FLUENT 2005 CFD Summit

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A Study of Chemical Agent Vaporization Modeling for Liquid Agent Mixed with Solid

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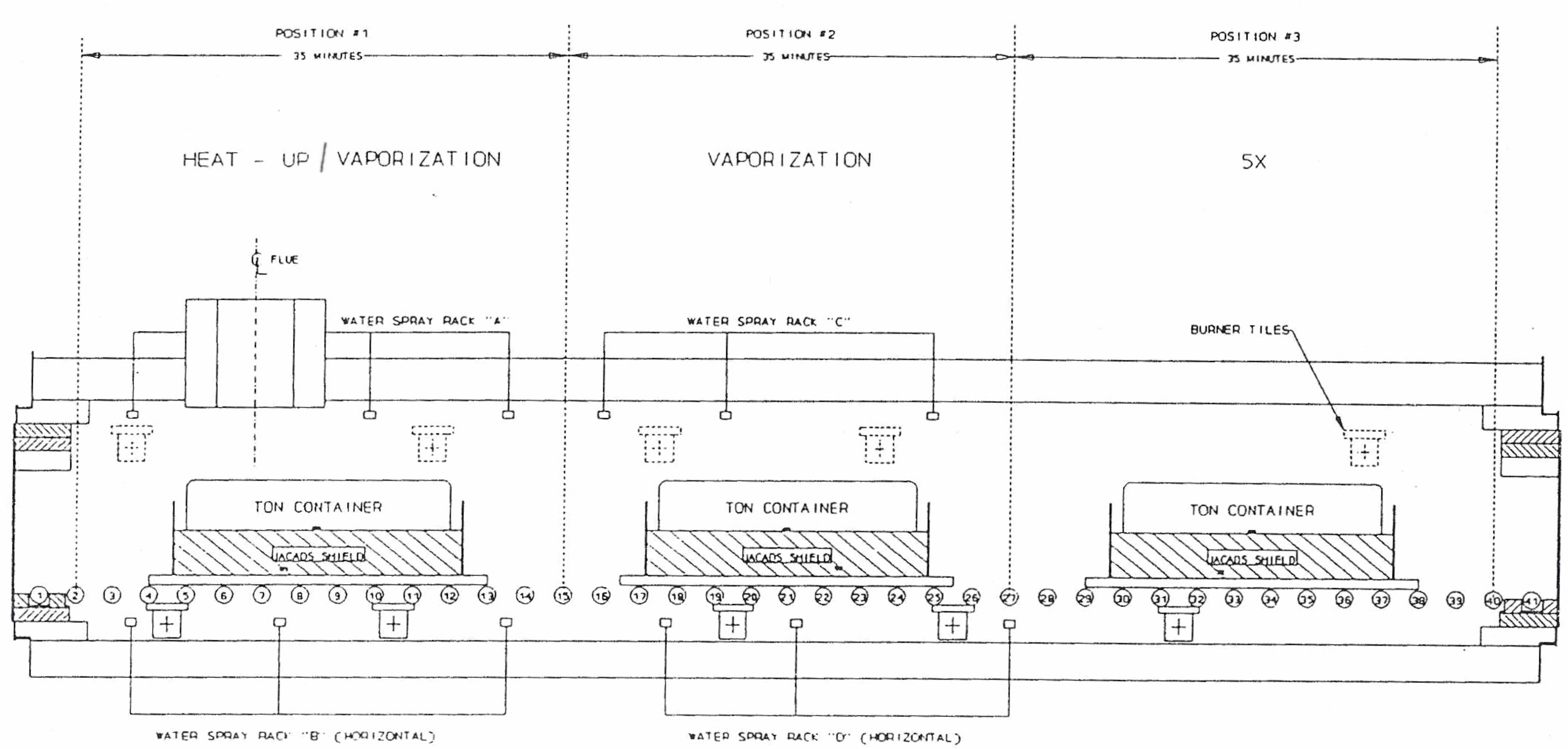
About Continental Research and Engineering, LLC

CR&E is the leading provider of engineering, research and operational support to a diverse group of clients with demanding expectations. Specific expertise encompasses Chemical, Mechanical and Electrical Engineering, Facilities Operations, Safety Analysis, Computer Modeling, Chemistry, Process Control and Project Management.

