

Utilizing CFD for Prediction of HD1.3 Pressure Loads in a Cell with Venting

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1 ABSTRACT

A methodology was presented at DDESB-2006 for the calculation of gas loading inside a room resulting from the ignition and burning of Hazard Class/Division (HD) 1.3 materials. That methodology, implemented in a spreadsheet, included thermodynamic sub-models for the burning material's creation of products, radiation heat loss to the walls, and time dependent venting to connected enclosures, such as a vestibule. The resulting pressure-time history was useful for the design of blast resistant walls and doors typically found in propellant containment or handling facilities.

This paper describes an improved method which uses computational fluid dynamics (CFD) to describe the HD 1.3 burning, gas loading, and venting. Advantages over the spreadsheet method include the ability to model convective heat transfer and water spray deluge along with being able to resolve local flow field characteristics using fundamental flow equations as opposed to treating the entire room as a single control volume as was done in the spreadsheet method.

The CFD method presented includes how the HD1.3 source term was modeled, including the important effects of burn rate, burning chemistry, sympathetic propagation, and the potential after burning of products in atmospheric air. Model setup is described for a recent analysis of a proposed chemical weapons disposal room processing solid rocket motors (SRMs) with and without venting and water spray. Details revealed by the model including venting size requirements and vent placing are reviewed. CFD results are compared to both the spreadsheet method and BlastX. Finally, model limitations are discussed, which include vent inertia and high speed flows.

2 BACKGROUND

The process for predicting HD 1.3 (propellants) gas pressure loads is not the same as that for HD 1.1 (high explosives) materials where the peak pressure is developed nearly instantaneously and reduces with time as venting occurs. HD 1.1 detonation in an enclosure will generate both shock and gas loading. The shock load includes short duration pressure spikes as the shock wave reverberates in the room. The gas load is a result of the heat released during the explosion and afterburning of explosives that was not consumed by the initial detonation. This happens in a very short period of time for HD 1.1 explosives and the gas load reaches a peak within milliseconds and venting present has little time to influence the formation of peak pressure, except in cases with very large vent areas that are either

Report Documentation Page

Form Approved
OMB No. 0704-0188

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1. REPORT DATE

JUL 2010

2. REPORT TYPE

N/A

3. DATES COVERED

-

4. TITLE AND SUBTITLE

Utilizing CFD for Prediction of HD1.3 Pressure Loads in a Cell with Venting

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)

ABSG Consulting Inc. 14607 San Pedro, Suite 215 San Antonio, Texas 78232

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

Approved for public release, distribution unlimited

13. SUPPLEMENTARY NOTES

See also ADM002313. Department of Defense Explosives Safety Board Seminar (34th) held in Portland, Oregon on 13-15 July 2010, The original document contains color images.

14. ABSTRACT

A methodology was presented at DDESB-2006 for the calculation of gas loading inside a room resulting from the ignition and burning of Hazard Class/Division (HD) 1.3 materials. That methodology, implemented in a spreadsheet, included thermodynamic sub-models for the burning materials creation of products, radiation heat loss to the walls, and time dependent venting to connected enclosures, such as a vestibule. The resulting pressure-time history was useful for the design of blast resistant walls and doors typically found in propellant containment or handling facilities. This paper describes an improved method which uses computational fluid dynamics (CFD) to describe the HD 1.3 burning, gas loading, and venting. Advantages over the spreadsheet method include the ability to model convective heat transfer and water spray deluge along with being able to resolve local flow field characteristics using fundamental flow equations as opposed to treating the entire room as a single control volume as was done in the spreadsheet method. The CFD method presented includes how the HD1.3 source term was modeled, including the important effects of burn rate, burning chemistry, sympathetic propagation, and the potential after burning of products in atmospheric air. Model setup is described for a recent analysis of a proposed chemical weapons disposal room processing solid rocket motors (SRMs) with and without venting and water spray. Details revealed by the model including venting size requirements and vent placing are reviewed. CFD results are compared to both the spreadsheet method and BlastX. Finally, model limitations are discussed, which include vent inertia and high speed flows.

15. SUBJECT TERMS

16. SECURITY CLASSIFICATION OF:			17. LIMITATION OF ABSTRACT SAR	18. NUMBER OF PAGES 45	19a. NAME OF RESPONSIBLE PERSON
a. REPORT unclassified	b. ABSTRACT unclassified	c. THIS PAGE unclassified			

Standard Form 298 (Rev. 8-98)
Prescribed by ANSI Std Z39-18

uncovered or have very frangible covers. Often, gas loading for HD 1.1 explosions is approximated as reaching the peak pressure instantaneously and reducing over time as venting relieves the pressure.

Established technical guidance and criteria for explosives safety design for accidental burn of HD 1.3 operating facilities is not as in-depth as it is for accidents involving HD 1.1 detonations. This includes the prediction of blast loads, incorporation of venting, and structural response calculations¹. Accidents involving HD 1.3 items would, under most conditions, burn over an extended period of time, thus, the peak does not occur instantaneously and venting will influence both the peak gas pressure and associated impulse. The gas pressure load history for HD 1.3 items is closely tied to the mass burn rate as well as the total quantity. The faster the burn rate, the more the gas loading mimics that of HD 1.1 explosion and the total quantity is very influential. The slower the burn rate, the greater influence venting has on the load history and the total quantity of material has less influence, with the exception of very small quantities.

The *HD 1.3 Passive Structural Systems Design Guide* HNDED-CS-93-7² specifies that all HD 1.3 in a room will be summed and converted to an equivalent TNT mass (based on energy), which will then be detonated. This process results in the near instantaneous release of all energy in the propellants, which generates significant gas loading as well as shock loading on the room. The actual burning process of HD 1.3 is much slower than a detonation; therefore, the time release of energy does not produce shock waves and gives a much slower pressure increase over time, to the point that heat transfer to the walls via radiation and convection as well as water spray can result in significant decreases in peak room pressures. CFD can model the timing of energy release as well as the above mentioned heat transfer mechanisms, and is therefore a more realistic representation of HD 1.3 burning than the conservative methods outlined in the design guide.

The design guide does allow for alternative methods which account for time dependent burning. This analysis therefore meets the design guide through the use of multiple blast design tools, including CFD and BlastX, to account for time dependent burning of HD 1.3 as described in this report. HNDED-CS-93-7 specifically allows this engineering approach; in addition, HNDED-CS-93-7 also states:

... there is no substitute for actual data about a specific HD 1.3 explosive material and its behavior. Such data should supersede any factors included in this procedure.

All data concerning the combustion properties utilized for the blast analysis were obtained from MIL-P-60071 *M28 Propellant Grain Specification* supplied to ABS Consulting. The composition of M28 was defined in the specification, while other properties such as heat of combustion and combustion products were calculated using the defined composition and fundamental thermodynamics. Therefore the use of CFD to provide input to the final venting size and location is compliant with *HD 1.3 Passive Structural Systems Design Guide*.

¹Whitney M.G., Harrison, B.F., Knight, G.K., "Explosives Safety Design for HD 1.3 Facilities," DDESB Explosives Safety Seminar, August 2006.

² Department of Defense Explosives Safety Board, "Hazard Division 1.3 Passive Structural Systems Design Guide", US Army Corps of Engineers Huntsville Division, HNDED-CS-93-7 (Rev 1), 1 November 1994.

In 2006, a paper³ was presented at DDESB describing the physics and calculation methods associated with the burning and venting of products and energy in an enclosed cell with frangible surfaces. A numerical procedure implemented in a spreadsheet tracked the burning of a HD 1.3 item in a controlled volume including the effects of venting and heat loss. The methodology relied on fundamental physics such as chemical reactions, radiation heat transfer, and fluid flow. Its methods were based on and extended from previous work by Ketchum and Whitney⁴ describing the methodology for the calculation of overpressure and temperature time histories for the burning of a HD 1.3 propellant in an enclosed cell.

The following CFD methodology was developed to analyze the vent area requirements and determine gas pressures for various processing rooms in a chemical munitions demilitarization building. The project evaluated the gas pressure loading in various rooms using different room dimensions, source terms, vent areas, and deluge rates. The analysis subsequently received DDESB approval.

The methodology is applicable to propellant burning only and does not address conditions that can cause transition from burning to more severe explosion or due to shock initiations.

3 CFD COMPARED TO HD 1.3 PASSIVE STRUCTURAL SYSTEMS DESIGN GUIDE

4 SOURCE TERM

Using CFD to model fluid flow involves describing the source term or driving mechanism which creates gradients in the flow domain. Typically described at a boundary of the flow domain, the source term may be a wind inlet condition for an external flow analysis or a velocity profile for flow through a pipe. In the current case, the source term represents the energy and mass being released by the HD 1.3 material as it burns. Modeling the actual time-dependant burning of the HD 1.3 material would require a very small mesh along with complex models for pyrolysis and combustion which would need to be compared to experimental data to ensure they correctly capture the fundamental physics. An alternative to modeling the burning of HD 1.3 in CFD would be to model just the products of the reaction as a source term at the boundary. Hand calculations with simplifying assumptions can be used to calculate the products. This is the approach taken in this work.

4.1 BURNING CHEMISTRY

M28 propellant is classified as a HD 1.3 material, and represents a potential deflagration hazard should an accidental ignition occur. The large quantities of heat and gaseous products expelled from the burning propellant will generate gas pressure inside the rooms that must be either contained or safely vented.

The M28 propellant grain is primarily composed of the materials shown below in Table 1 as defined in the M28 specification. Percentages were slightly adjusted to account for the remaining lubricant and

³Knight, G., Harrison, B., Whitney, M., *Utilizing Fundamental Thermodynamics Relationships for Prediction of HD1.3 Pressure Loads in a Cell with Directional Venting*, DDESB 2006.

⁴ Whitney, M. G., Ketchum, D., "Explosion Protection Structures for Munitions Testing, Phase I Report," SwRI Final Report 06-8348-001, Prepared for Department of the Air Force, Hill Air Force Base, August 1985. Note that the equation for unchoked mass flow has a sign typo, the term $\gamma/(\gamma+1)$ should be $\gamma/(\gamma-1)$.

stabilizer constituents, 2% Lead Stearate and 1.7% 2-Nitrodiphenylamine, which were neglected in this analysis. The combustion of the M28 propellant results in hot product gasses being discharged from the solid rocket motor (SRM). The M28 propellant is fuel rich with respect to the oxidizer it contains since only Nitroglycerin contains at least a stoichiometric amount of oxidizer, while the remaining components are all oxidizer deficient. A stoichiometric fuel plus oxidizer combination will result in only H₂O and CO₂ product gasses. Since the M28 propellant does not contain sufficient oxygen molecules, the product gasses will also contain some H₂ and CO.

Table 1. M28 Propellant Constituents

PROPELLANT	FORMULA	MASS %	MW (g/mole)	DENSITY (g/cm ³)
Nitrocellulose (12.2% N)	C ₆ H _{7.68} N _{2.32} O _{9.645}	61%	266.5	1.653
Nitroglycerin	C ₃ H ₅ N ₃ O ₉	25%	227	1.6
Triacetin	C ₉ H ₁₄ O ₆	11%	218.1	1.16
Dimethyl Phthalate	C ₁₀ H ₁₀ O ₄	3%	194	1.19

Propellant properties such as molecular weight and the moles of Carbon, Hydrogen, Oxygen, and Nitrogen per mole of propellant were determined using hand calculation methods as well as the Air Force Chemical Equilibrium Specific Impulse (AFCESI) Code⁵ and PROPEP via the GUIPEP⁶ interface. PROPEP is a version of the Propellant Evaluation Program (PEP) produced by the Naval Weapons Center. The theory and application of the PEP code is described by Cruise⁷. Both codes calculate the properties of a reactant as a function of its constituents as well as the solid rocket motor products both inside the pressurized motor and after expansion through the nozzle to atmospheric pressure.

Mole fractions for the contributing components are determined as shown below in Table 2. Mass of contributing components per mole M28 and resulting M28 molecular weight is shown in Table 3. The overall molecular weight of the propellant is 247 g/mole and the total moles of propellant per rocket are 35.43 moles. Finally, calculate the number of moles of C, H, N, and O per mole of M28. For example, considering Carbon, $6 \times 150.7 / 266.5 = 3.39$, $3 \times 61.8 / 227 = 0.82$, $9 \times 27.2 / 218.1 = 1.12$, and $10 \times 7.4 / 194 = 0.38$, the summation of which is 5.71 moles carbon per mole of M28. The ISP propellant code results in Figure 1 show the same values.

Table 2. M28 Propellant Mole Fractions

PROPELLANT	WEIGHT (g)	MOLES	MOLE %
Nitrocellulose (12.2% N)	61	0.2288	56.5%
Nitroglycerin	25	0.1101	27.2%
Triacetin	11	0.0504	12.5%
Dimethyl Phthalate	3	0.0154	3.8%

⁵ Air Force Chemical Equilibrium Specific Impulse (AFCESI) Code, Build Date 5.18.1992, <http://www.dunnospace.com/isp.htm>

⁶ GUIPEP Graphical User Interface to PROPEP, <http://www.lekstutis.com/Artie/PEP/Index.html>.

⁷ Cruise, D.R. "Theoretical Computations of Equilibrium Compositions, Thermodynamic Properties, and Performance Characteristics of Propellant Systems," Naval Weapons Center, China Lake, CA, April 1979.

