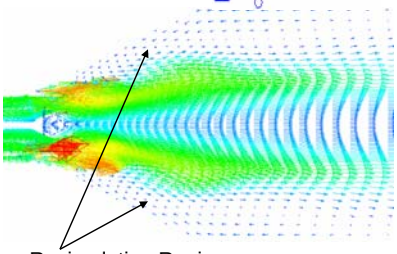
CMS Burner - Deposition Modeling









Recirculation Regions

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Value of Project to CMA

- Demonstrate reliability and performance of existing processes and equipment
- Assess
  - trouble shooting / problem solving
  - proposed design changes
  - process operation options & optimization
- Assist Site Operators & Support Contractors

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Path Forward

- Opportunities exist to apply modeling tools throughout the Chem Demil Program
- Baseline sites (TOCDF, ANCDF, UMCDF, PBCDF)
  - optimize processing
  - assistance with troubleshooting
- Non-baseline sites (where thermal treatment is required)
  - metal parts, dunnage, carbon

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