Outline

- Problem description
- Objective
- CR&E PVR model
- CFD model and melting/vaporization control code
- CFD model calibration
- CFD model results for liquid chemical agent mixed with solid

Problem Description



Metal parts furnace cross section

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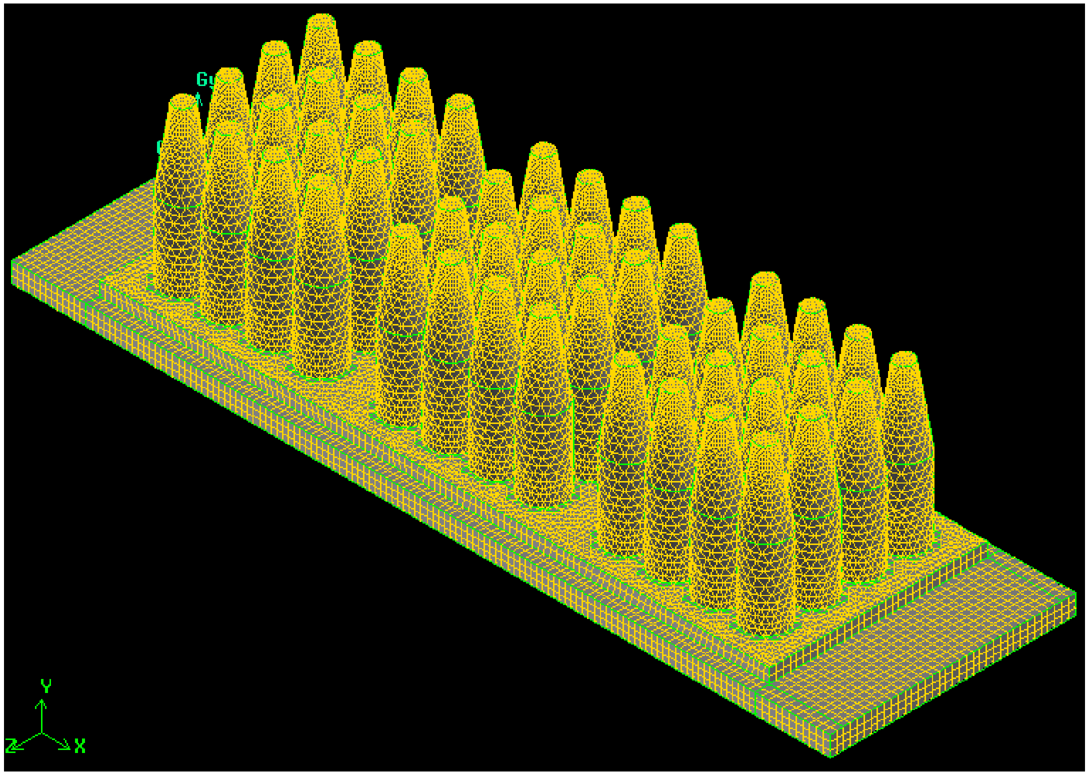
Problem Description

Different type of munitions: 4.2 inch mortar, 105mm projectile, 155 mm projectile on munitions tray



Objective

To determine vaporization rate profiles of liquid chemical agent mixed with solid for different kind of munitions (4.2 inch mortars, 105 mm projectiles, and 155 mm projectiles) in the full tray.

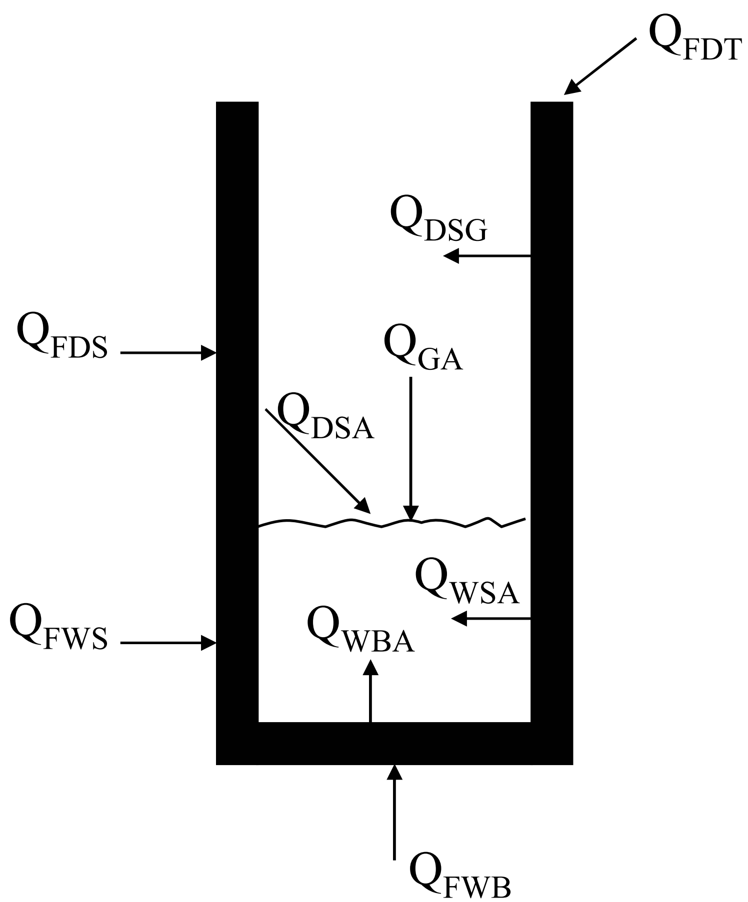
- Developing CFD model for heating process with vaporization code
- Calibrating CFD model with CR&E PVR model
- Using calibrated CFD model to predict the vaporization rate of liquid chemical agent mixed with solid

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.
- PVR model is based on the munitions family groups and radiation view factor. So PVR model only can be used for specific munitions family.