Table 3. M28 Propellant Overall Molecular Weight

PROPELLANT	MW (g/mole)	MOLES	MASS (g)
Nitrocellulose (12.2% N)	266.5	0.565	150.7
Nitroglycerin	227	0.272	61.8
Triacetin	218.1	0.125	27.2
Dimethyl Phthalate	194	0.038	7.4
TOTALS ->		1	247

Table 4. Moles of Elements per Mole M28

PROPELLANT	C	H	N	O	MASS (g)	MW (g/mole)	C (moles)	H (moles)	N (moles)	O (moles)
Nitrocellulose (12.2% N)	6	7.68	2.32	9.645	150.7	266.5	3.39	4.34	1.31	5.45
Nitroglycerin	3	5	3	9	61.8	227	0.82	1.36	0.82	2.45
Triacetin	9	14	0	6	27.2	218.1	1.12	1.74	0.00	0.75
Dimethyl Phthalate	10	10	0	4	7.4	194	0.38	0.38	0.00	0.15
Gram Atoms (moles) / mole M28->							5.71	7.83	2.13	8.80
ISP Gram Atoms / 100 g M28							2.31	3.17	0.86	3.56
ISP Gram Atoms / mole M28							5.71	7.82	2.13	8.80

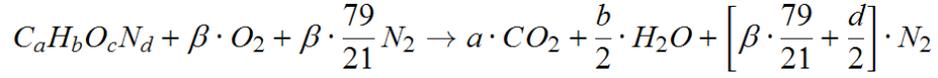
PROPELLANT	HF	DENSITY	WEIGHT	MOLES	VOLUME
NC	-172.2000	1.6530	.6100	.0023	.3690
NG	-90.7500	1.6000	.2500	.0011	.1563
TA	-316.1000	1.1600	.1100	.0005	.0948
DMP	-161.2000	1.1900	.0300	.0002	.0252
GRAM ATOMS/100 GRAMS					
H	3.1678	O	3.5618	N	.8611
		C	2.3112		
ENTHALPY = -67.81373			DENSITY =1.550		
		CHAMBER	EXH(SHIFT)		
PRESSURE (PSIA)	14.700		14.700		
EPSILON	.000		.000		
ISP	.000		.082		
ISP (VACUUM)	.000		95762.220		
TEMPERATURE(K)	2109.882		2109.984		
MOLECULAR WEIGHT	23.100		23.100		
MOLES GAS/100G	4.329		4.329		
CF	.000		.000		
PEAE/M (SECONDS)	.000		95762.130		
GAMMA	1.251		1.251		
HEAT CAP (CAL)	42.822		42.822		
ENTROPY (CAL)	275.146		275.145		
ENTHALPY (KCAL)	-67.813		-67.813		
DENSITY (G/CC)	1.33461E-04		1.33454E-04		
ITERATIONS	11		2		
MOLES/100 GRAMS (0.405 MOLES) of PROPELLANT					
H	.00594		.00595		
H2	.75230		.75228		
HO	.00081		.00081		
H2O	.82823		.82824		
NO	.00003		.00003		
N2	.43052		.43052		
CO	1.88971		1.88971		
CO2	.42150		.42149		

Figure 1. AFCESI Code Propellant Burning Results

Give the previously calculated elemental mole quantities per mole of propellant; a balanced stoichiometric equation for M28 can be determined as shown below in Equation 1. The quantities of gaseous products produced by each SRM at the nozzle and after external burning of the H₂ and CO are shown in Table 5. The Pre-Afterburning quantities are based on the chemical equilibrium calculations performed in the AFCESI code, scaled up based on the propellant grain weight. The Post-Afterburning quantities are based on the stoichiometric combustion equation below and include the consumed

atmospheric air. An example of the grain cross section can be seen below in Figure 2. Important grain geometry properties are listed below in Table 6.

Equation 1. Stoichiometric Equation for M28 Propellant



$$\beta = a + \frac{1}{4} \cdot b - \frac{1}{2} \cdot c, \quad a = 5.71, \quad b = 7.82, \quad c = 8.80, \quad d = 2.13$$

From the above equation it can be seen that for every mole of propellant burned, the secondary reaction of CO and H₂ with atmospheric air consumes β=3.265 moles of oxygen. The burning of CO and H₂ gasses once they exit the SRM and mix with air contributes an additional energy source that cannot be neglected.

Table 5. Solid Rocket Motor (SRM) Products

Species	Total Moles per Rocket	Total Mass per Rocket
At Nozzle (Pre-Afterburning)		
H2	65.8	131.7
H2O	72.5	1304.6
N2	37.7	1054.8
CO	165.4	4630.3
CO2	36.9	1623.0
(Post-Afterburning)		
H2O	138.5	2493.5
CO2	202.3	8901.2
+N2	472.9	13241.1
-N2	-435.2	-12184.6
-O2	-115.7	-3701.6
Net	262.9	8749.6

+ indicates added to domain

- indicates removed from domain

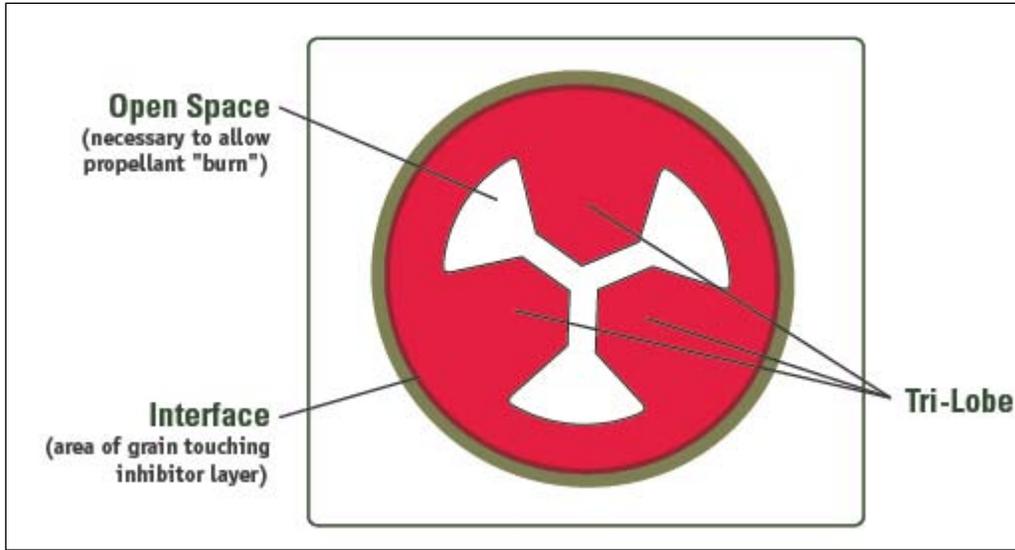


Figure 2. M28 Propellant Grain Cross Section⁸

Table 6. M28 Propellant Grain Properties

Length	83.4	cm
Diameter	11.3	cm
Density	1.55	g/cm ³
Void Area	17.4	cm ²
Void Perimeter	33	cm
Grain Cross Section Area	67.7	cm ²
Grain Volume	5646	cm ³
Grain Mass	8751	g
M28 Molecular Weight	247	g/mol
Grain Moles	35.43	mol

Having calculated the number of moles created and consumed during the burning and after burning of the propellant, we turn to the net energy production. Gas pressure in an enclosed room or volume is a function of both the number of moles added to the volume as well as the temperature of the volume. Assuming all species can be idealized as ideal gasses, the pressure in a closed volume takes the form of $P=n \cdot V^{-1} \cdot R \cdot T$. The significant temperature increase will have a much greater effect on pressure than the number of moles. Air at 20 °C has about 41.44 moles per cubic meter. Therefore, a 1200 m³ room has approximately 49,544 moles. A box of 20 SRMs contains 175 kg of propellant which will generate approximately 5258 moles of gas, effectively increasing the number of moles in the bay by a factor of 1.1 or 10 percent. The mean temperature of the bay can be expected reach 1100 °C resulting in a much larger increase factor for temperature which subsequently controls the pressure increase. Correctly modeling the temperature rise depends on accurately modeling the energy release of the combustion process, which is a function of the propellant properties as well as the burn rate.

⁸ U.S. Army Chemical Materials Agency, <http://www.cma.army.mil/m55rocketfires.aspx>

The energy released during combustion is a function of the heat of formation (ΔH_f) for M28 and the heat of formation of the products. The ΔH_f of M28 is a function of its constituents as shown in Table 7. The heat of combustion (ΔH_c) assuming the stoichiometric equation above (which includes afterburning with atmospheric oxygen) is calculated as shown below.

Table 7. M28 Heat of Formation

PROPELLANT	MOLE %	ΔH_f (kJ/mole)	kJ/mole M28
Nitrocellulose (12.2% N)	56.5%	-720.97	-407.60
Nitroglycerin	27.2%	-379.95	-103.37
Triacetin	12.5%	-1323.45	-164.82
Dimethyl Phthalate	3.8%	-674.91	-25.68
ΔH_f M28 (kJ/mole)			-701.47

$$\Delta H_c(M28) = -\Delta H_{rxn}(M28) = \sum \Delta H_f(\text{reactants}) - \sum \Delta H_f(\text{products})$$

$$\Delta H_f(M28) = -701.47 \frac{\text{kJ}}{\text{mole}} \quad \Delta H_f(H_2O) = -285.5 \frac{\text{kJ}}{\text{mole}} \quad \Delta H_f(CO_2) = -393.51 \frac{\text{kJ}}{\text{mole}}$$

$$\Delta H_f(N_2) = 0 \frac{\text{kJ}}{\text{mole}} \quad \Delta H_f(O_2) = 0 \frac{\text{kJ}}{\text{mole}}$$

$$\Delta H_c(M28) = \left(1 \text{mole} \cdot -701.47 \frac{\text{kJ}}{\text{mole}} \right) - \left(5.71 \text{mole} \cdot -393.51 \frac{\text{kJ}}{\text{mole}} + \frac{7.82}{2} \text{mole} \cdot -285.5 \frac{\text{kJ}}{\text{mole}} \right) = 2662.9 \frac{\text{kJ}}{\text{mole}}$$

$$\Delta H_c(\text{SRM}) = 2662.9 \frac{\text{kJ}}{\text{mole}} \cdot 8750 \text{g} \cdot \left(247 \frac{\text{g}}{\text{mole}} \right)^{-1} = 94,334 \text{kJ}$$

4.2 BURN RATE

The burn rate effectively sets the rate at which energy is added to the room. Adding the same amount of energy at a faster rate can significantly increase the peak pressure in a room depending on the venting configuration. A fast burn rate will increase pressure sufficiently fast to result in a peak gas pressure higher than the frangible vent release pressure. The pressure associated with a slow burn rate will nearly immediately begin to decrease once venting begins, and the peak gas pressure will be approximately the same as the vent panel release pressure. Two different burn rates were considered in this work.

Under normal operations the M55 rocket igniter would initiate burning along the length of the motor over the exposed internal surface of the tri-lobe propellant. This produces significant pressure rise in the motor which increases the burn rate of the propellant. The M28 propellant grain specification⁹ indicates a range of action times (burn time) depending on temperature. A burn time of three seconds was used in this analysis for motors initiated by their igniter. This ignition will hereby be called a normal ignition.

⁹ MIL-P-60071 M28 Propellant Grain Specification, 6-15-1966.

An alternative ignition may occur in the M28 propellant at the interface between the propellant and inhibitor layer. External heating of the rocket which produces hot spots could produce such an ignition, as could an impact to the rocket of sufficient magnitude. The burning behavior of the rocket would be very different from a normal ignition. Burning would occur much slower resulting in lower internal rocket motor pressures. A total burn time of approximately 78 seconds with powered flight possible after 40 seconds was used. This ignition will hereby be called a soft ignition.

4.3 PROPAGATION

Propagation of one burning SRM to neighboring SRMs was necessary to ensure a conservative worst case assessment. The mode of propagation has a direct impact on the number of SRMs burning simultaneously and therefore the overall burn rate for the room which directly affects pressure build up. All SRMs in the same storage box are assumed to propagate instantly and burn at the same time. Propagation from one box to a neighboring box is assumed as soon as SRMs in the first box attain powered flight (40 seconds for a soft ignition). Propagation between rooms was not considered due to the low probability of a SRM finding its way through the relatively small connecting vent.

5 MITIGATION

5.1 WATER SPRAY

Water droplets have the potential to evaporate during an event, producing additional moles of gas which will increase the gas pressure in the room. This evaporation will also decrease the temperature of the air and walls of the room, which will decrease the room pressure based on the ideal gas equation of state. Therefore, sprinklers produce competing effects which may serve to increase or decrease a room's gas pressure depending on specific conditions such as water flow rate, the deflagration rate of propellant, heat capacity of the walls, and room volume. For the scenarios modeled, the cooling effects of sprinklers produced a decrease in room pressure.

A sprinkler activation temperature of 74 °C was assumed. This value is the standard activation temperature used in FDS. A higher temperature would delay sprinkler activation; however, since in many cases the upper elevations of the rooms reach high temperatures very quickly, the effect of activation temperature is negligible.

6 CFD MODEL

6.1 FIRE DYNAMICS SIMULATOR (FDS)

The relationships between cell pressure, temperature, source term (propellant), venting, and heat transfer modes are complex. Therefore, a full CFD solution was sought which implicitly incorporated all of the necessary physics. The open source code *Fire Dynamics Simulator*¹⁰ (FDS) produced by National Institute of Standards and Technology (NIST) was used.

FDS is a computational fluid dynamics model of fire-driven fluid flow. The software solves numerically a form of the Navier-Stokes equations appropriate for low-speed, thermally-driven flow, with an emphasis

¹⁰ Fire Dynamics Simulator, NIST, Version 5.5, <http://fire.nist.gov/fds/>

on smoke and heat transport from fires. While primarily developed for the simulation of fires, FDS has evolved into a useful general purpose CFD code with excellent capabilities related to general fluid flow and heat transfer. The methodologies of the various features in FDS can be found in the Technical Reference Guide¹¹ and/or Users Guide¹².

6.2 LIMITATIONS

A distinguishing feature of a CFD model is the regime of flow speeds (relative to the speed of sound) for which it is designed. High speed flow codes involve compressibility effects and shock waves. Low speed solvers, however, explicitly eliminate compressibility effects that give rise to acoustic (sound) waves. Since FDS was written primarily for solving low speed fire growth and propagation, the equation set assumes that pressure is composed of a “background” component and a perturbation component. This numerical treatment effectively filters out high speed flow acoustic waves and compressibility effects, simplifying the equation set and allowing for larger time steps and faster solutions.

