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Vaporization Model for Solid Agent Contaminated Charcoal

Yunhan Zheng, Ph.D.
Research Engineer
Continental Research and Engineering

About Continental Research and Engineering, LLC

Continental Research and Engineering (CR&E) is well known in the demilitarization industry for providing, design/research engineering, laboratory and field testing, process numerical modeling, project management, new technology research and testing, and providing solution to processing problems.

Technology Requirements

Demilitarization Technologies

- Reverse disassembly of munitions
- Thermal treatment of liquid agents
- Thermal treatment of explosive components
- Thermally decontaminate metal parts at 1000^{o}F for 15 minutes.
- Technologies required for decontamination / destruction of secondary and closure wastes

Vaporization Model for Solid Agent Contaminated Charcoal

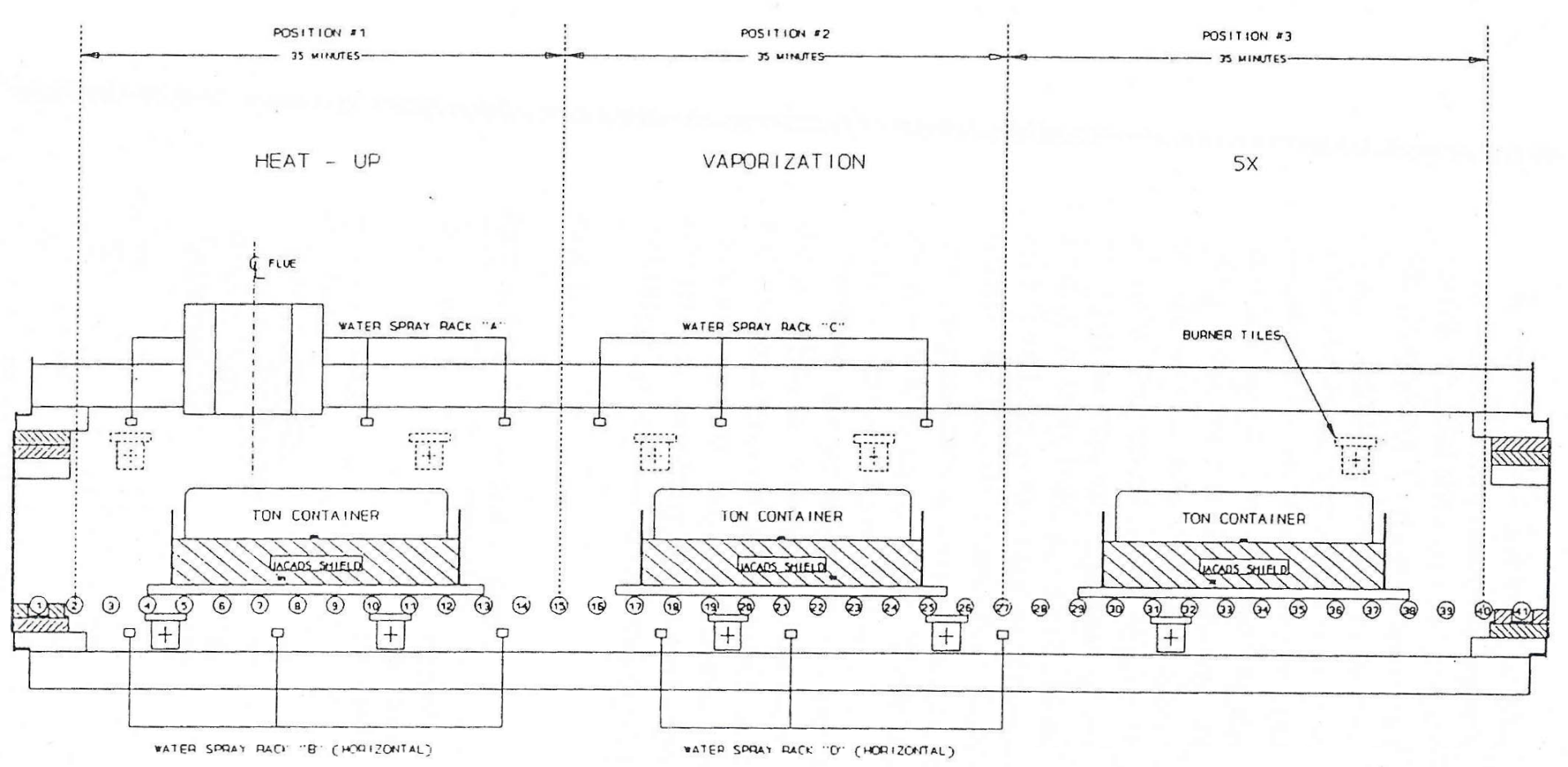
Agent Contaminated Charcoal

Activated charcoal used in the following process is considered secondary waste:

- As a filter for chemical agent
- Agent collection system filters
- Heating, ventilation, and air conditioning (HVAC) filters
- Pollution abatement system filtration

Vaporization Model for Solid Agent Contaminated Charcoal

Problem Description



Vaporization Model for Solid Agent Contaminated Charcoal

Test one – Verify normal secondary waste process times used to 5X the charcoal. 4/28/2008

Test two – Identify extended processing time required to burn the charcoal to ash. 4/29/2008

Vaporization Model for Solid Agent Contaminated Charcoal

Objective

The contaminated charcoal heats up to 1000 ^{0}F very quickly while it continues to burn for an extended period of time. This study is to determine the heating process of different chemical agent contaminated charcoal to achieve 5X decontamination.

- Developing general vaporization model for heating process with melting/vaporization control code using dynamic moving mesh
- Calibrating the vaporization model with test data and CR&E Peak Vaporization Rate (PVR) model
- Using calibrated CFD model to predict the heating process of different chemical agent contaminated charcoal

Vaporization Model

Fluent CFD coupled with melting/vaporization control code using dynamic moving mesh

- k-ε turbulence model
- Discrete Ordinates (DO) radiation model
- Melting/vaporization control UDF
- Dynamic moving mesh

Melting and Vaporization Control UDF

Two scalars are used in the vaporization control code

First scalar - to measure the solid agent mass fraction

- Solid begins to melt when temperature of a computational cell reaches melting point
- Calculating the cell heat flux and adjust the solid mass fraction according to melting/vaporization equation
- Adjust the energy source term and momentum source term

Second scalar - to measure the liquid mass agent fraction

$$\frac{d(\rho \forall_{cell} \in_{cell})}{dt} = -\frac{Q_{cell}}{L}$$

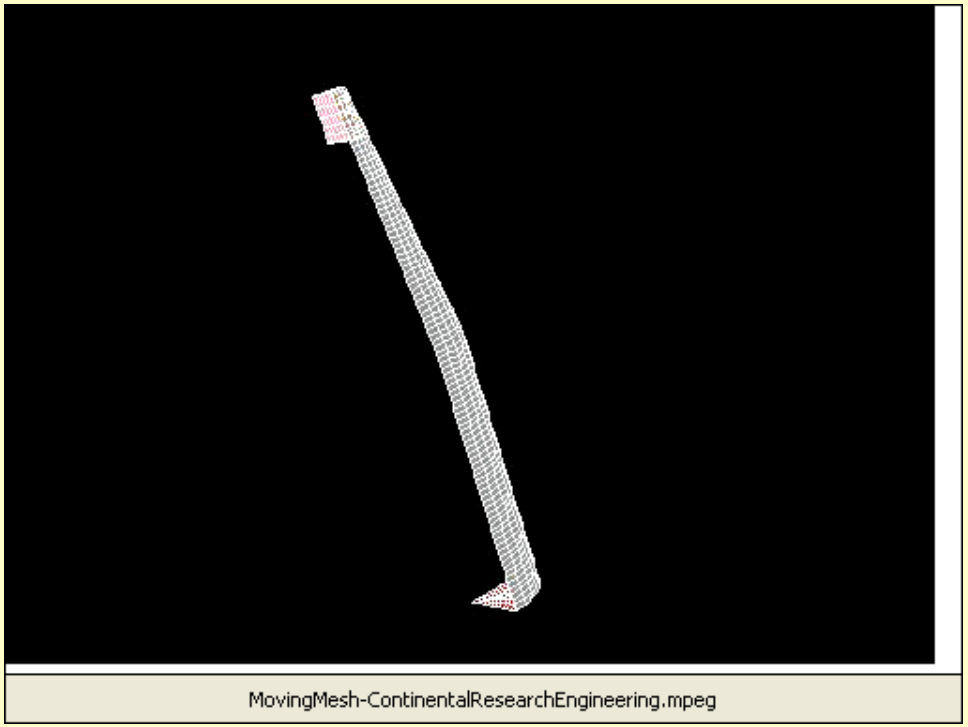
Vaporization Model for Solid Agent Contaminated Charcoal

Dynamic Moving Mesh

- DEFINE_EXECUTE_AT_END and DEFINE_GRID_MOTION were used to control the behavior of the dynamic moving mesh during the chemical agent vaporization
- The dynamic moving mesh was based on the total heat flux of cells, current time step, latent heat of chemical agent, density of chemical agent, dimension of munitions
- Next slide shows an example of dynamic moving mesh animation of a quarter munitions

