Integrated Violence Model of 1.3 Events with Example Test Results

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ABSTRACT

The Integrated Violence Model (IVM) has been successfully used to determine the necessary vent area to prevent damage to process equipment and building structures from excessive pressure during deflagration events. It has also been used to determine the potential effects (fragmentation and overpressure) from a lack of sufficient venting that can result in an explosion. Accidental ignitions of 1.3 substances like propellants can transition from a deflagration to an explosion if the gases generated by the substance are not properly vented. This paper provides an overview of the Integrated Violence Model that is specific to 1.3 materials. Application of the Integrated Violence Model to the test scenarios outlined in NAWCWD TM 8742 is highlighted showing the relationship for predicted structural failure between vent area ratio and the loading density for the tested conditions as well as multiple other conditions. The model predictions of structural failure and internal pressures agree with the experimental results.

INTRODUCTION

Burning or 1.3 type reactions are characterized by a non-instantaneous consumption of the substance such that the substance reacts and gives off heat and or gas. If that heated gas is produced in a sufficient quantity and is not vented properly the confining medium will yield and potentially explode. The confining medium may be the processing equipment or the building in which the substance is located. Ideally, the amount of substance allowed in the processing equipment or building structure and the associated venting conditions necessary to prevent an explosion would be determined experimentally; however, completing such a large amount of experimental test is cost and time prohibitive. Modeling based on small-scale testing is an effective way to obtain accurate estimates of the necessary vent area to prevent an explosion of a small or large structure containing 1.3-type substances.

There are multiple different methods to complete modeling of the pressurization of a structure based on critical parameters including gas generation rate of the reacting substance, size and location of vent areas, vent panel mass, vent opening pressure, internal volume, and strength of the structure. The modeling scale can range from including the molecular interactions and reactions (e.g. molecular dynamics), to the treatment of collections of molecules in defined volumes interacting with each other (e.g. computational fluid dynamics), and to the treatment of larger areas of gases (e.g. ballistics-type codes including the Integrated Violence Model). Unfortunately, the time to complete modeling evaluations at smaller and smaller sizes increases exponentially. The modeling methodology selected should be the one that yields the most accurate result with the least number of parameters. The accuracy of the model is evaluated on whether or not the model can predict pressures and impulses that correspond to those observed experimentally. The Integrated Violence Model has been accurate in matching small-scale experimental results and in accurately predicting large-scale experimental results. An example application of the Integrated Violence Model to the test scenarios outlined in NAWCWD TM 8742 (Farmer, 2015) is highlighted below.

2 BACKGROUND

The Integrated Violence Model (IVM) provides conservative time-pressure curves for deflagration events inside small and large equipment or structures. The pressure-time curves are found from explicit integration of the propellant burn (including the pressure dependence) as well as afterburn effects. IVM has been used to accurately estimate the internal pressure and associated outcome for burning/deflagrating substances including the following scenarios where the model outcome matched experimental results:

- The internal pressure and associated pressure rate-of-rise for propellant burning inside a heated steel tube. Velocities of the associated low-speed fragments were also matched (Butcher 2011).
- The internal pressure of a large chamber into which an MLRS rocket motor was fired. Prior to completing the experiment, IVM conservatively predicted the results within 10% of that observed experimentally.
- The required vent sizing for a dust cloud explosion versus the calculation scheme presented in NFPA 68, Eq. 8.2.2 (NFPA 2013). IVM predicts a slightly larger vent size is required for a given condition.
- The violence outcome (internal pressure and whether or not the structure fails) of 3 or 8 drums of M1 propellant in a concrete structure with varying vent areas as referenced in A. Farmer, K. Ford, J. Covino, T. Boggs, A. Atwood, "Combustion of Hazard Division 1.3 M1 Gun Propellant," Naval Air Warfare Center Weapons Division, August 2015. Modeling approach and purely predictive results highlighted below.