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

CR&E PVR Model

4.2 Inch Mortars on Munitions Tray
96/tray in 6 x 16 array
Identified by Vaporization Family Group

2	2	3	2	2	3	4	3	2	4	3	2	2	3	2	2
2	4	4	4	4	5	6	5	5	6	5	5	4	4	4	2
3	4	6	6	7	7	8	8	8	8	7	7	6	6	4	3
3	4	6	6	7	7	8	8	8	8	7	6	6	6	4	3
2	4	4	4	5	6	6	5	5	6	5	4	4	4	4	2
2	2	3	2	2	3	4	2	3	4	3	2	2	3	2	1

Tray Feed →

Family no.	Munitions/Family
1	1
2	21
3	14
4	22
5	9
6	14
7	7
8	8

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4.2 Inch Mortar Munitions Tray Layout
By Vaporization Family

SIZE	DWG NO.	REV
A	A-03013-2-0	0

SCALE	DATE	SHEET
None	Nov. 17, 2003	1 OF 1

CR&E PVR Model

105mm Projectiles on Munitions Tray
96/tray in 6 x 16 array
Identified by Vaporization Family Group

1	3	4	2	2	3	4	2	2	4	3	2	2	3	1	1
2	4	4	5	5	5	5	5	5	5	5	5	4	4	4	2
3	4	6	6	6	6	6	6	6	6	6	6	6	5	4	3
3	4	6	6	6	6	6	6	6	6	6	6	6	6	4	3
2	4	4	5	5	5	5	5	5	5	5	5	5	4	4	2
1	3	3	2	2	3	4	2	2	4	3	2	2	3	1	1

Tray Feed →

Family no.	Munitions/Family
1	6
2	16
3	13
4	18
5	20
6	23

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105mm Projectile Tray Layout
By Vaporization Family

SIZE	DWG NO.	REV
A	A-03013-3-0	0

SCALE	DATE	SHEET
None	Nov. 18, 2003	1 OF 1

CR&E PVR Model

155mm Projectiles on Munitions Tray
48/tray in 4 x 12 array
Identified by Vaporization Family Group

2	2	3	3	3	5	5	3	3	4	2	1
2	6	9	6	6	9	10	6	6	8	6	2
2	6	8	6	6	10	9	6	6	7	5	2
2	2	3	3	3	5	4	3	3	2	2	1

Tray Feed

Family no.	Munitions/Family
1	2
2	11
3	10
4	2
5	4
6	11
7	1
8	2
9	3
10	2

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155mm Munitions Tray Layout
By Vaporization Family

SIZE	DWG NO.	REV
A	A-03013-1-0	0

SCALE	DATE	SHEET
None	Nov. 17, 2003	1 OF 1

CFD Model

Fluent CFD coupled with vaporization control code

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

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 melting 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