The first effect of this “low mach number assumption” is that FDS does not handle flows approaching the speed of sound (340 m/s) and will not accurately model compressible flows (approximately >100m/s). The manifestation of this limitation in the current problem relates to the opening of venting surfaces. While FDS allows surfaces to “fail” or “release” at a given pressure, the differential pressure across the surface should be limited to not much more than 1 psi. Larger differential pressures result in numerical instabilities, causing the solution to fail in most instances. For solutions that do not fail, the fast flow changes can result in some numerical oscillation of pressure. This oscillation does not appear to affect the overall accuracy of the general trend.

A limitation related to the above is that releasing surfaces disappear instantaneously rather than over a period of time as they are pushed away by the load. Actual failing surfaces will require time to move out of the way and result in higher cell pressure. This instantaneous removal is partially responsible for the limitation above on maximum differential pressure. A more desirable behavior would be to linearly increase porosity of the surface over a time period to model the failure while not subjecting the pressure solver to any instantaneous changes in pressure.

The second effect of splitting pressure into background and perturbation components is that FDS by default assumes the entire domain shares the same background pressure. This is an undesirable condition when trying to model multiple cells connected by small vent areas. The condition can be partially remedied through the use of the ZONE command in FDS which assigns each room its own background pressure; however, once venting begins (via the removal of an obstruction between the two ZONES thereby opening up a hole) between two ZONES, the background pressures are merged over a few seconds, which may not be the actual time scale. A better alternative is to specify a leak area between the ZONES as opposed to removing an obstruction. Invoking leak area uses a sub-grid model

¹¹ K.B. McGrattan, S. Hostikka, J.E. Floyd, H.R. Baum, and R.G. Rehm. Fire Dynamics Simulator (Version 5), Technical Reference Guide Volume 1 – Mathematical Model. NIST Special Publication 1018-5, National Institute of Standards and Technology, Gaithersburg, Maryland, October 2007.

¹² K.B. McGrattan, B.W. Klein, S. Hostikka, and J.E. Floyd. Fire Dynamics Simulator (Version 5), User’s Guide. NIST Special Publication 1019-5, National Institute of Standards and Technology, Gaithersburg, Maryland, October 2007.

for leaks between pressure zones. The only limitation to using leak areas between ZONES is the current leak rate calculation uses an incompressible form which will overestimate leak rate for any significant upstream to downstream pressure ratio. The solution is to re-compile the code using the equation for volumetric flow of compressible gasses including the possibility of choked flow.

6.3 MODELING THE SOURCE TERM

Modeling the source term in FDS can be done in two different ways. The first approach is to specify a reaction equation for the fuel and a heat release rate at an inlet surface. FDS will inject fuel into the domain from the inlet surface which will then burn on mixing with oxygen in the air. This method is simple since it only requires that the user specify the reaction stoichiometry and heat release rate, both previously determined values. The drawback is that since FDS uses a mixture fraction approach for burning fuel, it is not possible to specify a fuel which contains its own oxidizer. Oxygen from the atmosphere will be consumed to burn the fuel and create the products specified by the stoichiometry. Also, the burning rate is not directly controllable by the user and is dependent on the mixing of fuel and oxygen. Internal constants designed for fires can be changed such that FDS burns the fuel faster than normal.

The second approach, and the one taken in the current work, is to add reaction products to the domain at a temperature which equates to the desired heat release rate (heat of combustion). The quantities of products were previously determined in the stoichiometric calculations. The temperature at which to add the products can be determined iteratively by guessing a temperature, running FDS, and then examining the time integral of the FDS output quantity CONV_LOSS, which tracks the energy added to the domain according to Equation 2. The temperature which gives the desired total integrated energy that equals the heat of combustion is the correct temperature. This procedure is equivalent to using the temperature enthalpy relationships in the JANNAF tables for each product to determine the temperature which gives the desired energy for the system while accounting for pressure-volume (pV) work. For the current work, a products temperature of 3000 °C gave approximately 94,181 kJ per SRM, which is very close to the desired value of 94,334 kJ per SRM.

Equation 2. Heat Flow through Inlet

$$\dot{Q}_{conv} = \int_A c_p \rho (T - T_\infty) \mathbf{u} \cdot d\mathbf{S}$$

6.4 VENTING BETWEEN CELLS

Venting between cells may occur when opening or frangible surfaces connect two adjacent cells. Both cases should be handled by using a ZONE for each cell in FDS along with a specified leak area and leak path between the ZONES. In the current work, the first cell represents an unmanned cutting and shearing room which processes the SRM by cutting the propellant and removing the chemical agents. No more than two SRMs are present in the cutting room at any one time. The potential for a normal ignition during the cutting process is a possible outcome. A soft ignition of the second SRM due to impact from the first during powered flight is also simulated. Therefore, the source term includes one SRM which burns for three seconds and a second SRM which burns for 78 seconds.

The general configuration of the cells is shown in Figure 3. More complex cell geometry including equipment is possible. Reduced room volume taken up by equipment will increase pressure for a given thermal loading. In the cutting and shearing cell, inlet surfaces are defined for both the normal ignition SRM and soft ignition SRM. In FDS, a RAMP is used to control the rate of products flowing through each inlet. Similar outlets exist for removing afterburning oxidizer and associated nitrogen. A vent connecting the two cells may either be initially open or set to open on based on any condition in the donor cell such as pressure, temperature, or time. In the current case the vent was open at time zero since it was a pass through portal for SRMs moving to additional processing stages.

Velocity contours at a slice plane through the source inlets and vent are shown in Figure 4. An advantage of a CFD approach is the ability to show variations in temperature and flow across a cell. This can be especially useful when considering the thermal loading on personnel from a venting scenario. In this case, both convection and radiation heat transfer modes can be considered. FDS includes the ability to track variables at discrete locations as well as integrate them across planar and volume regions. Figure 5 shows the integrated mass flow through the vent.

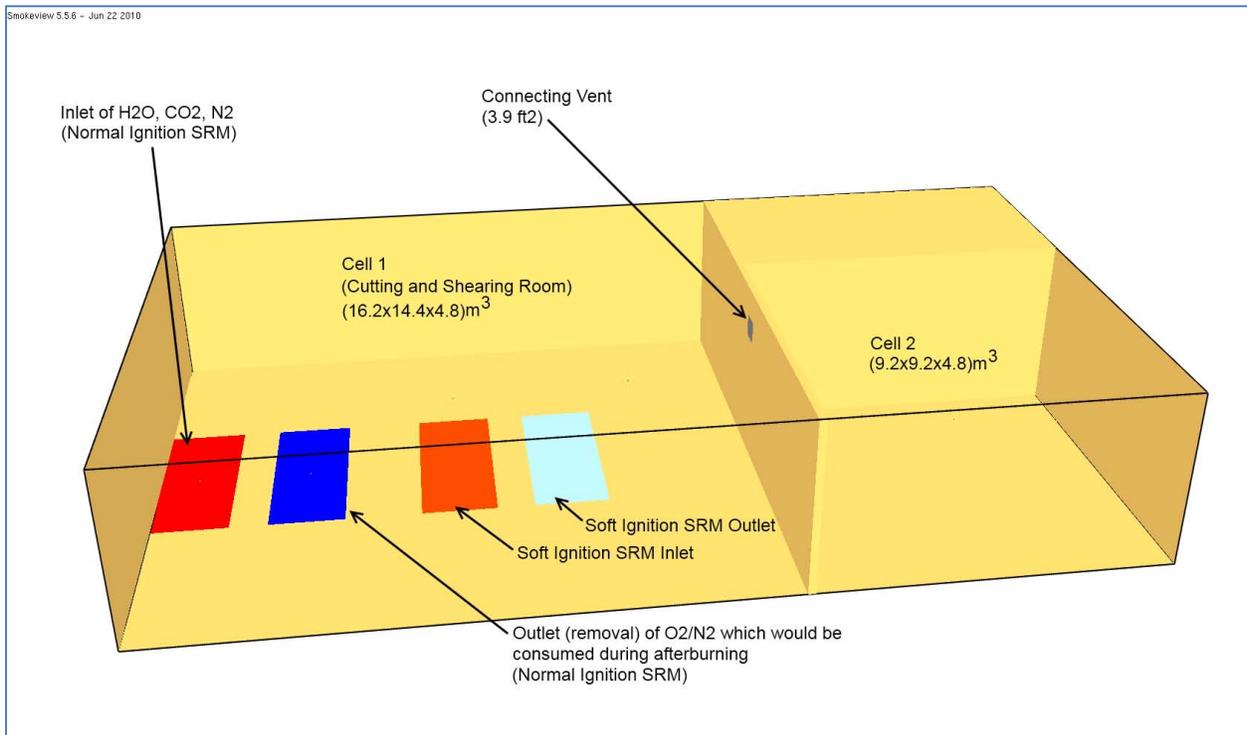


Figure 3. Venting Between Cells

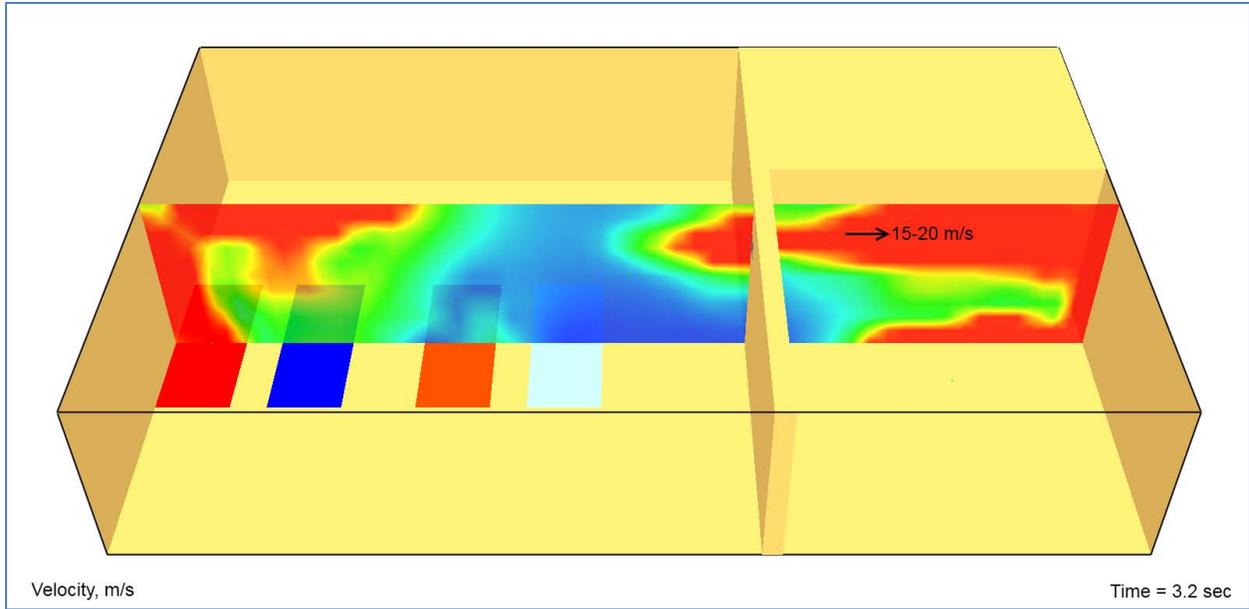


Figure 4. Velocity Contours at 3.2 Seconds

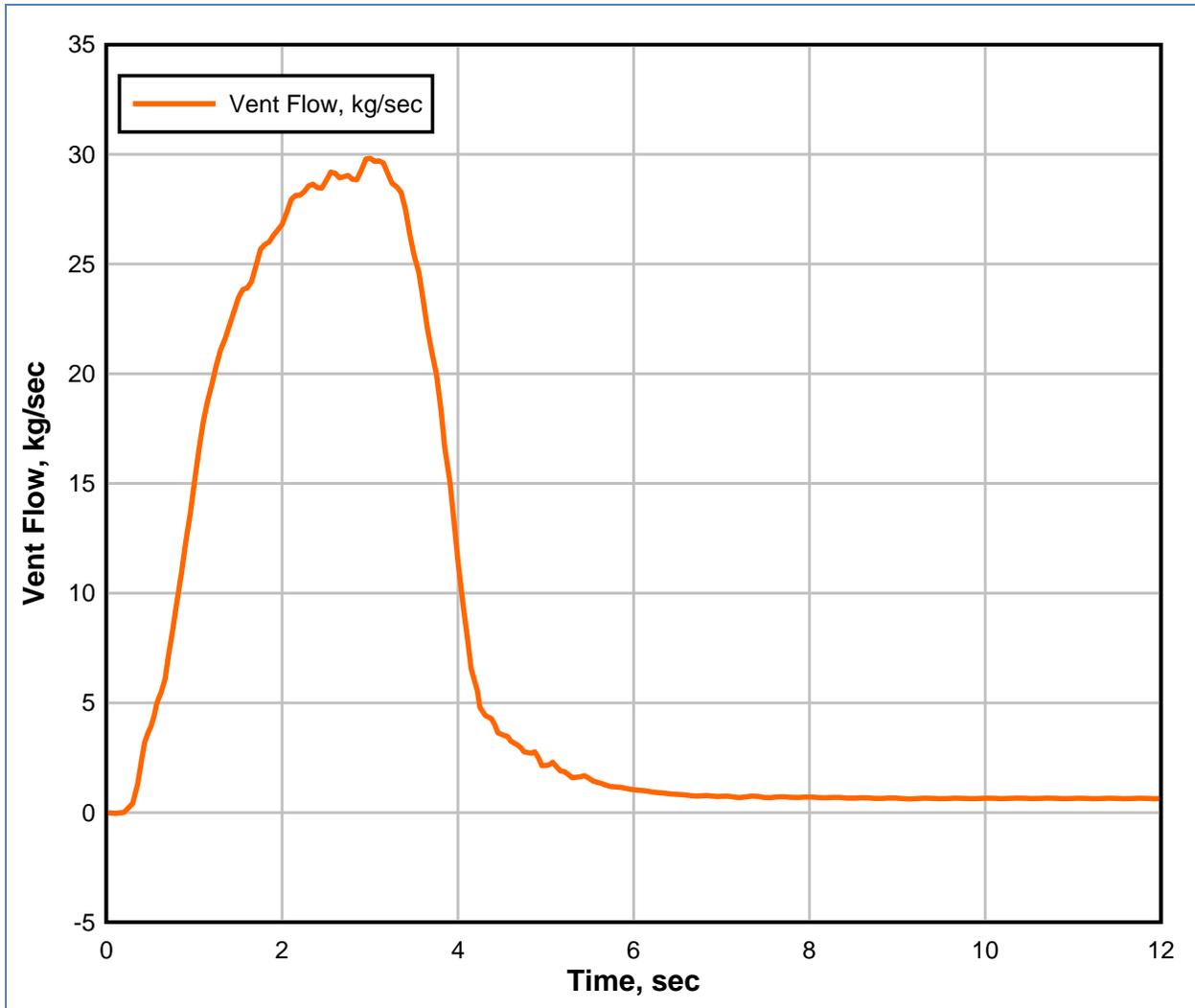


Figure 5. Vent Flow between Cells

The pressure vs. time history in each cell is shown in Figure 6 and Figure 7 after the first SRM burnout and second SRM burnout, respectively. Due to the large vent area relative to the thermal loading rate, the pressure differential between cells is not very large. The maximum difference is approximately 13 percent at 2.5 seconds for the actual case (concrete walls with convection and radiation heat transfer modes). After the normal ignition SRM has burned out, the two cells equalize since the thermal loading rate of the soft ignition SRM is low.

