

# *Reaction Engineering International*

## Advanced Computer Simulations Of Military Incinerators

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**Reaction Engineering International**

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*23<sup>rd</sup> Army Sciences Conference, November 29, 2004, Orlando, FL USA*

Funding Provided Under DOD-Army SBIR Phase II/II+ Program  
Contract #DAAD19-01-C-0050  
Program Manager Dr. Robert Shaw (ARO)

## Outline

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

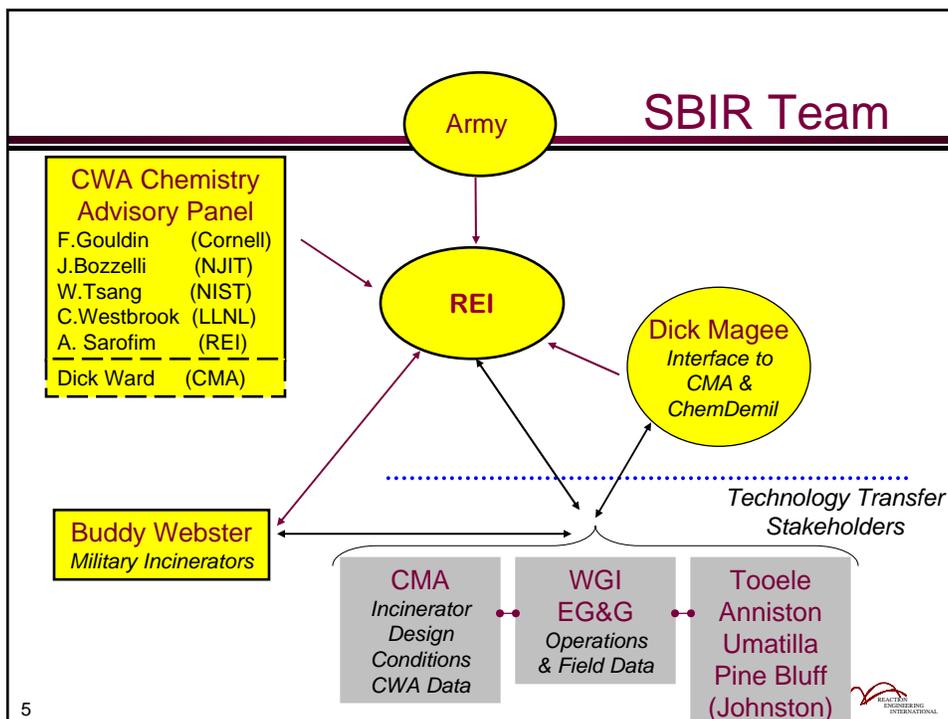
# Report Documentation Page

*Form Approved*  
*OMB No. 0704-0188*

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1. REPORT DATE <b>00 DEC 2004</b>	2. REPORT TYPE <b>N/A</b>	3. DATES COVERED <b>-</b>	
4. TITLE AND SUBTITLE <b>Advanced Computer Simulations Of Military Incinerators</b>		5a. CONTRACT NUMBER	
		5b. GRANT NUMBER	
		5c. PROGRAM ELEMENT NUMBER	
6. AUTHOR(S)		5d. PROJECT NUMBER	
		5e. TASK NUMBER	
		5f. WORK UNIT NUMBER	
7. PERFORMING ORGANIZATION NAME(S) AND ADDRESS(ES) <b>Reaction Engineering International</b>		8. PERFORMING ORGANIZATION REPORT NUMBER	
9. SPONSORING/MONITORING AGENCY NAME(S) AND ADDRESS(ES)		10. SPONSOR/MONITOR'S ACRONYM(S)	
		11. SPONSOR/MONITOR'S REPORT NUMBER(S)	
12. DISTRIBUTION/AVAILABILITY STATEMENT <b>Approved for public release, distribution unlimited</b>			
13. SUPPLEMENTARY NOTES <b>See also ADM001736, Proceedings for the Army Science Conference (24th) Held on 29 November - 2 December 2005 in Orlando, Florida. , The original document contains color images.</b>			
14. ABSTRACT			
15. SUBJECT TERMS			
16. SECURITY CLASSIFICATION OF:			17. LIMITATION OF ABSTRACT
a. REPORT <b>unclassified</b>	b. ABSTRACT <b>unclassified</b>	c. THIS PAGE <b>unclassified</b>	<b>UU</b>
			18. NUMBER OF PAGES <b>11</b>
			19a. NAME OF RESPONSIBLE PERSON