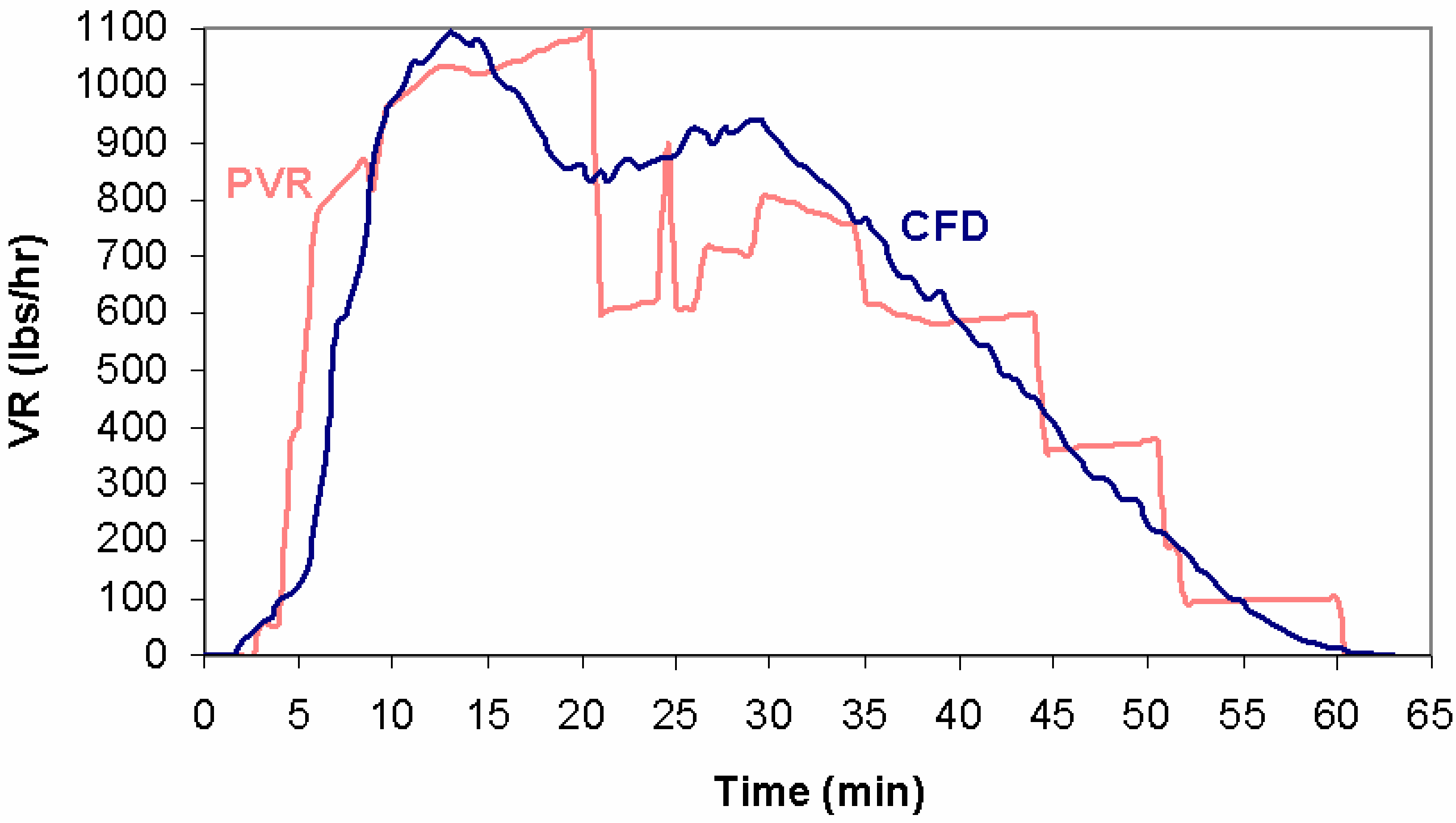
$$\frac{d(\rho\forall_{cell} \in_{cell})}{dt} = -\frac{Q_{cell}}{L}$$

CFD Model Calibration

Comparing CFD model results with PVR model results of liquid chemical agent.

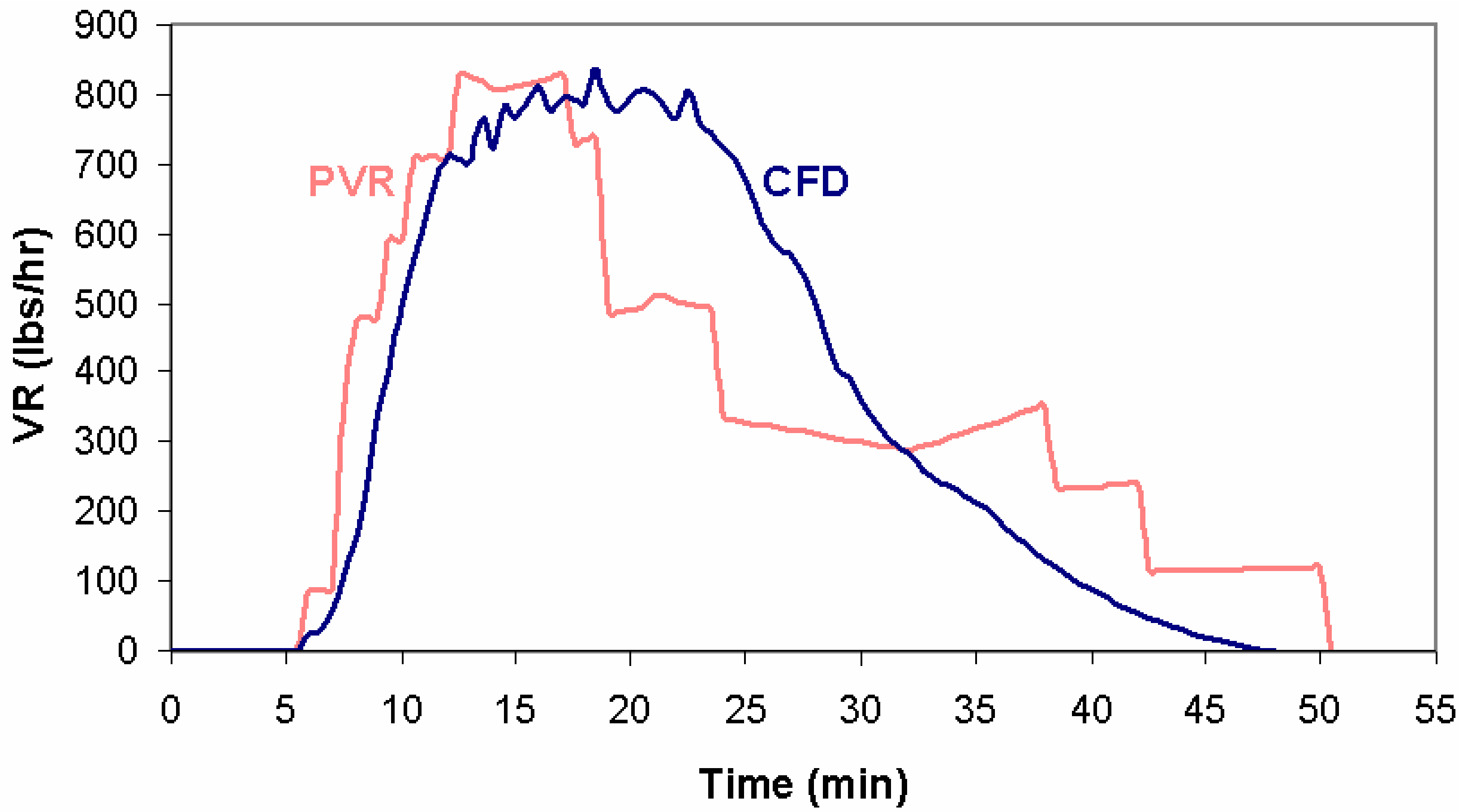
- 4.2 inch mortars (96 munitions/tray)
- 105 mm projects (96 munitions/tray)
- 155 mm projects (48 munitions/tray)