2 IVM MATHEMATICAL FORMULATION

IVM is based on thermodynamics principles with gas flows into and out of the internal void volume of the structure. Additional volumes can be included to more accurately represent systems with more tortuous flow patterns between volumes. A limited amount of parameters are used in the model: structure volume, gas generation rate from the reacting substance, gas temperature, bulk density of the substance, burn rate pressure exponent, fraction of gases produced that are combustible, vent areas, vent geometries and masses with burst pressures, combustion gas compositions, after-burn rate and heat of combustion, ratio of product moles to reactant moles for afterburning, and the mass of the substance reacting. The parameter values are determined from small-scale testing or from literature values. Gases are treated as ideal with immediate thermal and pressure equilibrium with the venting of the gases per the choked and unchoked flow in Perry's Chemical Engineering Handbook (Perry, 1997). Calculation of the Mach number of the exiting gases is included and effects of a choked or unchoked flow condition are included in the model. Governing equations are given below.

$$\frac{dnU}{dt} = \dot{n}H_{in} - \dot{n}H_{out} + q_{gen} \tag{1}$$

$$\frac{dn}{dt} = \dot{n}_{in} - \dot{n}_{out} \tag{2}$$

where t is time, n moles, U the internal energy, H enthalpy, and q heat. The dot used above the n in the mass balance represents a rate. q_{gen} accounts for afterburning of the unburned carbon monoxide and hydrogen that mixes with the oxygen in the air inside the structure as given below.

$$q_{gen} = k_a \cdot P_{CO} \cdot P_{O2} \cdot H_{comb} \tag{3}$$

where k_a is the afterburn constant (units of mol per second per pressure squared) and P_{CO} is the partial pressure of the reactant gases (like CO) and P_{O2} is the partial pressure of the oxidizing gases (like oxygen) H_{comb} is the combustion heat of reacting gases (CO) afterburning with the O_2 in the air inside the chamber.

The energy balance above was simplified to

$$\frac{nR}{(\gamma-1)} \cdot \frac{dT}{dt} = \dot{n}_{in} \cdot (H_{in} - H + RT) - \dot{n}_{out}[RT] + q_{gen} \tag{4}$$

where *gamma* is the heat capacity ratio inside the control volume (which is a function of the temperature and composition of the gases), R is the gas constant, T is the temperature of the gases, H is enthalpy. The moles of gas coming in is

$$\dot{n}_{in} = -g_{gen} \frac{dm_s}{dt} \tag{5}$$

where g_{gen} is the moles of gas generated per mass of propellant and

$$\frac{dm_s}{dt} = -k \left(\frac{P}{P_{ref}}\right)^{\alpha} \tag{6}$$

where k is the atmospheric burn rate of the propellant, P is the control volume pressure, alpha is the pressure exponent, and ref indicates the reference or atmospheric pressure.

Typically, 4 gases are tracked as a function of time through the simulation: inert gases (modeled as CO2), reactive gases (modeled as CO), oxidizing gases (modeled as O2), and water vapor. The heat capacity and enthalpy of the gases are explicitly modeled throughout the simulation and are a function of temperature. Time dependent equations are explicitly solved using the Velocity Verlet algorithm and the Taylor Series Expansion to the second order.

4 IVM SETUP AND RESULTS

IVM was applied to the structure (volume) and conditions (propellant type, mass, and vent area) used in the NAWCWD TM 8742 testing. IVM parameters were not determined from the test results but from literature values of approximate burn rates of the M1 propellant (Walsh 2012). Thus, the model results presented here are predictive in that the modeling results could have been entirely obtained prior to the testing.

The conditions of the testing are outlined in the below table, where each drum was ignited inside the 2m x 2m x 2m Kasun reinforced concrete structure. Two difference propellant types were tested. The model differentiated burning rates between the two types purely on the surface area. The vent was an uncovered circular orifice in the center of one of the four walls. Further details of the test setup are not included here and readers are referred to the publicly available TM 8742 technical report for additional information.

Table 1: Experimental Setup in 2m x 2m x 2m Kasun Reinforced Concrete Structure

Test	M1 Propellant	Mass, lb	Drums	Vent Diameter, cm
1	Single Perforation	296	3	79
2	Single Perforation	1176	8	39
3	Multiple (7) Perforation	264	3	79
4	Multiple (7) Perforation	1108	8	39

Based on the literature for M1 Propellant (Walsh 2012) the burn rate used in the model was calculated to be 3.8 kg/s and 0.76 kg/s per drum for the single and multi-perforation propellant, respectively. Additional parameters for the IVM model were estimated to be 0.7 for the burn rate pressure exponent with a gas generation per kilogram of propellant of 39 moles which are typical for smokeless powder. Combustion gas temperatures were estimated at 2400 K with a fraction of combustion gases that can participate in afterburning to be 0.3 based on an estimate for M1 propellant from a thermochemical calculation program (Cheetah). Afterburning was included with the oxygen initially present in the structure with a heat of combustion of 285 kJ/mol CO.