## 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

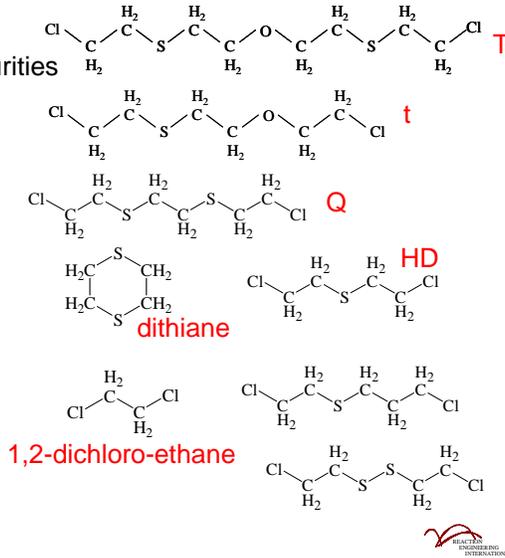
$$\begin{array}{c}
 | \quad | \quad | \\
 \text{Cl-C-C-S-C-C-Cl} \\
 | \quad | \quad |
 \end{array}
 \longrightarrow
 \begin{array}{c}
 | \quad | \quad | \\
 \text{Cl-C-C-S-C=C} \\
 | \quad | \quad |
 \end{array}
 + \text{HCl}$$

$k = 1.85 \times 10^{13} e^{(-58.75/RT)} \text{ sec}^{-1}$

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## Thickeners & Impurities

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

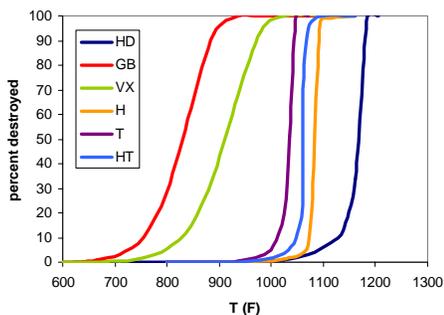


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## Calculated Incinerability Rankings

### Approximation to UDRI Incinerability Ranking

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

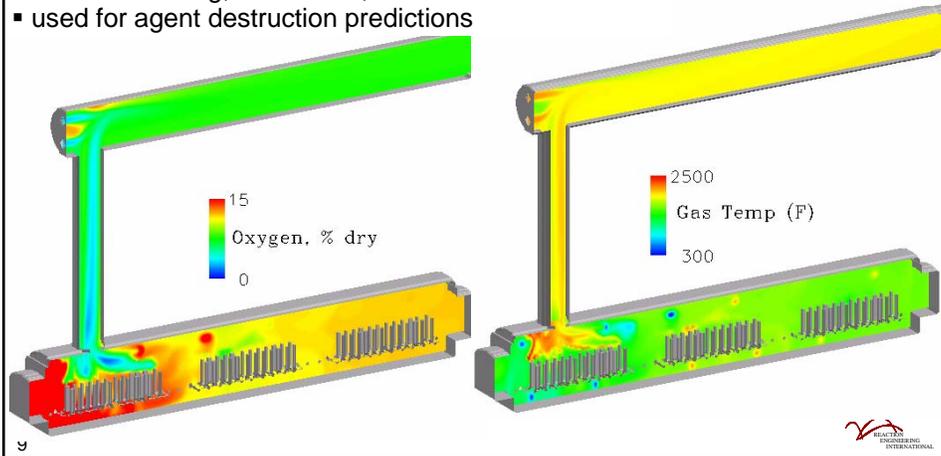


Compound	T99(2)	Class
Benzene	1150 C	1
Toluene	895 C	2
Vinyl Chloride	770 C	3
Trichloroethane	635 C	4
<b>HD</b>	<b>628 C</b>	<b>4</b>
<b>H</b>	<b>603 C</b>	<b>4</b>
<b>HT</b>	<b>578 C</b>	<b>5</b>
<b>T</b>	<b>562 C</b>	<b>5</b>
Chloroform	545 C	5
<b>VX</b>	<b>541 C</b>	<b>5</b>
Hexachloropropene	505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

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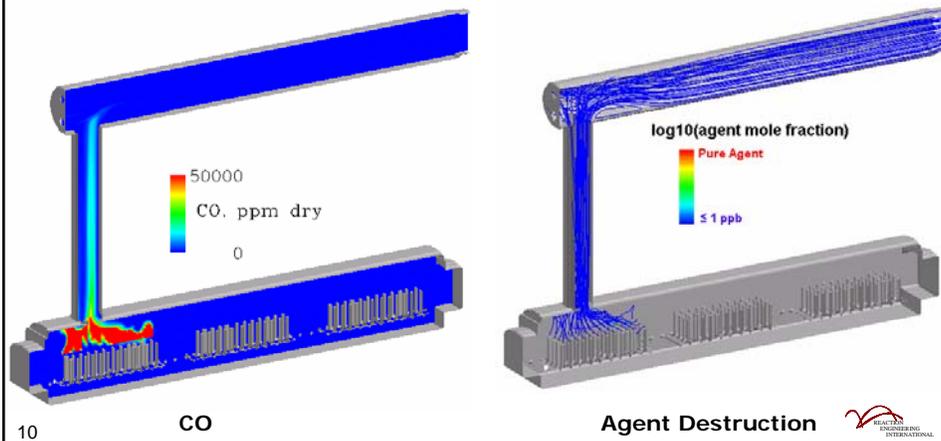
## CFD Combustion