CFD Model Calibration



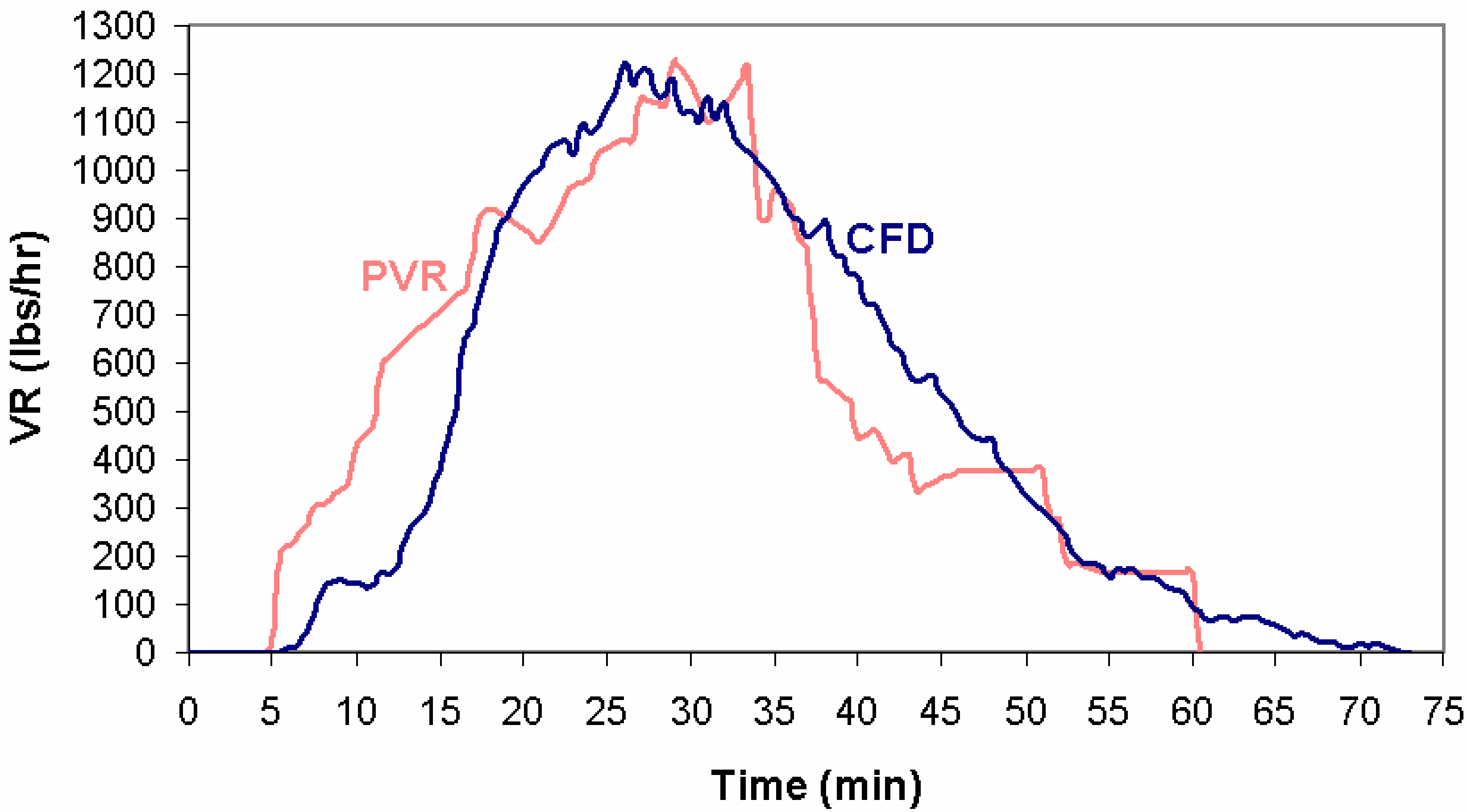
4.2 inch 100% Liquid HD Vaporization Rate Results