The effect of different wall boundary conditions is presented in each figure. The most conservative boundary condition is an adiabatic condition where no heat is lost from the system. The peak pressure after the first SRM was approximately 3.5 psi rising to nearly 5.5 psi by the end of the second SRM. Because no heat was lost during the long duration second SRM burn, its effects were more pronounced for the adiabatic boundary condition than the other boundary conditions.

Modeling the walls as concrete had a significant effect on the peak pressure, reducing it to 55 percent of the adiabatic value when both convection and radiation heat transfer modes were included account.

Since FDS includes 1D conduction heat transfer at boundaries, the ability to model the thermal flux and temperature of objects in the room both at their surface and into the material is another advantage of CFD over more simplified analyses.

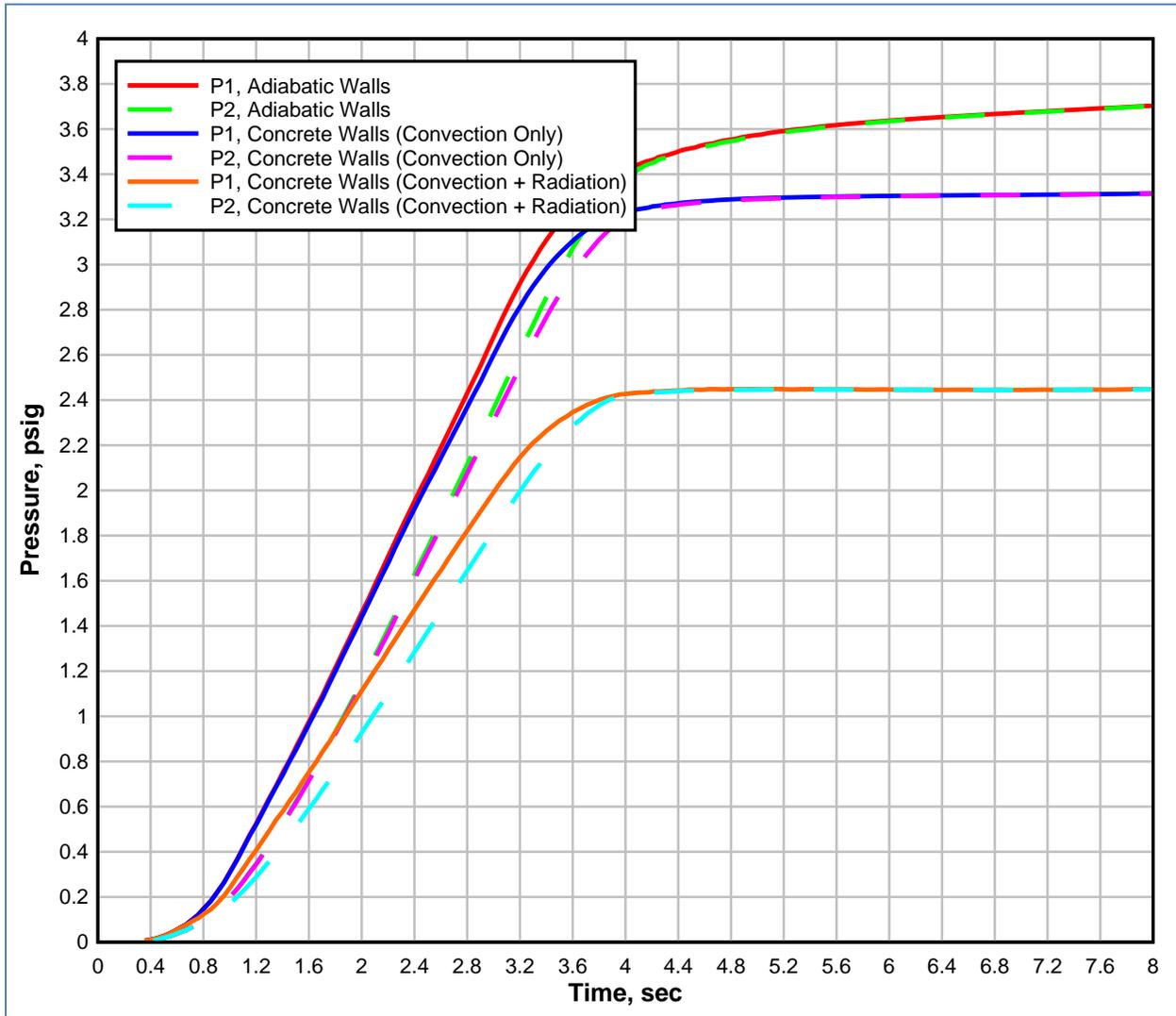


Figure 6. Cell 1 & 2 Pressures after 1st SRM Burnout

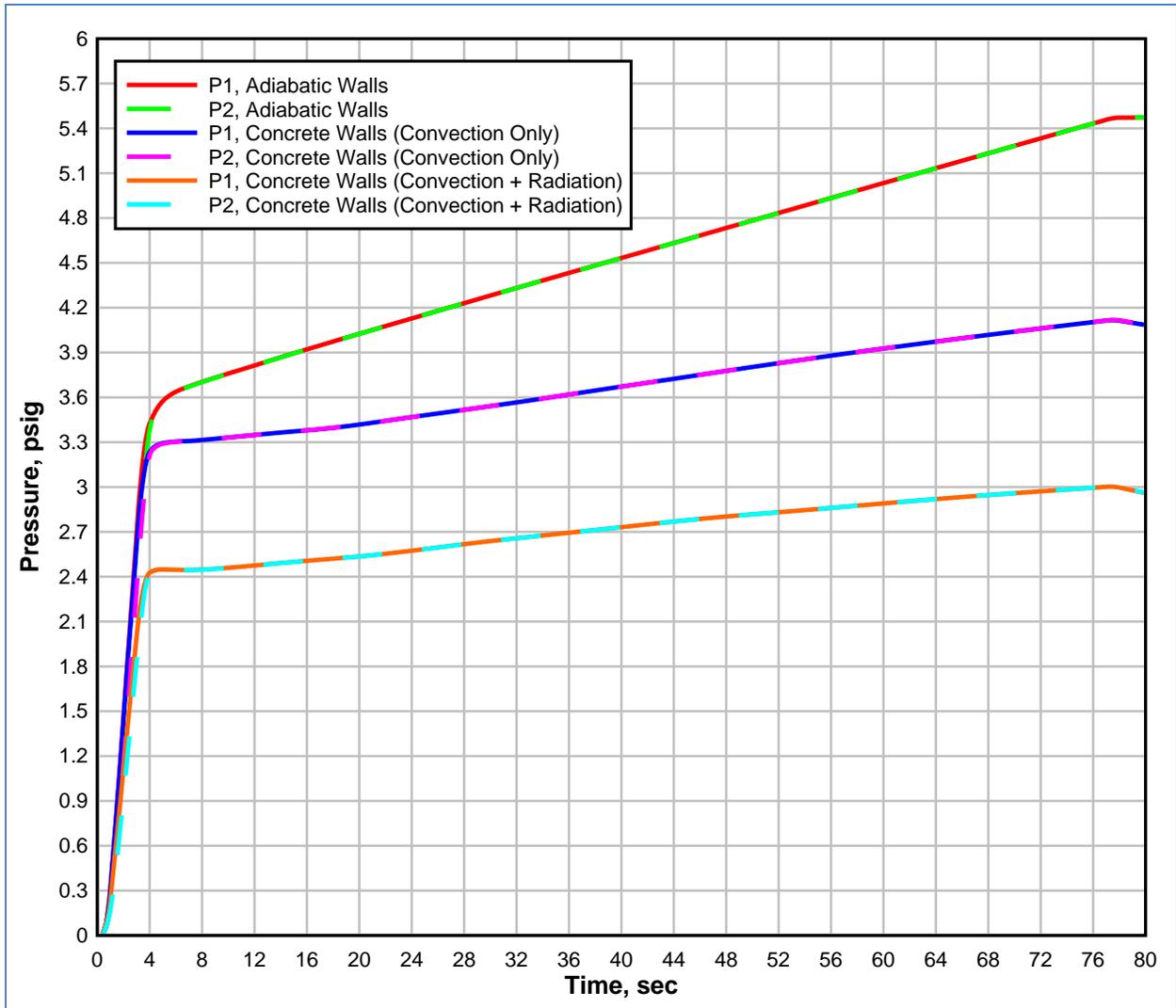


Figure 7. Cell 1 & 2 Pressures after 2nd SRM Burnout

6.5 VENTING OUTSIDE

The venting of products outside or to a sufficiently large volume such that the downstream pressure remains ambient is a common requirement. In the current work, a 1200 m³ cell containing boxes of SRMs (20 each) stored vertically was modeled to determine the minimum vent area required to maintain less than 2 psi overpressure in the room. The vent relief opening pressure was 1.5 psi. Since FDS cannot model vent inertia, artificially increasing the opening pressure level can be used as a pragmatic way to account for vent mass. The room was rectangular with concrete boundary conditions and included all heat transfer modes. A general configuration of the model can be seen in Figure 8.

The source term modeled the simultaneous normal ignition and burning of all 20 SRMs in a box. The mechanism for such an ignition was not explicitly defined. Although such an ignition is unlikely, the case represented a conservative scenario for design purposes. Propagation to other boxes was considered but rejected. Propagation by thermal heating of the acceptor SRMs was deemed unlikely due to the time necessary for convection heating to penetrate the storage box and SRM casing and heat the propellant sufficiently to initiate a soft ignition. Similarly, propagation via impact from a donor SRM which has obtained powered flight was deemed unlikely due to the protection afforded the acceptor SRMs via the storage containers.

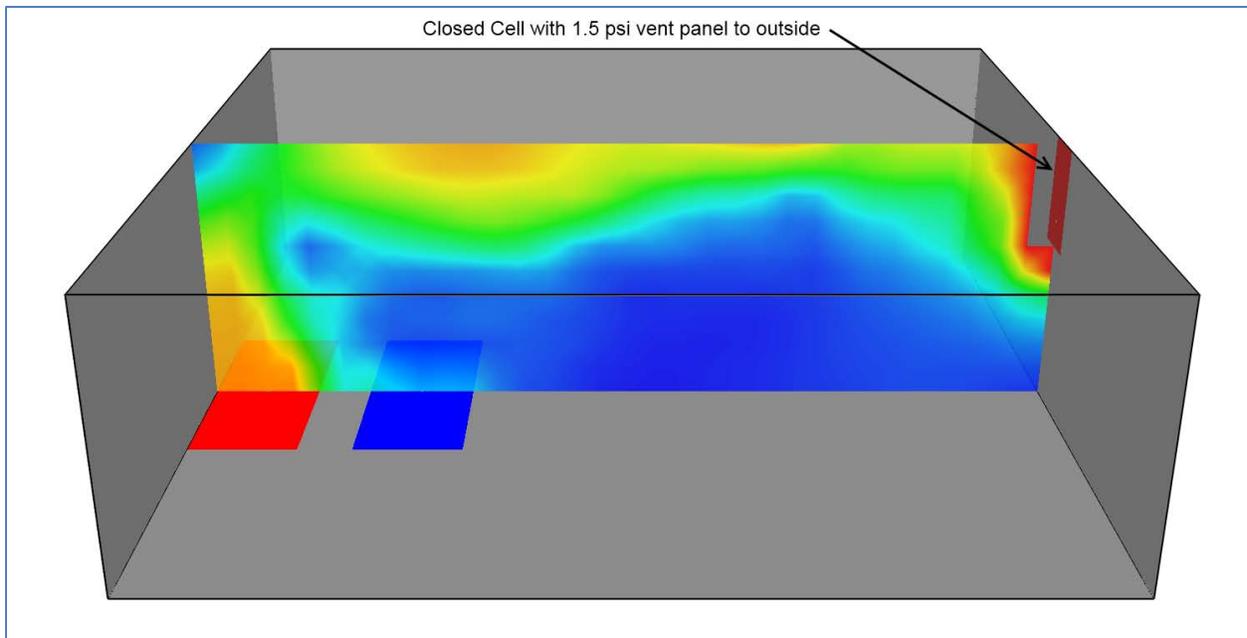


Figure 8. Closed Cell Venting to Atmosphere through 1.5 psi Vent Panel

Pressure time histories for various vent areas are shown in Figure 9. Peak pressure in the room without venting was 55 psi. Vent opening occurs at 0.6 seconds when 1.5 psi cell pressure is reached. Vent areas of 1 m², 2 m², and 4 m² significantly decreased the peak pressure, but failed to maintain the desired 2 psi maximum cell pressure. A vent area slightly greater than 6 m² was found to be necessary to maintain a 2 psi cell pressure.