Vaporization Model for Solid Agent Contaminated Charcoal

Dynamic Moving Mesh



Double click to see moving mesh animation

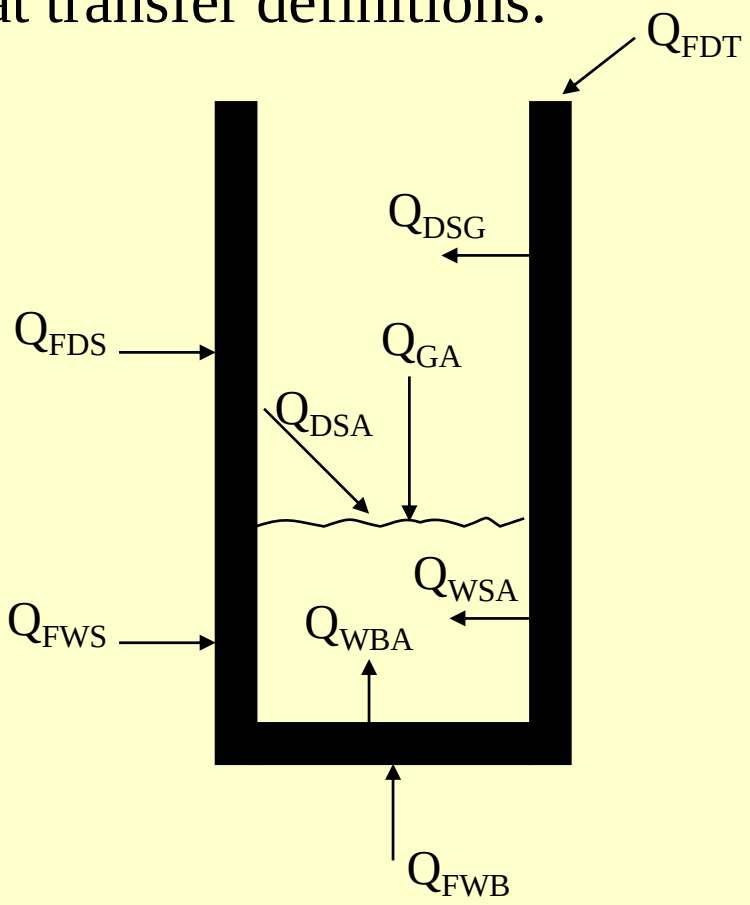
CR&E PVR Model

- CR&E PVR model for chemical agents GB, VX, HD and their simulants from drained projectiles on a full standard tray was developed in 1988
- The PVR program was updated and calibrated to test data in 1994.
- The PVR model is based on the munitions family groups and radiation view factor. So the model only can be used for specific munitions family

Vaporization Model for Solid Agent Contaminated Charcoal

CR&E PVR Model

Heat transfer definitions:



Q_{FDT} – Furnace to Dry Top

Q_{FDS} – Furnace to Dry Sides

Q_{FWS} – Furnace to Wet Sides

Q_{FWB} – Furnace to Wet Bottom

Q_{DSA} – Dry Side to Agent

Q_{DSG} – Dry Side to Gas

Q_{GA} – Gas to Agent

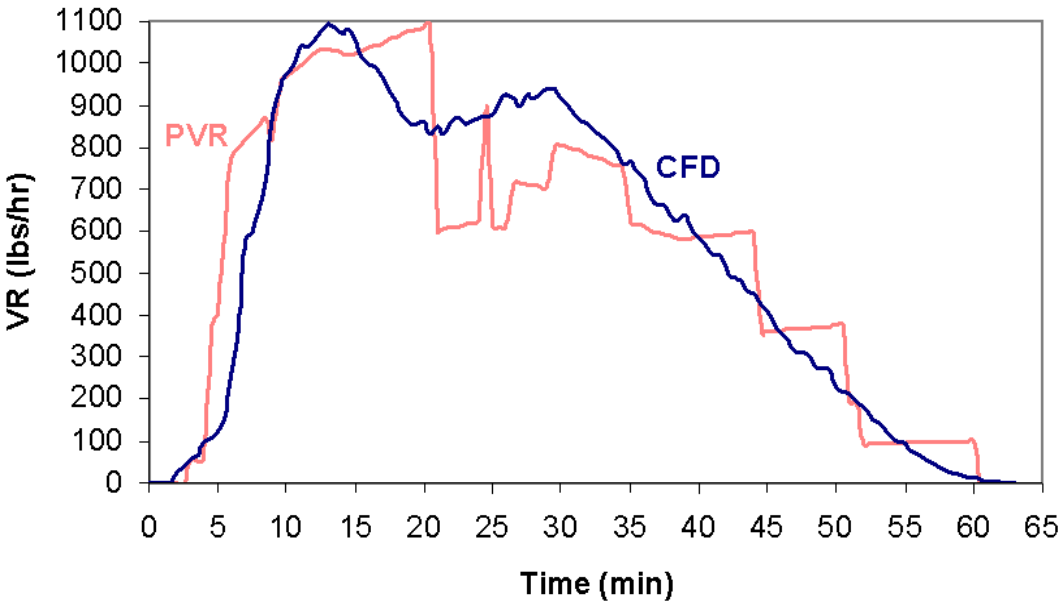
Q_{WBA} – Wet Bottom to Agent

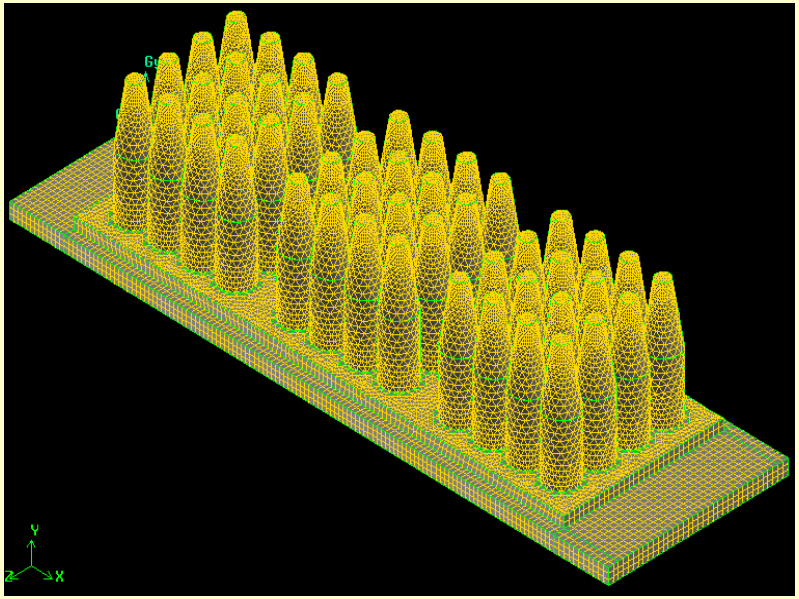
Q_{WSA} – Wet side to Agent

Vaporization Model for Solid Agent Contaminated Charcoal

Model Calibration

(1) Munition vaporization model - the model has been verified accurate based on empirical data gathered during testing at the demilitarization facilities.





4.2 inch 100% Liquid HD Vaporization Rate Results

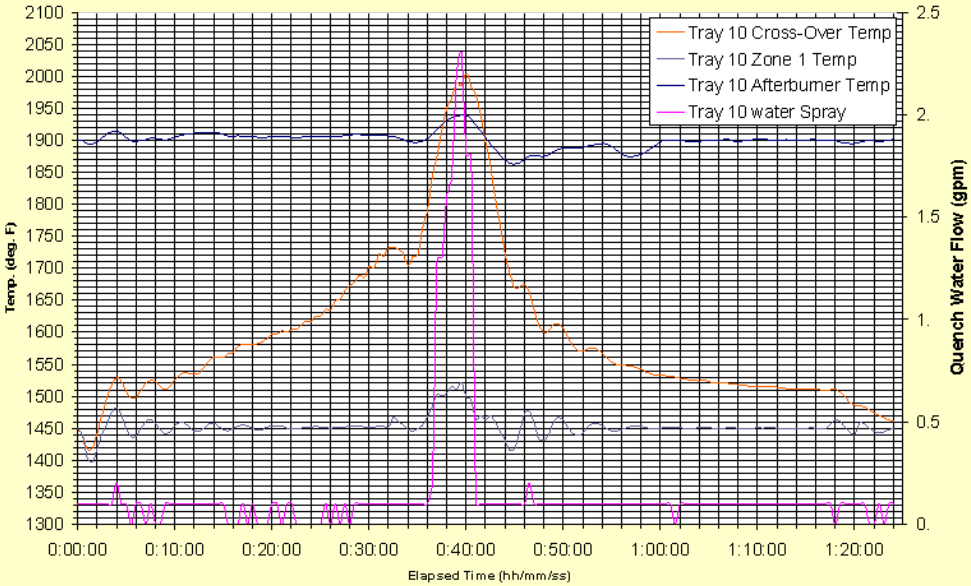
Vaporization Model for Solid Agent Contaminated Charcoal

Model Calibration

(2) Ton Container vaporization model - 45 lbm VX ton container

Tray No.	Vap. Start Time (min)	Peak Vaporization time (min)
2	22:30	37:30
3	21:00	40:30
4	19:00	40:00
5	19:30	37:30
6	18:30	41:00
7	24:00	34:30
8	19:00	40:00
9	22:30	43:30
10	20:00	39:30
11	23:30	41:00
Average	21:00	39.30