CFD Model Calibration



105 mm 100% Liquid HD Vaporization Rate Results

CFD Model Calibration



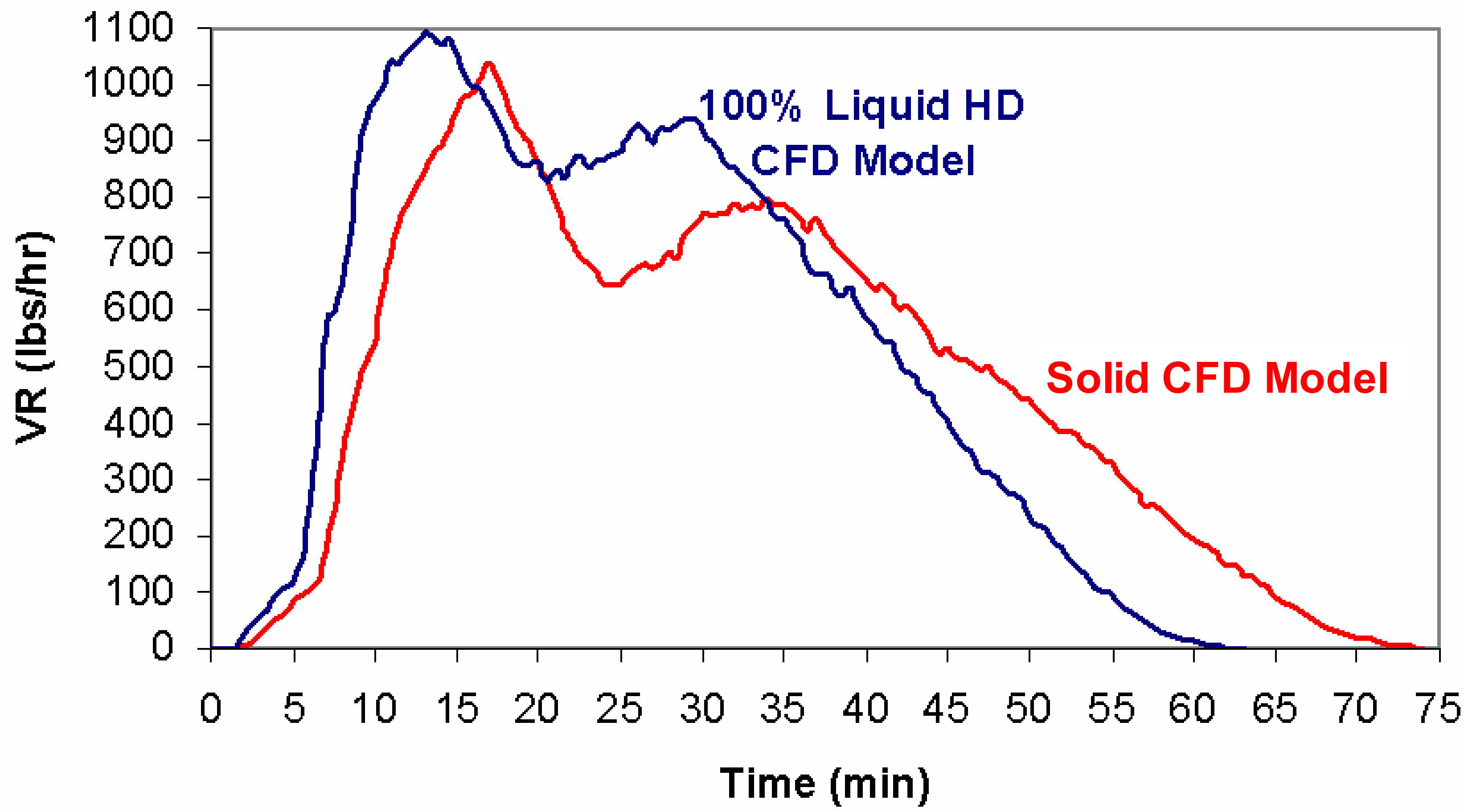
155 mm 100% Liquid HD Vaporization Rate Results