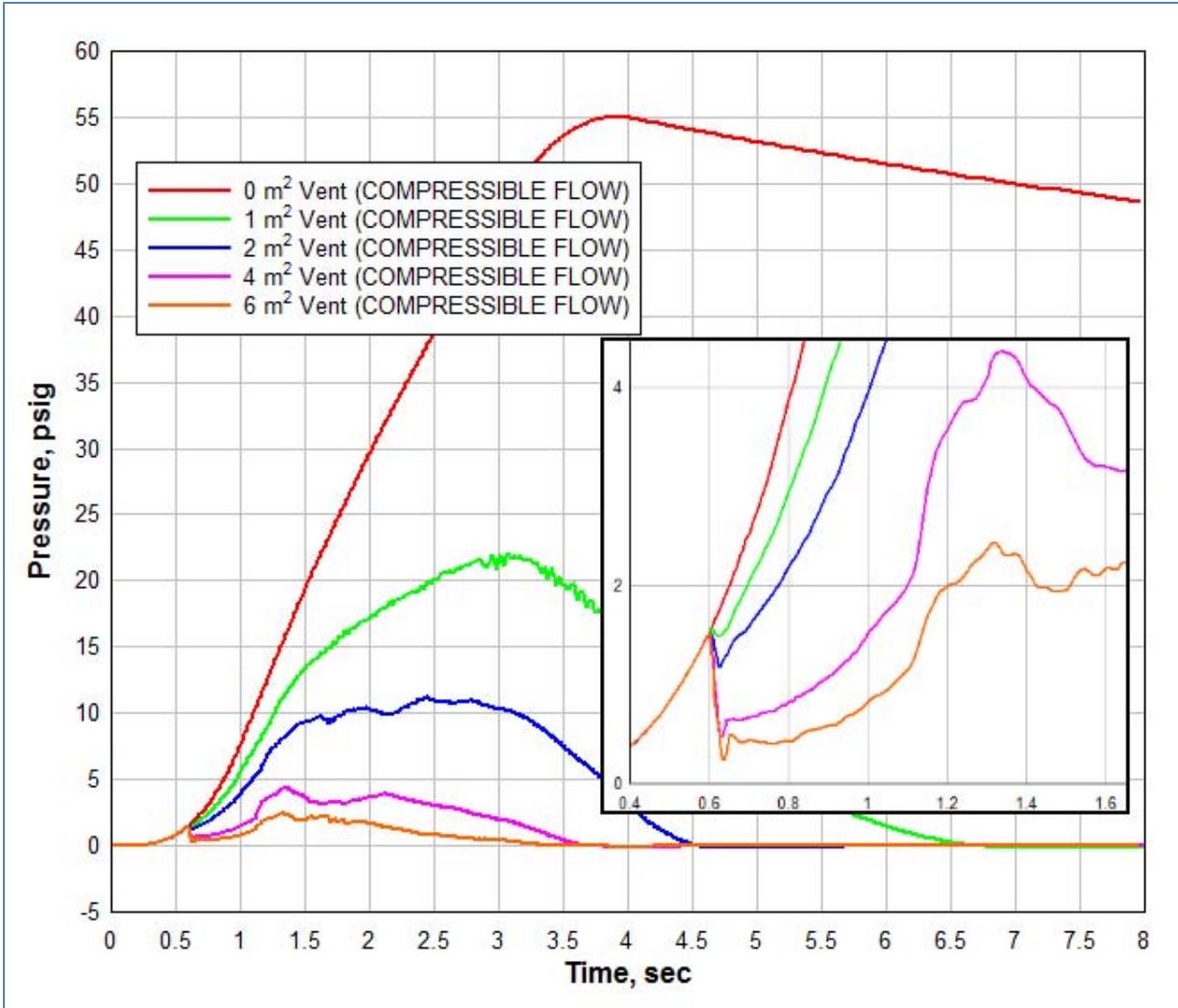


Figure 9. Cell Pressure for Various 1.5 psi Vent Areas

6.6 WATER SPRAY

The effect of including water spray is primarily to cool the environment thereby decreasing the pressure via the equation of state. The effects of water spray were modeled in a closed cell with approximately 1200 m³ volume. Cases for 1 SRM and 20 SRMs were modeled, both modeling a normal ignition. In both cases, water spray was shown to have little effect on the initial pressure and temperature in the room due to the time necessary to initiate the spray. After a few seconds, the water spray begins to cool the cell resulting in a decrease in overall peak pressure and temperature. After peak pressure has occurred and the SRMs have finished burning, water spray cooling has a significant effect on the rate of pressure and temperature decrease. Results for 1 SRM can be seen in Figure 10. Peak pressure decreased 10 percent with water spray. At 8 seconds the pressure decrease was 37 percent. Results for 20 SRMs can be seen in Figure 11. Peak pressure decreased 11 percent with water spray. At 8 seconds the pressure decrease was 18 percent.

The decrease in room temperature was higher for the high thermal loading case (20 SRMs, 46%) compared to the low thermal loading case (1 SRM, 37%). Since the low thermal loading case had the higher pressure decrease over time, this indicates that the phase change of water during cooling of the high thermal loading case may be responsible for offsetting the pressure reduction through the creation of additional moles of water vapor. Therefore, the effects of water spray on peak pressure were moderate and appear to increase with thermal loading; however, the pressure mitigation after burning was complete was higher for low thermal loading cases.

Water spray is expected to have a more significant effect for slow burn rate accidents. The same 1 SRM case as above was modeled with a soft ignition slow burn rate (78 second). As seen in Figure 12, the peak pressure was decreased 59 percent by the water spray compared to the no water spray case.