Processing Data of March 13, 2004



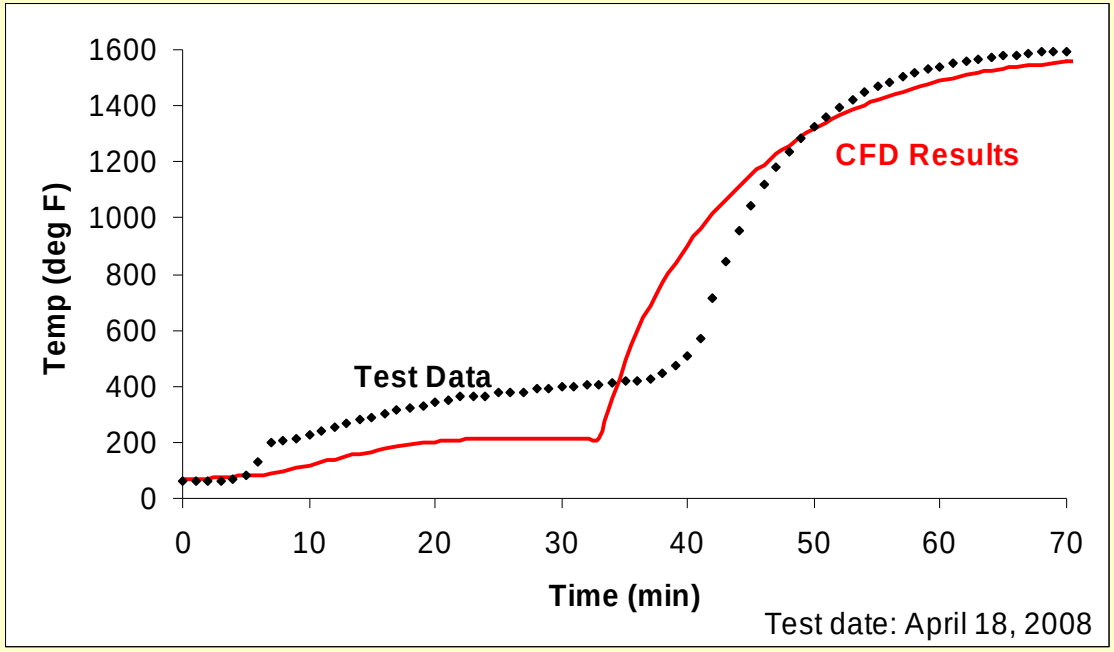
	Vap. Start Time (min)	PVR time (min)	Vap. End Time (min)
TOCDF data	21:00	39:30	
PVR model	20:00	32:00	43:00
CFD model	23:00	35:00	41:00

Vaporization Model for Solid Agent Contaminated Charcoal

Model Calibration

(3) Wet Charcoal Heating Process Model -

- 2inx6inx6in charcoal test tray
- 23 oz charcoal
- 18 oz total water adsorbed by the charcoal
- Kiln temperature 1600 ^{0}F



Vaporization Model for Solid Agent Contaminated Charcoal

Model Application

The vaporization model with dynamic mesh has been successfully used in the processing wastes (liquid, solid, or liquid-solid mixture) through the Metal Part Furnace including the following wastes:

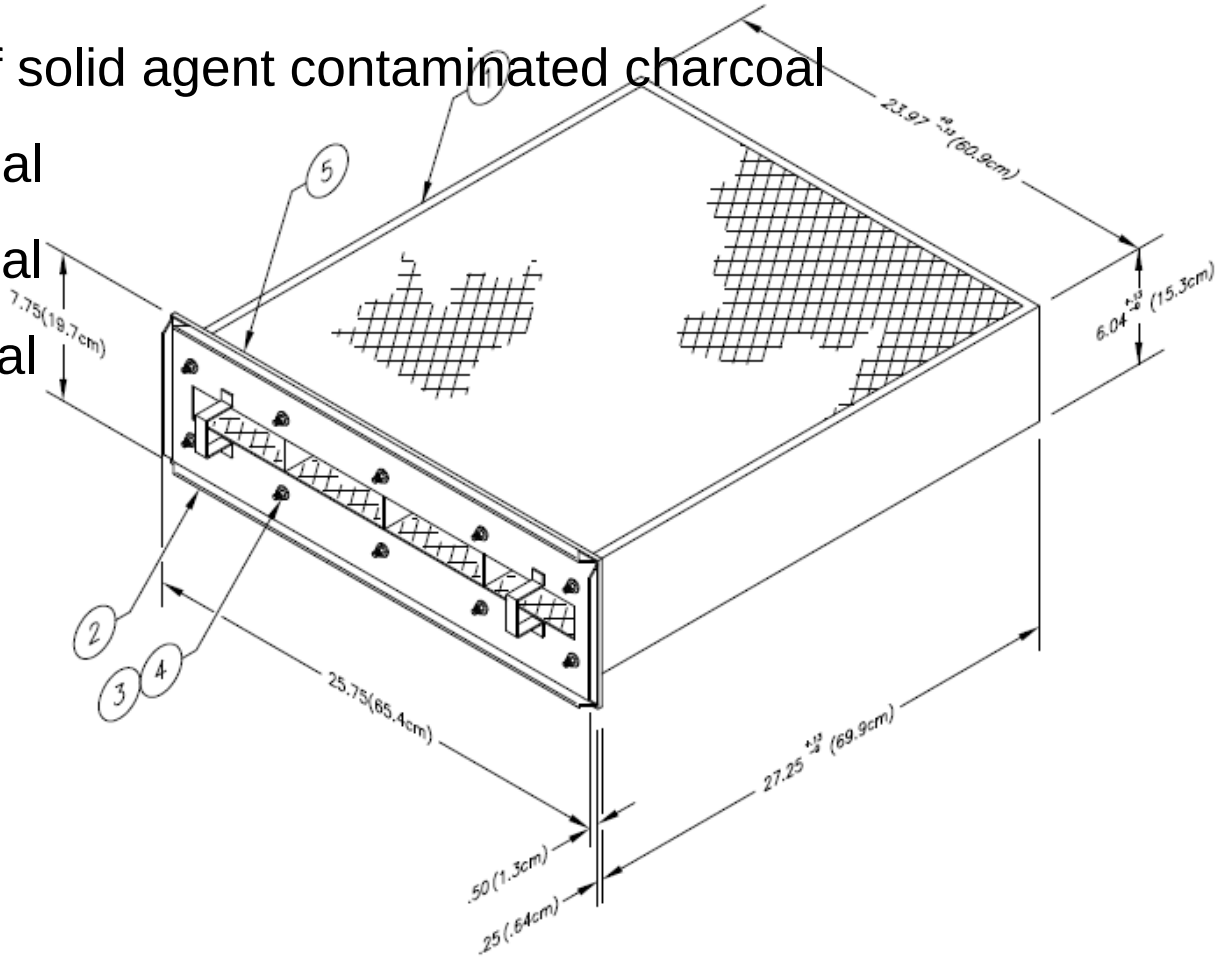
- Chemical warfare agents (HD, GB, VX)
- DPE suits
- Sludge
- VX hydrolysate
- Scrabbled concrete
- Secondary and closure waste
- Contaminated charcoal

Vaporization Model for Solid Agent Contaminated Charcoal

Solid Agent Contaminated Charcoal

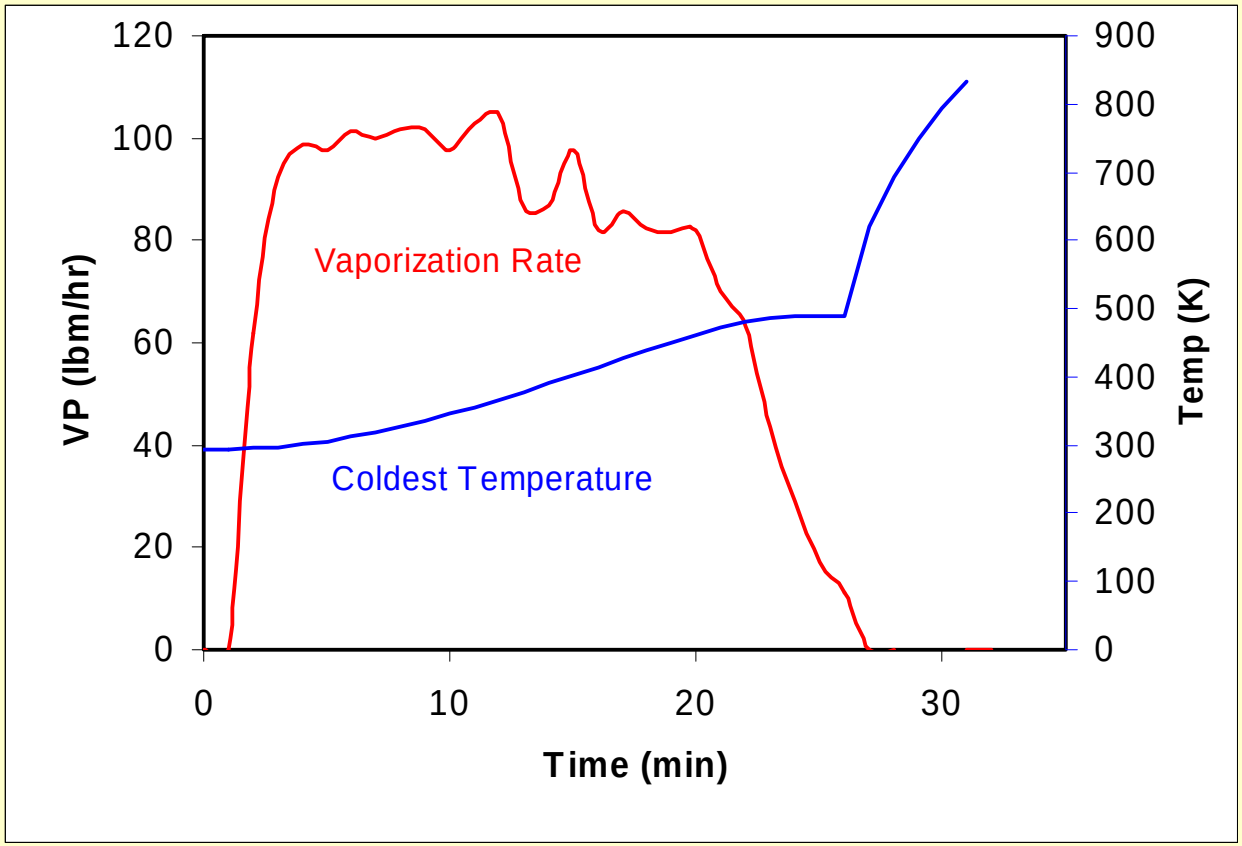
Vaporization model results of solid agent contaminated charcoal