The pressure inside the structure as a function of time was found using IVM for each test condition as described above. The pressure as a function of time for Test 4 is shown below in Figure 1. Although not reproduced here, the experimental internal pressure for Test 4 was similar in that the maximum pressure was 34 psi and the time to reach that pressure was approximately 1 second.

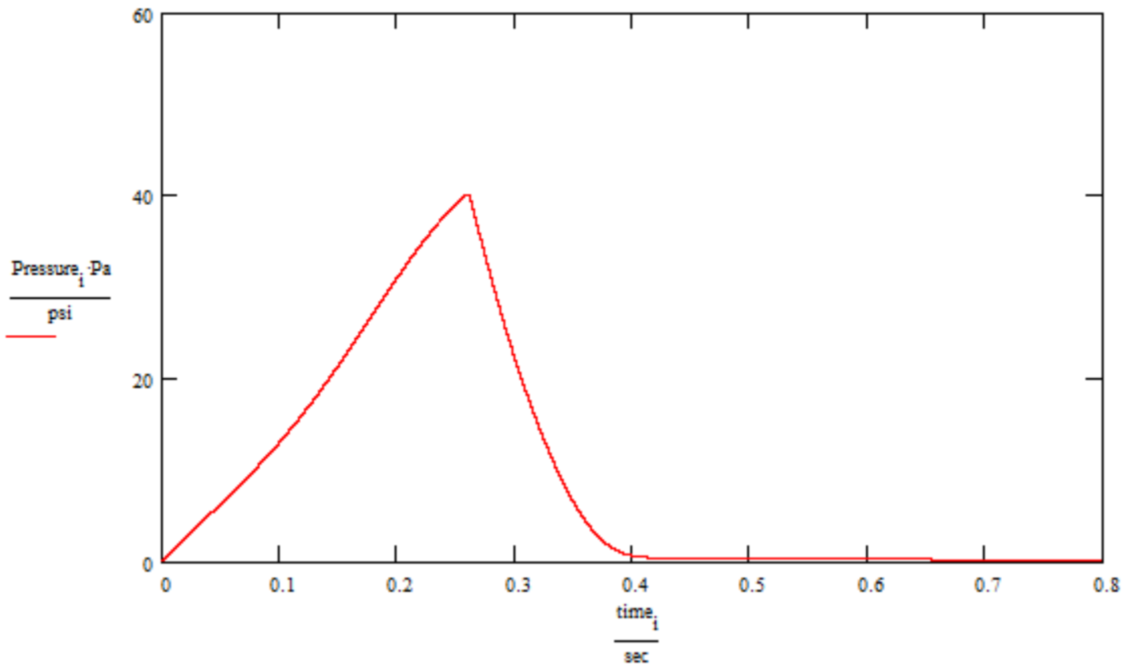

Figure 1: IVM prediction of the pressure (psi) as a function of time (seconds) inside the structure for Test 4. Although not reproduced here, the experimental internal pressure for Test 4 was similar in that the maximum pressure was 34 psi and the time to reach that pressure was approximately 1 second.

Note that the IVM pressure reaches a maximum at 40 psi as this is the pressure at which a reinforced concrete structure is expected to fail given the pressure impulse has reached 2 psi-sec as reported by Wheaton et al. in ATLSS Report No 05-08 (Wheaton 2005). This is the condition (40 psi pressure and 2 psi-sec impulse) used by IVM to determine if the structure fails. Thus, it was predicted that the structure would fail in Test 4 which is what happened experimentally.

Shown below in Table 2 are the IVM predictions and the experimental results. The agreement between model and experiment is very good in that the violence outcome agree exactly, the maximum internal pressures are within 5 psi or 18% (whichever is greater).

Table 2: Model and Experimental Results Compared

	Violence Outcome		Max Pressure, psig		Impulse, psi-s	
Trial	Model	Experiment	Model	Experiment	Model	Experiment
1	Burn	Burn	7.4	<2	-	-
2	Explosion	Explosion	54	47	2	5
3	Burn	Burn	0.34	<2	-	-
4	Explosion	Explosion	40	34	7.2	5

Although not discussed here, IVM can be used to estimate the distance fragments from the structure may be thrown given a fragment size distribution. This is based on the gas pressure and volume as the structural fragments are accelerated away from the structure by the decreasing gas pressure.