Liquid Chemical Agent Mixed with Solid

CFD model results of liquid chemical agent mixed with solid

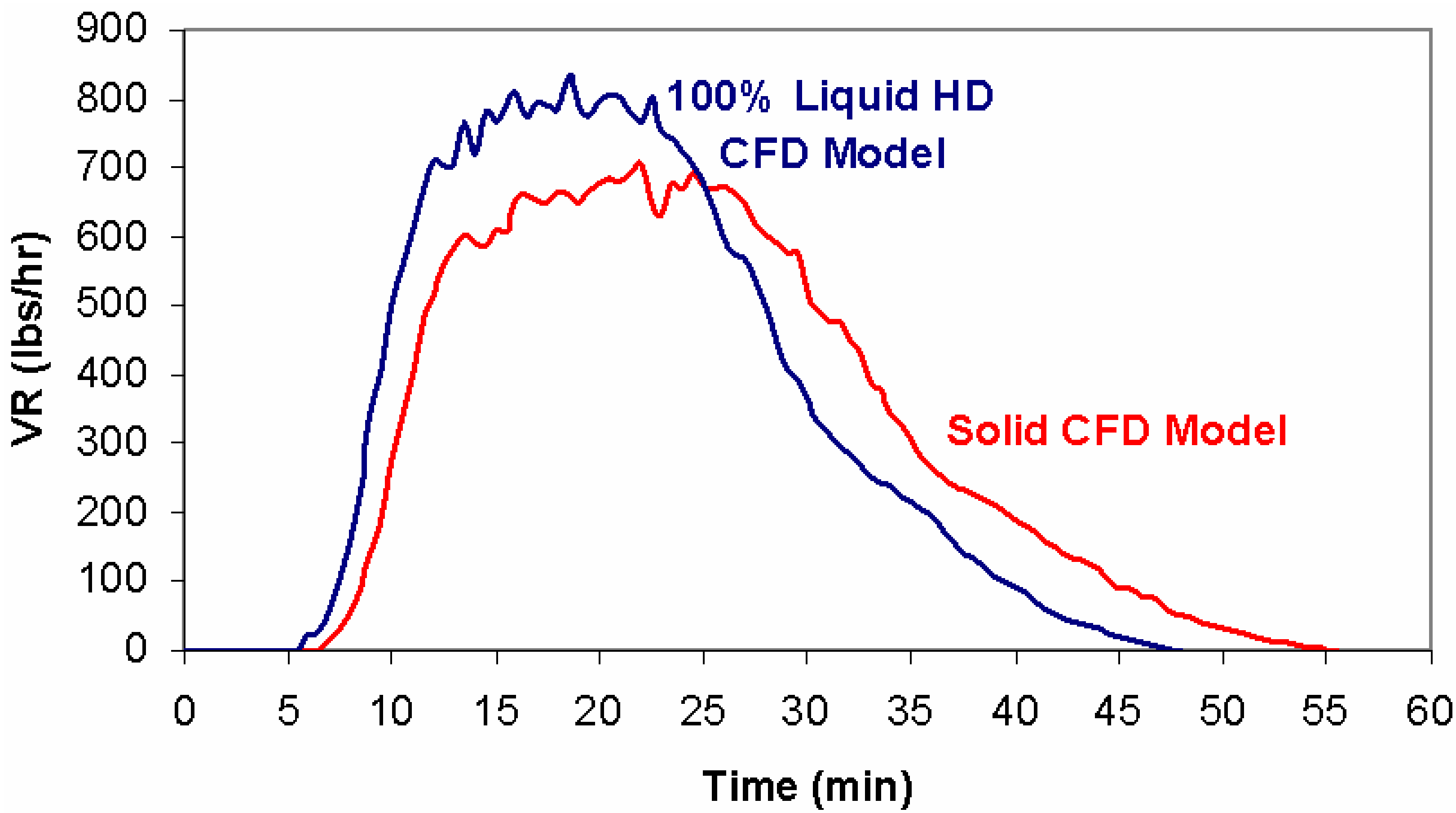
- 4.2 inch mortars (96 munitions/tray)
- 105 mm projects (96 munitions/tray)
- 155 mm projects (48 munitions/tray)