- HD contaminated charcoal
- GB contaminated charcoal
- VX contaminated charcoal



Vaporization Model for Solid Agent Contaminated Charcoal

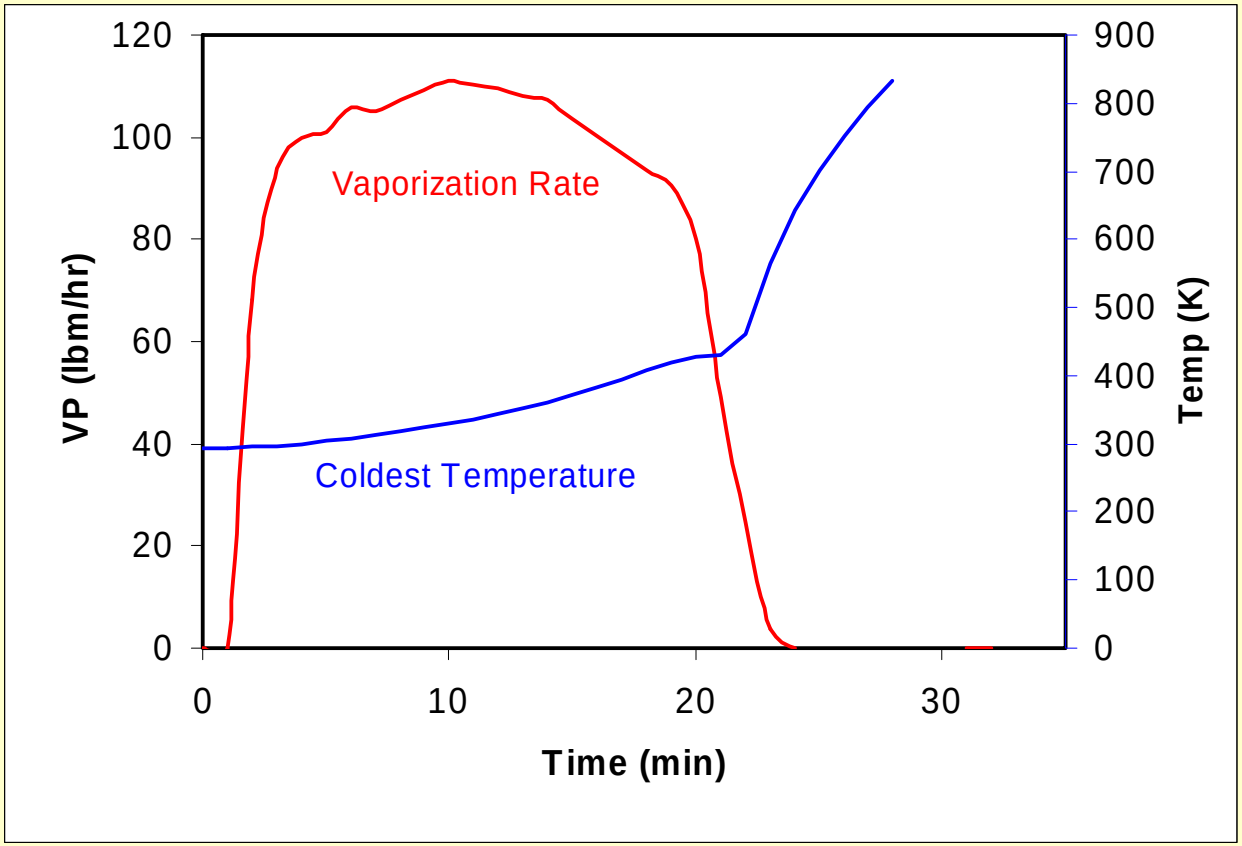
Vaporization Model Results



Vaporization Rate and Coldest Temperature Curve of 33 lb Agent HD with 50 lb Charcoal