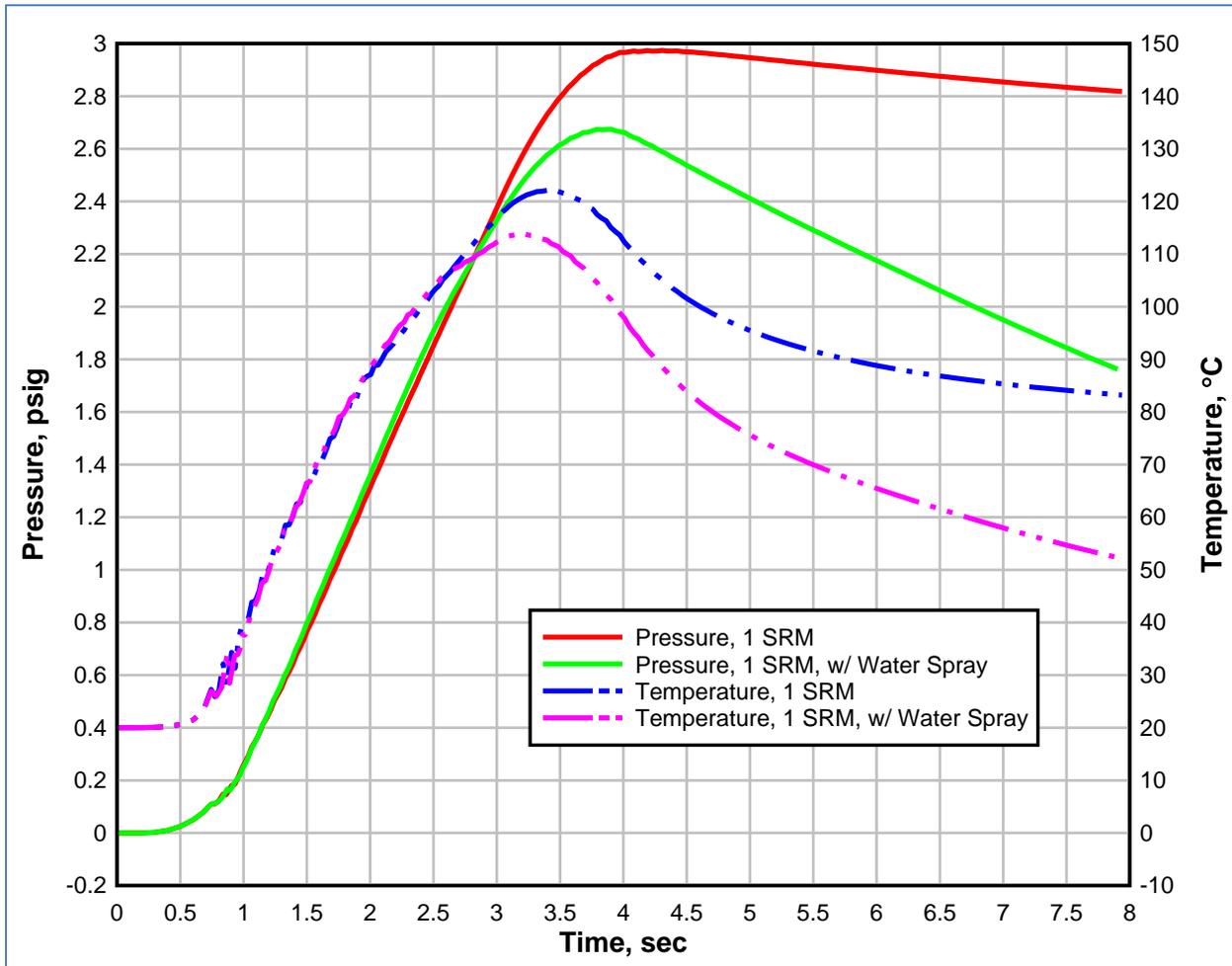


Figure 10. Cell Pressure and Temperature for 1 SRM with and without Water Spray

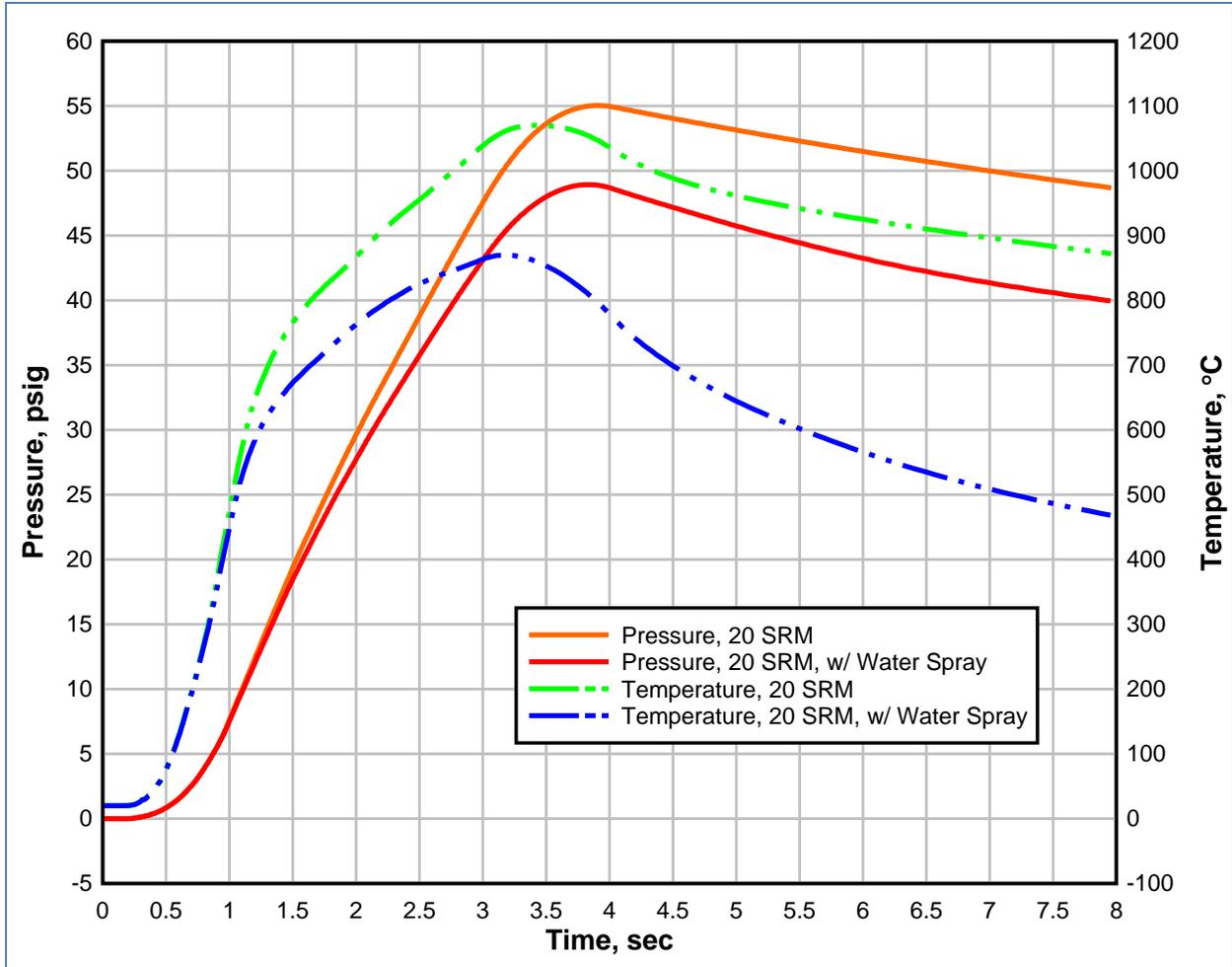


Figure 11. Cell Pressure and Temperature for 20 SRM with and without Water Spray

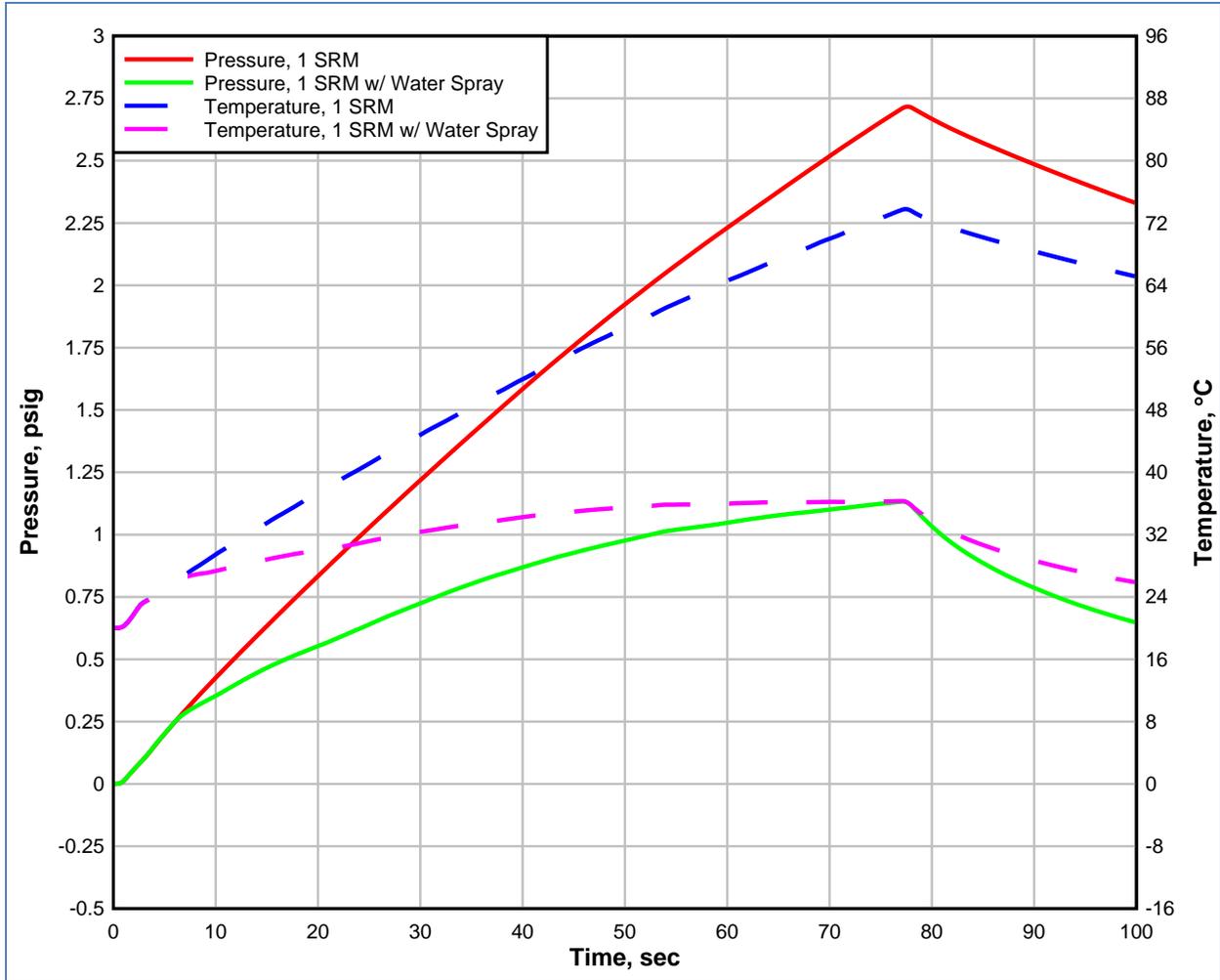


Figure 12. Cell Pressure and Temperature for 1 SRM (slow burn) with and without Water Spray

7 COMPARISONS

7.1 BLASTX

BlastX¹³ calculates the internal airblast loading for both shock and gas loading phases. Both high explosive and HD 1.3 propellants can be simulated. BlastX is not a computational fluid dynamics code, but rather an analytical model based on theory as well as empirical data. BlastX models a propellant by releasing energy into the room based on a user defined duration and propellant mixture, which defines the heat of combustion. While convection losses to the walls are accounted for, radiation losses are not included. Radiation losses become more important when significant energy release heats the room up to high temperatures. Also, the effect of sprinklers cannot be accounted for in BlastX.

¹³ BlastX, V6.4.2.2, US Army Engineer Research and Development Center.

BlastX considers each room as a single control volume. The energy added during a time step is uniformly distributed over the entire control volume, resulting in a uniform room temperature. Venting between rooms or to the outside is accomplished assuming steady isentropic flow through a perfect nozzle.

A limitation exists in BlastX concerning the definition of M28. M28 is composed of four primary components. The BlastX library only contains the first two, nitrocellulose and nitroglycerin. An approximate M28 formulation of 70% nitrocellulose and 30% nitroglycerin was used in BlastX. This results in a lower heat of combustion than the actual M28 formulation. The actual M28 heat of combustion was 94,334 kJ/SRM while the approximate M28 formulation used in BlastX was only 80,438 kJ/SRM, or 85 percent. While BlastX does not give the heat of combustion it uses as an output, one can infer from the change in room energy (which is a given output) what the heat of combustion was, approximately. For this to work, the convection calculations must be disabled by the use of a zero convection constant in the BlastX room inputs. For the approximate M28 formulation, the change in room energy was 75,555 kJ/SRM, which is close to the value calculated above. The difference may be due to incomplete burning of combustion products or slight differences in heats of formation for nitrocellulose and nitroglycerin. In order to compensate, the mass of explosive was increased to 10,926 g/SRM such that the energy per SRM in BlastX was equal to that used in FDS (94,334 kJ/SRM).

Comparisons between BlastX and FDS were made for two connected cells similar to Figure 3. Figure 13 shows peak pressure for a 1 m² vent area. There was no significant pressure difference between cells for any model. The BlastX peak pressure was approximately 1 psi higher after the first SRM and 1.75 psi higher after the second SRM burned out. The results between BlastX and FDS (without radiation) were closer, but BlastX still predicted higher pressures. If the mass of explosive is not increased as described above in BlastX, the peak pressure was found to be between the FDS results with and without radiation.

In order to compare the venting differences between BlastX and FDS, a small 0.25 m² vent area was modeled between rooms. As shown in Figure 14, BlastX predicted a higher peak pressure after the first SRM burns out, but both codes predicted similar pressure differentials between cells. The BlastX pressure rise time is lower than FDS since FDS includes a one second ramp up and down for the first SRM while BlastX burns the SRM linearly over the first three seconds.

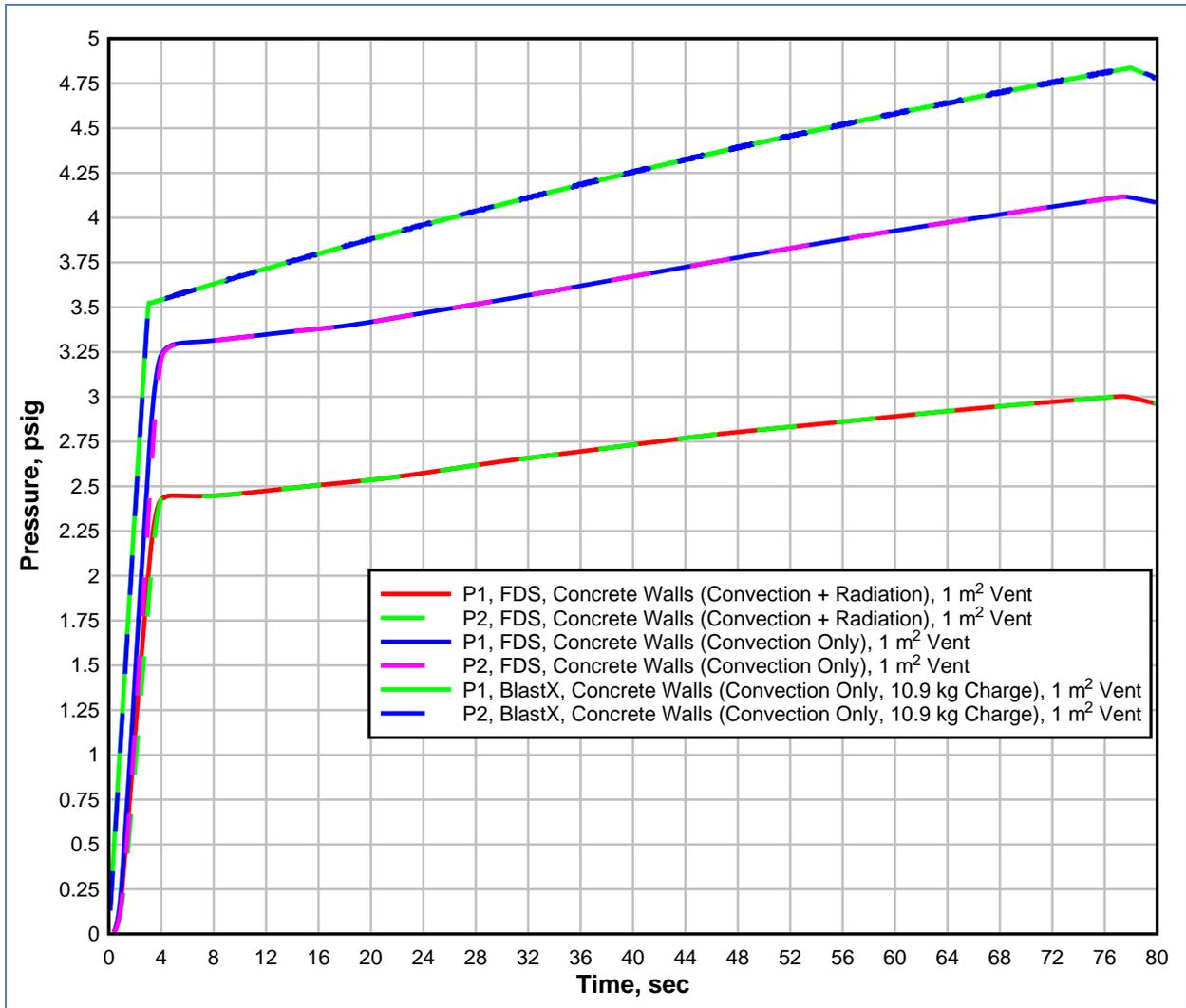


Figure 13. BlastX to FDS Comparison for 2 SRMs and 1 m² Vent Area

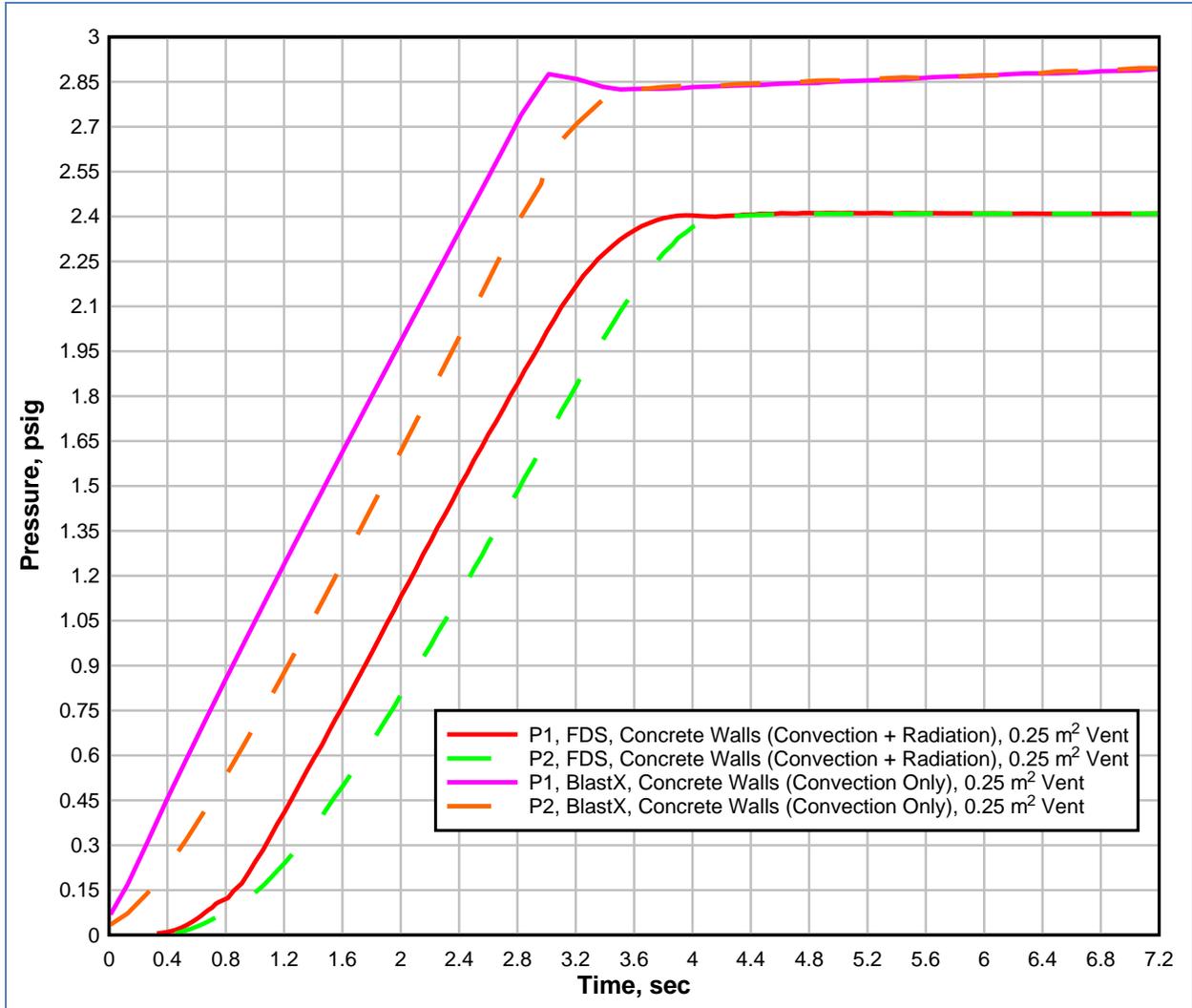


Figure 14. BlastX to FDS Comparison for 2 SRMs and 0.25 m² Vent Area

7.2 SPREADSHEET

The spreadsheet calculates the internal gas loading resulting from a HD 1.3 burning propellant. It considers each room as a single control volume. The energy added during a time step is uniformly distributed over the entire control volume, resulting in a uniform room temperature. Venting between rooms or to the outside is accomplished assuming steady isentropic flow through a perfect nozzle.