- 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



## CFD Model Results & Agent Destruction

CFD Results provide details about agent destruction along streamlines

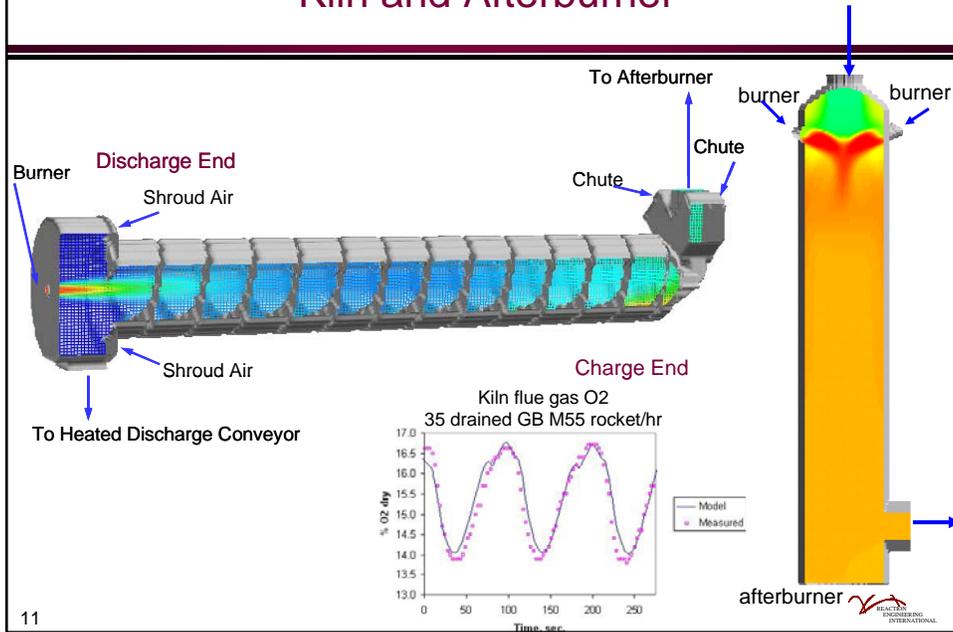


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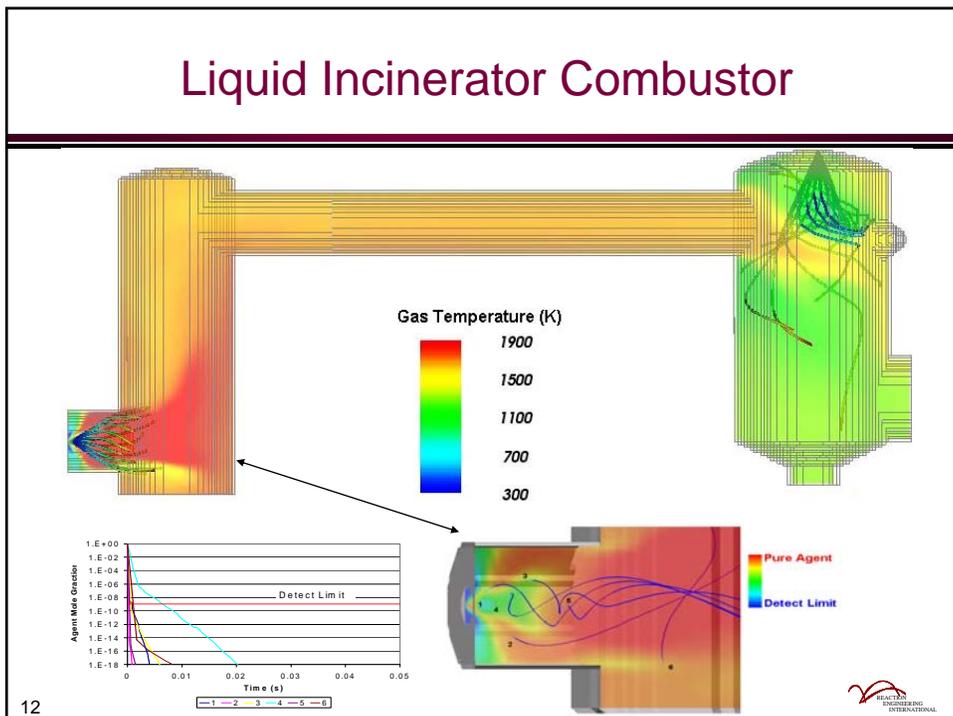
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Agent Destruction