Vaporization Model for Solid Agent Contaminated Charcoal

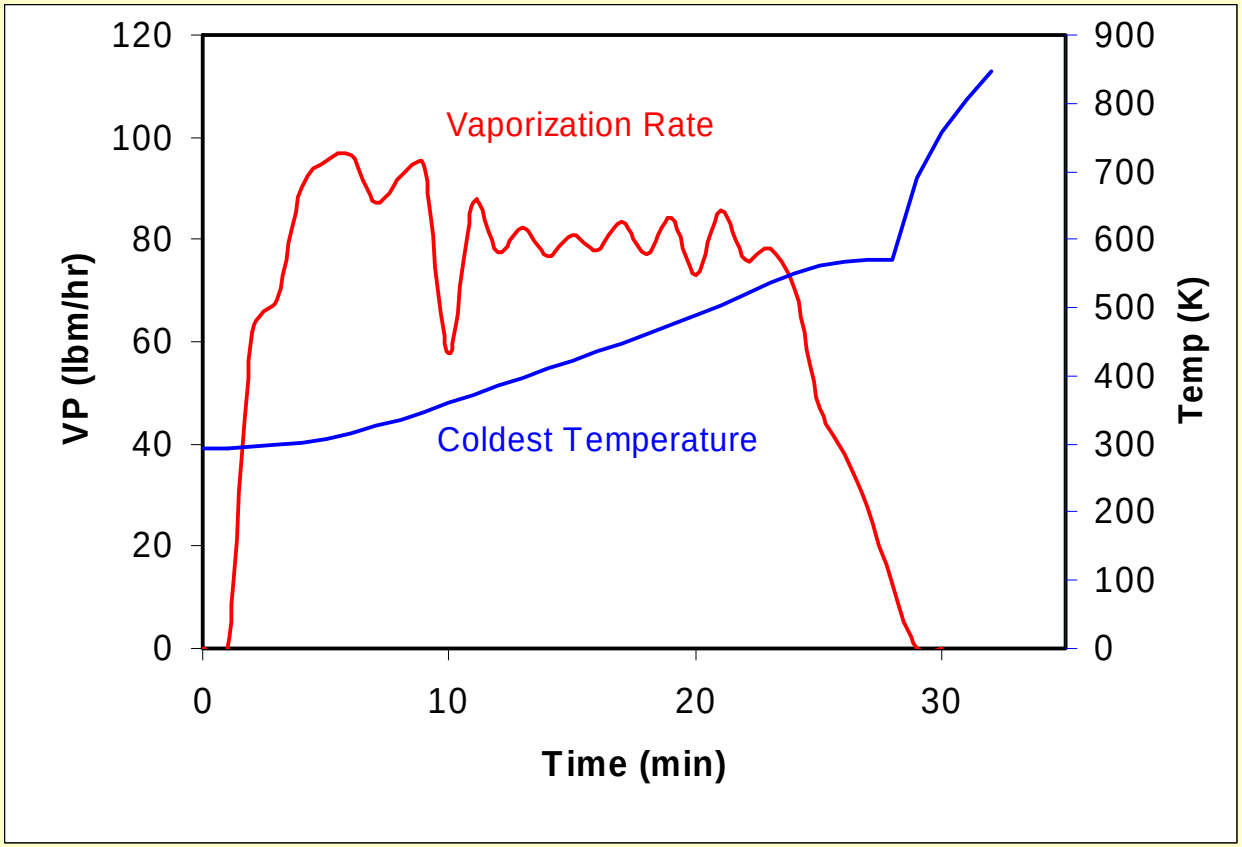
Vaporization Model Results



Vaporization Rate and Coldest Temperature Curve of 33 lb Agent GB with 50 lb Charcoal

Vaporization Model for Solid Agent Contaminated Charcoal

Vaporization Model Results



Vaporization Rate and Coldest Temperature Curve of 33 lb Agent VX with 50 lb Charcoal

Conclusion

1. CFD model coupled with melting/vaporization code using dynamic moving mesh has been developed.
2. The vaporization model was calibrated by test data and CR&E PVR model. The predicted vaporization model results were in good agreement with PVR model results and test data.
3. This calibrated melting/vaporization dynamic model can simulate heating processing of any liquid, solid, and liquid-solid mixture. The model results have provided a guide for disposal of chemical wastes.

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Contaminated Charcoal Solution

Chemical warfare agent contaminated charcoal decontamination / destruction has been problematic

- Charcoal micronization / incineration utilized in 2000. High cost, high maintenance, problematic operation.
- Complete incineration in filter casings requires very long residence times.
- Test data and CFD model show that heating the charcoal to 1000 ^{0}F for 15 minutes utilizing existing thermal treatment system is a cost effective, simple solution for a complex problem.

Acknowledgement

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Thank You