CFD Model Results



4.2 inch Solid HD Vaporization Rate Results

CFD Model Results



105 mm Solid HD Vaporization Rate Results

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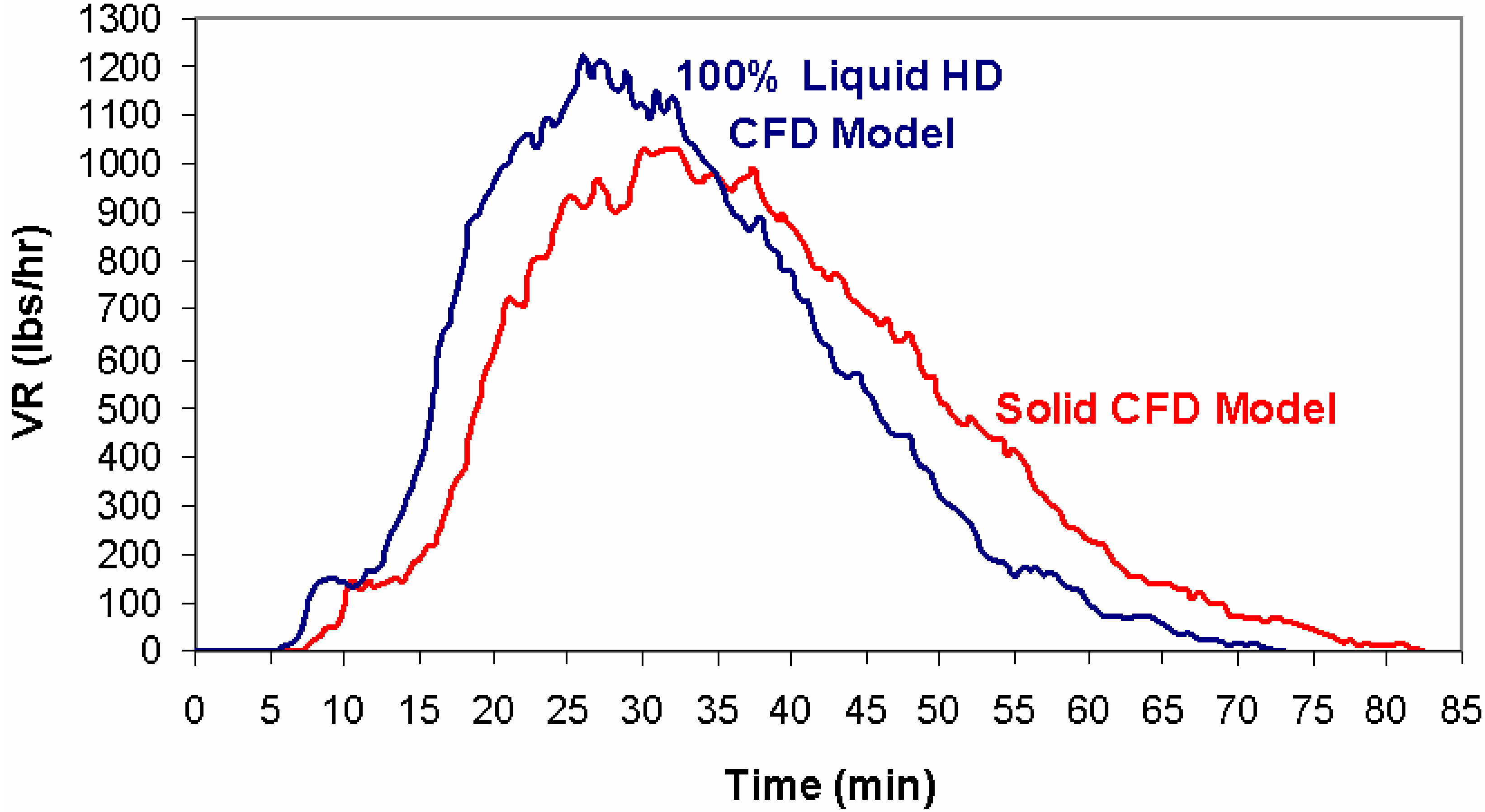
CFD Model Results



155 mm Solid HD Vaporization Rate Results

Results

Model		Peak Vaporization Rate (PVR)	PVR time	Vaporization End Time
		(lbm/hr)	(min)	(min)
4.2 inch Mortars	PVR model	1094	20.5	60.5
	100% liquid HD CFD model	1095	13	63
	Solid HD CFD model	1044	17	74
105mm Projectiles	PVR model	828	13	50.5
	100% liquid HD CFD model	833	18.5	48
	Solid HD CFD model	706	22	55.5
155mm Projectiles	PVR model	1226	28.3	60.5
	100% liquid HD CFD model	1224	26	73
	Solid HD CFD model	1030	32	82.5

Conclusion

1. Fluent CFD model coupled with melting/vaporization code has been developed.

2. CFD model for liquid chemical weapon agent was calibrated by CR&E PVR model. The predicted results of CFD model and PVR model for three different kinds of munitions were in good agreement.

3. The current PVR model does not have the capability to simulate the overall vaporization rate for chemical agent that has been solidified. The calibrated CFD model can simulate the necessary heat and mass transfer for the solidified agent found in the munitions.

Acknowledgement

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Thank You