## Deactivation Furnace System Kiln and Afterburner



## Liquid Incinerator Combustor



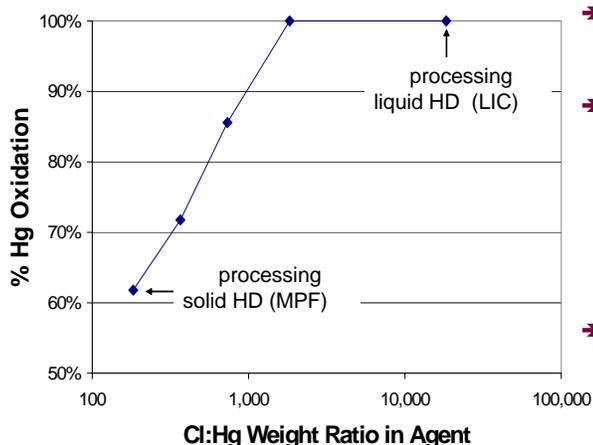
## Impact of SBIR Project on Chem Demil Program

- 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<sup>0</sup> 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<sup>0</sup> is restricted to brine wastes
  - ◆ Low Hg removal efficiency
    - carbon in the PFS is also contaminated by Hg<sup>0</sup>.

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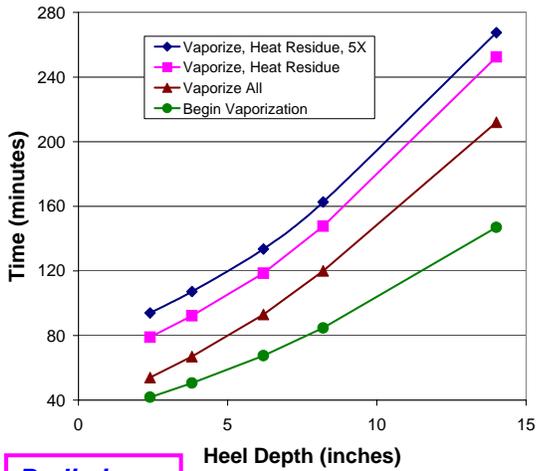
## Processing Partially Drained TCs in MPF

- 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



- ❖ 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

**Preliminary Results**

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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

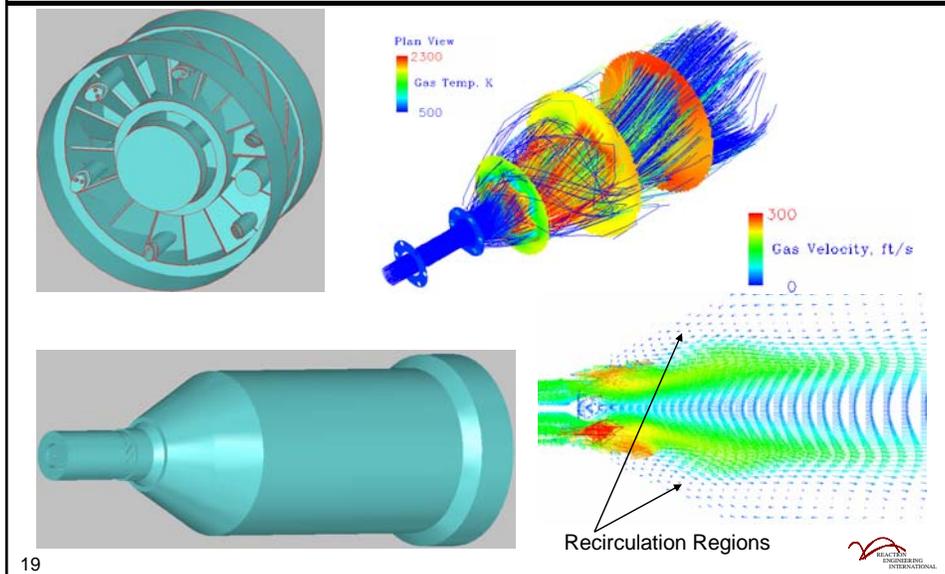
Partial listing of issues raised in one or more of the following studies:

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

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## CMS Burner - Deposition Modeling



## 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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## Acknowledgements

- The authors would like to acknowledge the contributions of
  - ◆ Dr. Charlie Westbrook (LLNL)
  - ◆ Dr. Wing Tsang (NIST)
  - ◆ Alfred G. Webster (CR&E)
  - ◆ Dave Hoecke (Enercon Systems)
  - ◆ Kevin Gildner, Dr. Dick Ward, Cheryl Maggio (CMA)
  - ◆ Washington Demilitarization Company
  - ◆ Washington Group
  - ◆ International and EG&G, Inc.

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