While similar to FDS and BlastX, the spreadsheet had some fundamental differences as described below in Table 8. For comparison purposes, a single room model (1200 m³) with venting to the atmosphere was modeled using FDS and the spreadsheet. The source term was 20 SRMs all with normal ignition. Figure 15 shows comparisons of peak pressure for no venting, 1 m², and 2 m² vent area cases. The spreadsheet overpredicted pressure partly due to the fact that the spreadsheet neglects convection heat transfer.

Table 8. Differences between Spreadsheet, FDS, and BlastX

Feature	Spreadsheet	BlastX	FDS
Convection Heat Transfer	No	Yes	Yes
Radiation Heat Transfer	Yes	No	Yes
Time dependent Venting	Yes	No	Yes

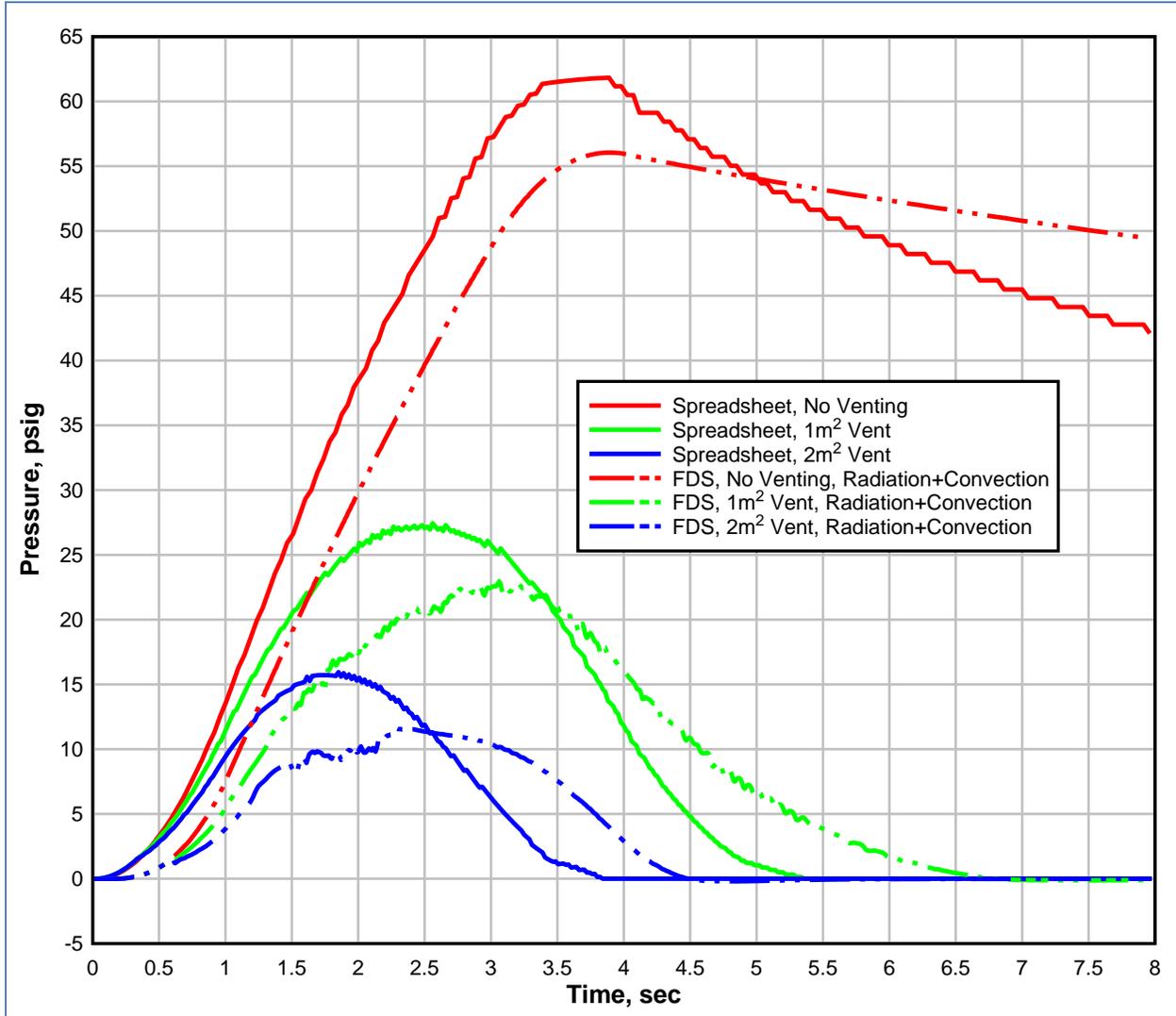


Figure 15. Comparison between FDS and Spreadsheet

8 CONCLUSIONS

The use of CFD for time dependent burning of HD 1.3 material represents an improvement over previous spreadsheet models. CFD includes the ability to model pressure and time dependent vents, all heat transfer modes, and water spray mitigation. Further, it has been used successfully in the design of a chemical weapons demilitarization facility vent analysis that was subsequently approved by DDESB.

The methodology is applicable to propellant burning only and does not address conditions that can cause transition from burning to more severe explosion or due to shock initiations.

Utilizing CFD for Prediction of HD1.3 Pressure Loads in a Cell with Venting

Author: Greg Knight

Presented by: Mark Whitney

Presentation Overview

- Problem Defined
- Caveats
- Current Practices
 - Benefits & Limitations
- Proposed Methodology
 - CFD Code FDS
 - Source Term
 - Examples of Use
- Comparison to BlastX and Spreadsheet Methods
- Conclusions

Caveats

- Methodology proposed applies to
 - Propellant burning in rooms with vent panels
 - Scenarios where propellant burning generates only gas loading
 - Scenarios where burning takes place in seconds not milliseconds
 - Scenarios where the burn rate is known
- The methodology does not address conditions such as
 - Transition from burning to more severe explosions
 - Shock initiations that cause detonations

Problem Defined

- HD 1.1 Gas Loading
 - Peak reached in milliseconds
 - Venting
 - Insufficient time to affect peak gas (except for very large vent areas)
 - Can affect duration
 - Peak is function of W and V
- HD 1.3 Gas Loading
 - Pressure rise dependant on burn rate
 - Venting affects peak pressure
 - Burn rate is critical

Current Practices

- Technical guidance for HD 1.3 not as in-depth as for HD 1.1
- *HNDED-CS-93-7 - HD 1.3 Passive Structural Systems Design Guide*
 - All HD 1.3 in room summed and converted to TNT
 - 1.2 Safety Factor Applied
 - TNT Gas Load Curves
 - Allows for alternative methods
- Alternate Methods we have used
 - Spreadsheet methods (presented at DDESB 2006)
 - BlastX
 - CFD

Benefits/Limitations of Spreadsheet and BlastX

- Both model rooms as a single control volume
 - uniform pressure and temperature
- Both have incomplete heat transfer modes
 - Spreadsheet currently includes radiation but not convection
 - BlastX includes convection but not radiation
 - *(Note: CFD shows that radiation important at high temps and convection important for long durations)*
- Spreadsheet models failing vents, including inertia effects
- BlastX can only model constant vents (no failing vents)
- Neither models effects of water sprays

FDS (Fire Dynamics Simulator) by NIST

- FDS

- Developed for the simulation of fires
- Evolved into a useful general purpose CFD code
- General fluid flow and heat transfer capabilities

- Benefits of FDS

- Fast running; 10's of minutes to hours instead of days
- Good documentation and examples
- Open source with a large community of users
- Low computing requirements, but parallel capable

FDS Limitations

- FDS makes a “low mach number assumption”
 - Cannot handle high speed flows including compressibility effects and shock waves
 - Great deal to do with FDS’s fast run times
- FDS is more suitable for burn rates in seconds than milliseconds

FDS Assets

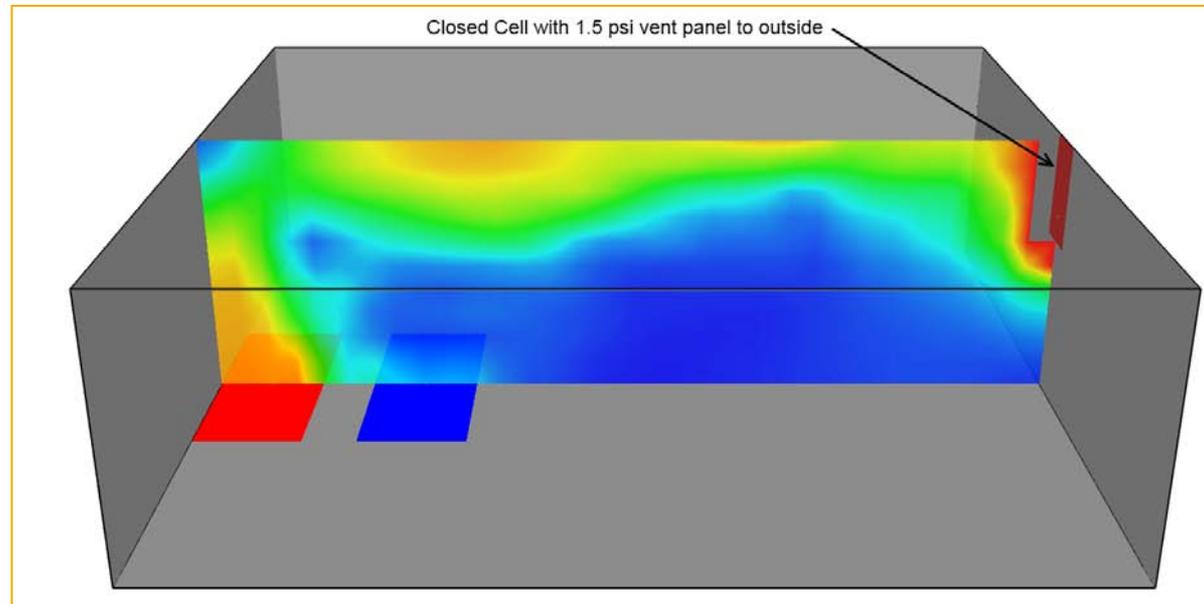
- FDS can model each room and vents between rooms
 - Vents can open on pressure or any other criteria
 - Overall vent area can be time dependent by opening additional vents over time
 - Vents open instantaneously; no direct capability for translating vents which gradually open
 - Venting is via an incompressible flow submodel; ABS has recompiled FDS with a compressible version that will be submitted to NIST for inclusion in FDS
- FDS can include water spray activated on temperature or any other criteria

FDS Methodology - Source Term

- HD 1.3 burning is a complex, so instead of modeling pyrolysis and combustion, we model only the reaction products as a source term
- Hand calculations used to define source term
 - Includes initial combustion of fuel and oxidizer and combustion of intermediate products with air (if any)
 - Heat of combustion is determined either from the literature or through the use of heats of formation ($\Delta H_c = \sum H_{f_{\text{reactants}}} - \sum H_{f_{\text{products}}}$)
- Source Term
 - Hot products are injected into the domain while after-burning reactants (O₂/N₂) are removed (if any)
 - Injection rate is based on the burn rate of the propellant
 - Temperature of products is based on matching heat flow (FDS variable) to the heat of combustion

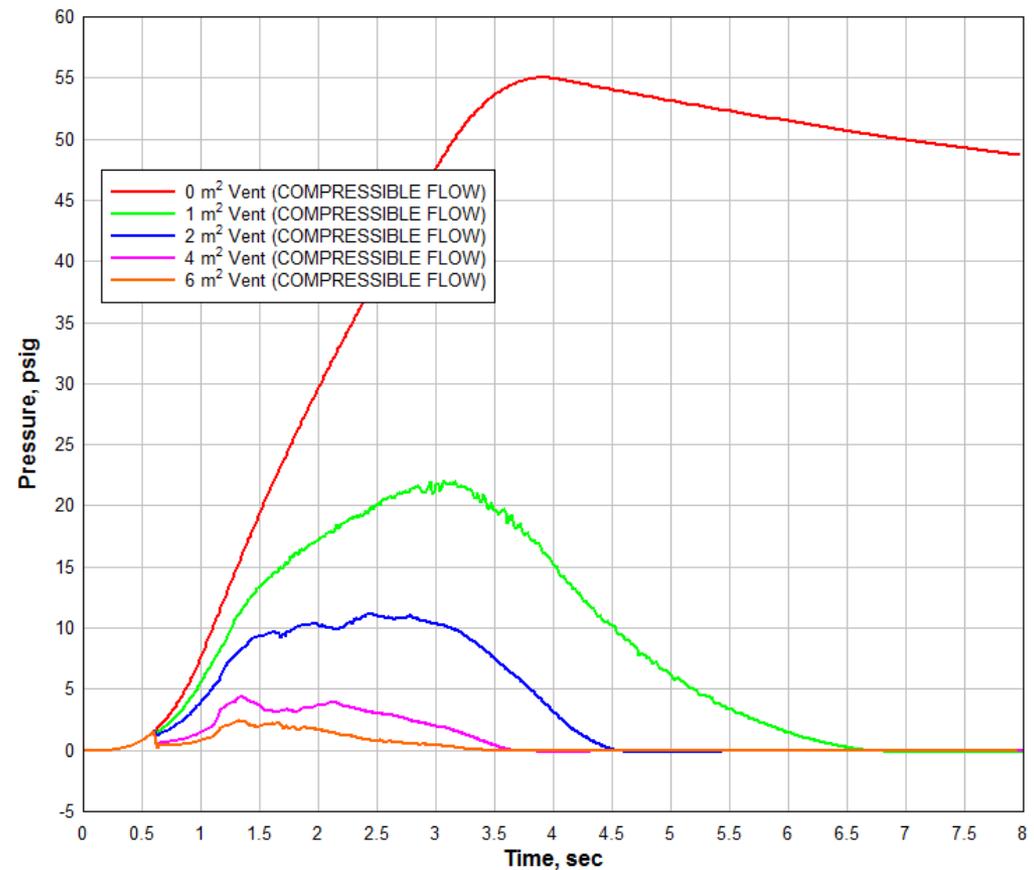
FDS – Example 1

- Storage room with box of 20 rocket motors
- Scenario has all burning in 3 seconds
- Storage room has vents to outside
 - Vent does not open (stay closed)
 - Vent opens at 1.5 psi – vent area varied