Additional IVM results were predicted for different vent area ratios (ratio of the vent area to the volume to the 2/3 power) and loading densities (mass of the reacting substance to the structure volume) for the Kasun structure used in the TM 8742 testing. This relationship has been used to relate the point at which a structural failure could result by other scientists and engineers. Below is a plot of the IVM prediction of the vent area ratio and loading density for the single perforation M1 propellant in a Kasun structure indicating at which conditions a structural failure can be expected. Also indicated on the plot are the Test 1 and 2 conditions and results.

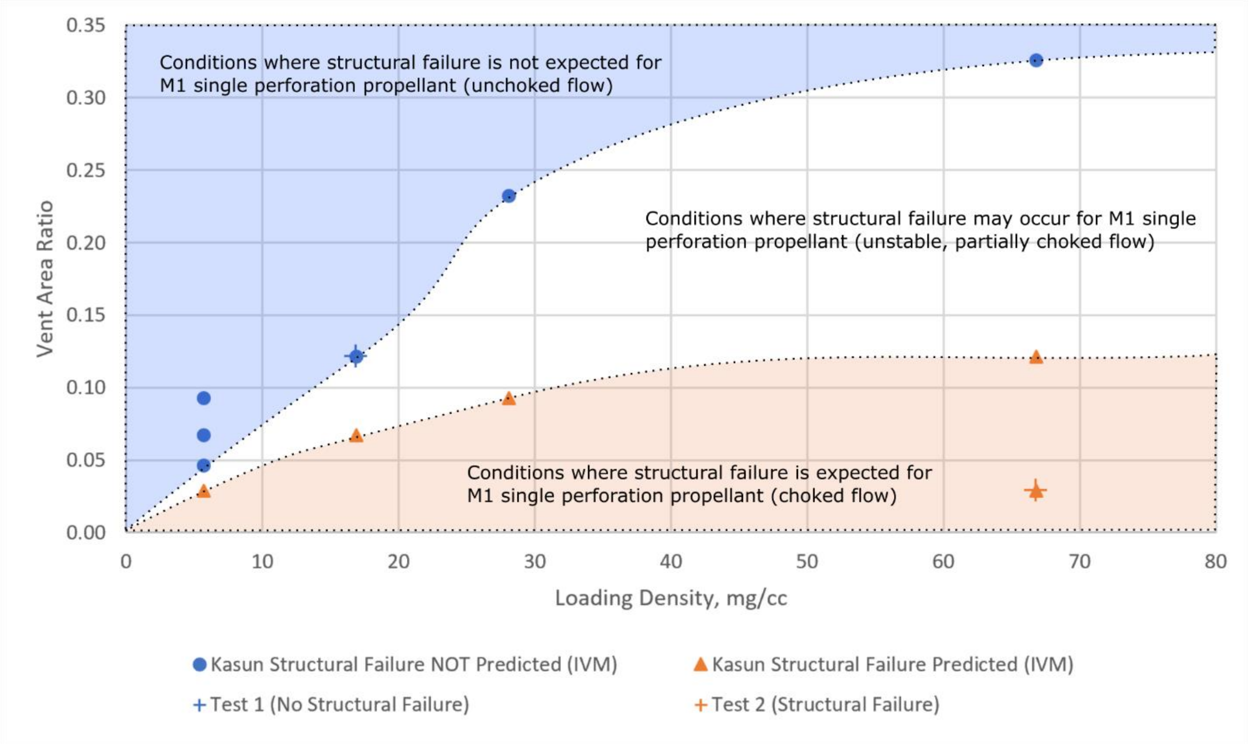

Figure 2: IVM prediction of the vent area ratio and loading density for the single perforation M1 propellant in a Kasun structure indicating at which conditions a structural failure can be expected. Also indicated on the plot are the Test 1 and 2 conditions and results.

5 CONCLUSION

The Integrated Violence Model, with relatively few parameters, can be used to accurately predict necessary vent areas to prevent internal pressures from reaching a dangerous condition should ignition of a reacting substance occur. IVM has been used successfully in multiple scenarios and has recently been applied to the testing of a concrete structure with burning M1 propellant to accurately predict the outcome regarding structural failure and internal pressures. The Integrated Violence Model is not a one-size-fits-all method and requires literature values of critical parameters or small-scale testing results. It can be used in concert with other methodologies for safely handling, processing, and storing reactive substances.

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