FDS – Example 1

- No venting
 - Peak pressure is 55 psi
- With vent area
 - Peak drops with vent area
 - All overshoot vent release pressure
 - At 6 m² peak pressure ~ 2 psi



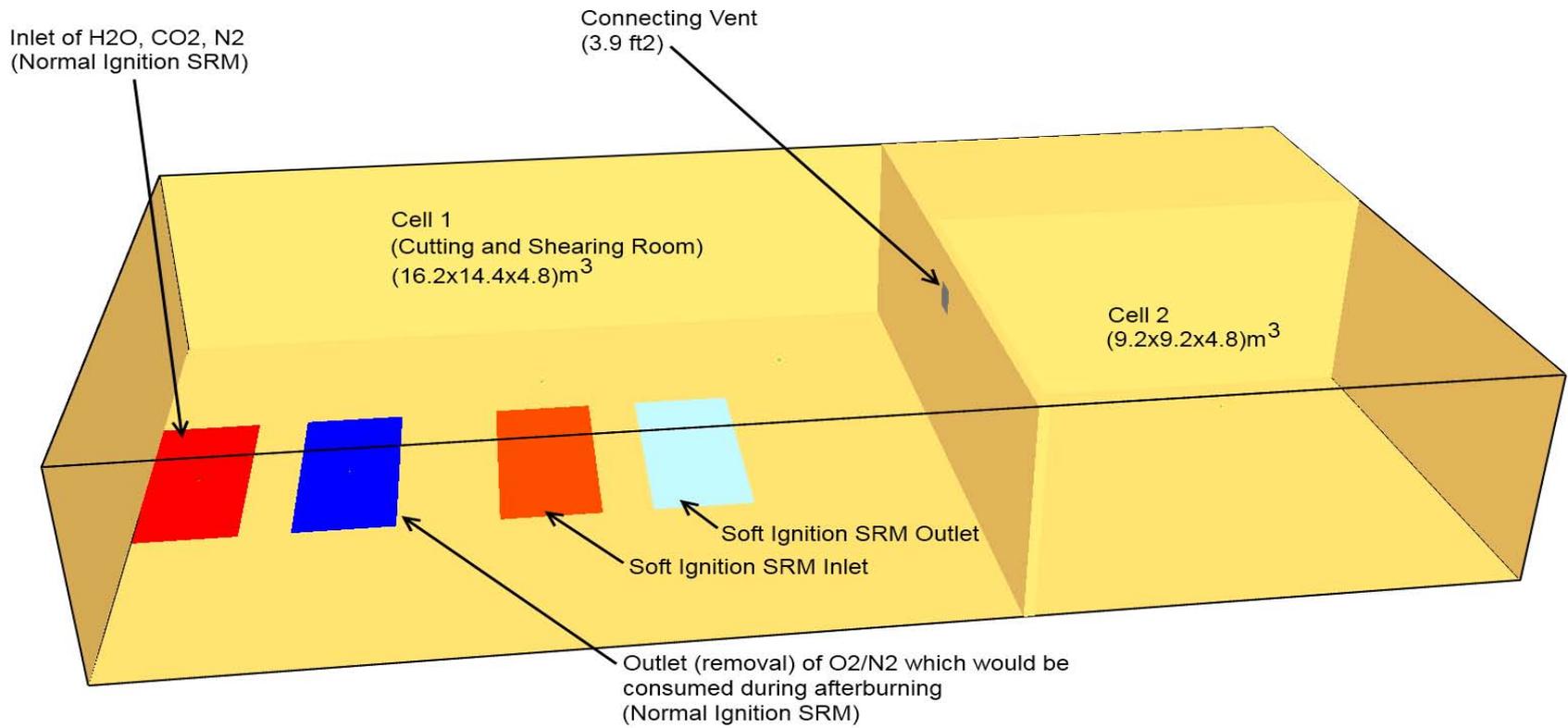
Examples of Use – Example 2

- Demilitarization of chemical weapons, M55 rockets containing M28 propellant grains (8.7 kg) are cut and sheared in an automated, multi-room process
- Two solid rocket motors (SRMs) are present in the cutting room; a small pass-through vent connects the cutting room to another room
- Scenario involves the burning of two SRMs defined as:
 - One with a fast burn rate (3 seconds)
 - The second with a slow burn rate (78 seconds)

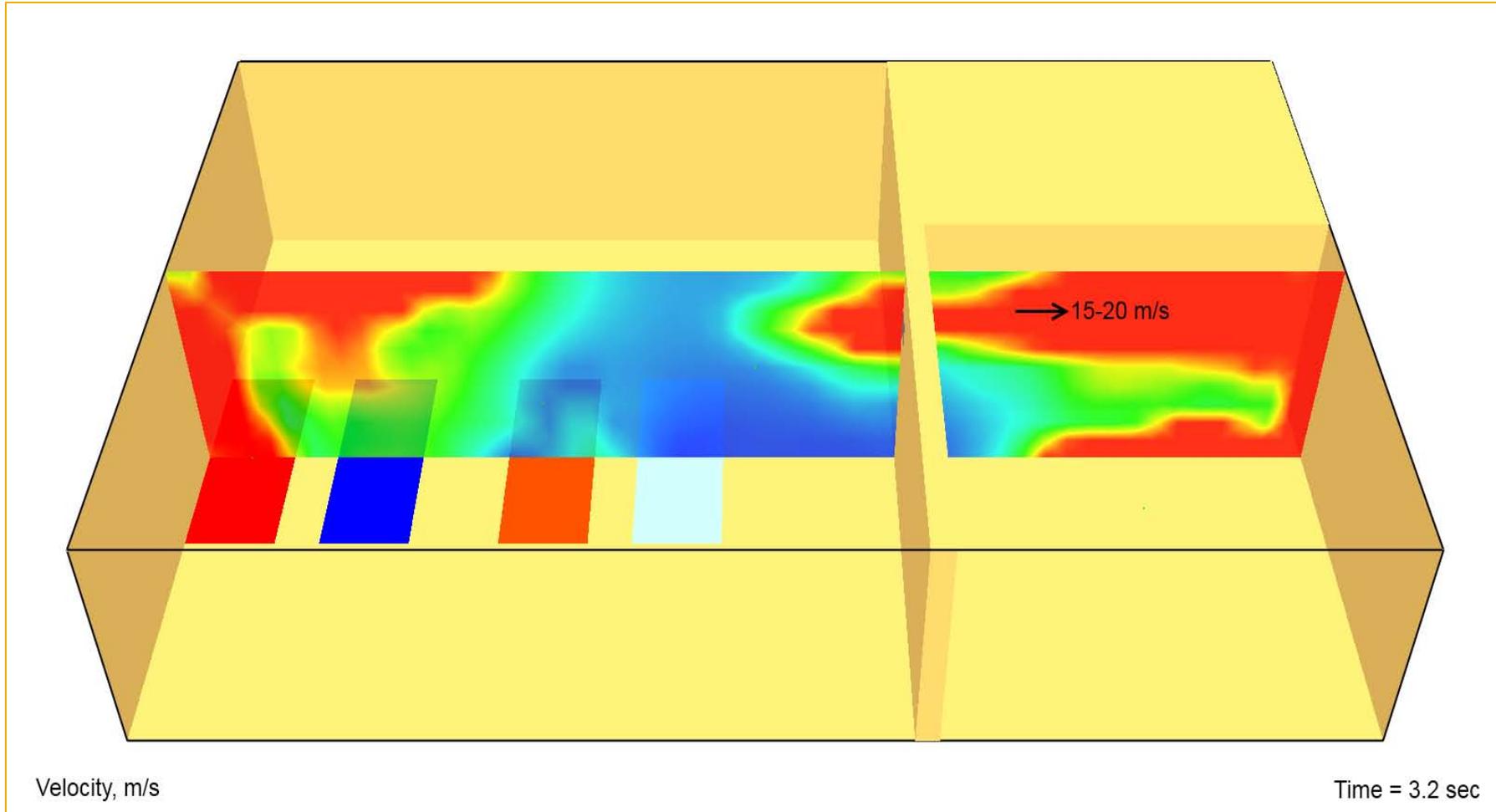
FDS – Example 2

FDS model includes two rooms, vent, and source term inlets

Smokeview 5.5.6 – Jun 22 2010

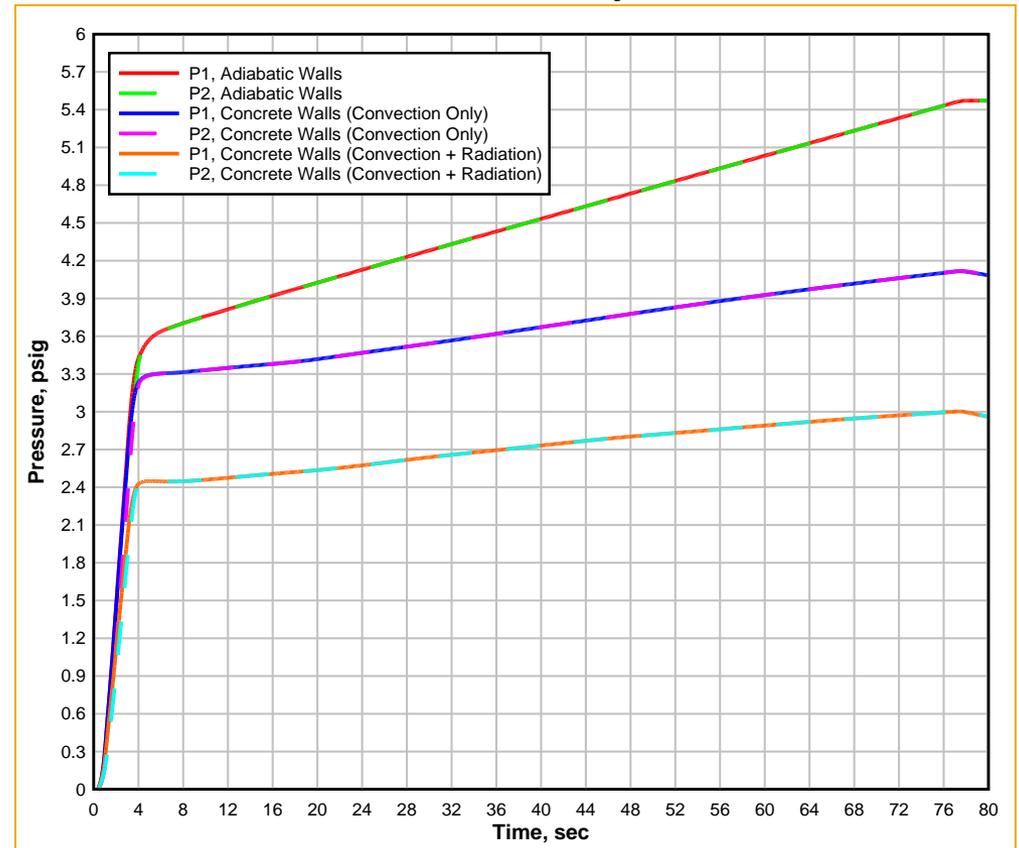


FDS – Example 2



FDS – Example 2

- Boundary conditions and heat transfer modes matter
- Initial pressure slope due to SRM #1 followed by SRM#2
- Adiabatic walls gives maximum pressure
- Concrete walls with convection and radiation results in peak pressure of 3 psi
- Venting allowed essentially same pressure in both room after SRM#1 burnout



FDS – Mitigation Example

- Water spray cools the room, which decreases the pressure via the equation of state $pV=nRT$
- Water spray has the greatest effect on low burn rates and less of an influence on high burn rates
- The paper includes examples for fast and slow burn rates
 - Fast burn - peak pressure reduced 13 %
 - Slow burn – peak pressure reduced 59%

Comparison to BlastX and Spreadsheet Methods

- The paper includes a discussion on how FDS compares with BlastX and the early Spreadsheet Method
 - FDS with/without convection and radiation
 - With and without vents
 - Venting between rooms
- Similar results with comparing apples to apples (i.e., FDS with convection and/or radiation turned off)
- FDS with convection and radiation on – always resulted in lower peak pressure

Conclusions

- CFD has many advantages over simplified methods for HD 1.3 burning modeling in enclosed environments including:
 - Ability to model local flow effects and temperature gradients (personnel hazards)
 - Time dependent venting between rooms and to outside
 - All heat transfer modes included in the model
 - Ability to model water spray mitigation
- DDESB has accepted an ABS Consulting CFD analysis for HD 1.3 modeling in a chemical weapons demilitarization facility