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Analysis of a Full Scale Blowdown Due to a Mechanical Failure of a Pressure Relief Device in a Natural Gas Vehicle Maintenance Facility

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Abstract

A computational fluid dynamics (CFD) analysis of a natural gas vehicle experiencing a mechanical failure of a pressure relief device on a full CNG cylinder was completed to determine the resulting amount and location of flammable gas. The resulting overpressure if it were to ignite was also calculated. This study completes what is discussed in Ekoto et al. [1] which covers other related leak scenarios. We are not determining whether or not this is a credible release, rather just showing the result of a possible worst case scenario.

The Sandia National Laboratories computational tool Netflow was used to calculate the leak velocity and temperature. The in-house CFD code Fuego was used to determine the flow of the leak into the maintenance garage. A maximum flammable mass of 35 kg collected along the roof of the garage. This would result in an overpressure that could do considerable damage if it were to ignite at the time of this maximum volume.

It is up to the code committees to decide whether this would be a credible leak, but if it were, there should be preventions to keep the flammable mass from igniting.

Keywords: Natural Gas Vehicle Maintenance Facility, Pressure Relief Device Failure, CFD

ACKNOWLEDGMENTS

The authors would like to thank Bill Houf (SNL-Retired) for his assistance with setting up and post-processing of the numerical simulations. We would also like to thank DOE’s Clean Vehicle Education Foundation and Vehicle Technologies Office Clean Cities program for funding this research.

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NOMENCLATURE

CFD	Computational Fluid Dynamics
CNG	Compressed Natural Gas
DOE	Department of Energy
EOS	Equation of State
HAZOP	Hazardous and Operability Study
LNG	Liquid Natural Gas
PRD	Pressure Relief Device
SNL	Sandia National Laboratories

1. INTRODUCTION

Sandia National Labs is using a leak calculation tool coupled with computational fluid dynamics (CFD) to model leak scenarios in a maintenance garage to help the codes and standards community understand the consequences and outcomes of these leaks. In this report we describe the “worst case scenario” of a complete venting of a CNG cylinder due to a faulty pressure relief device (PRD). This can then be compared to more likely but less severe cases.

As previously reported in [1], three leak scenarios were identified by a HAZOP study to be simulated using computation fluid dynamics to gain a better understanding of the conditions in a maintenance garage during the leaks. The first two, a dormant LNG blow-off and a crack in a CNG or LNG fuel system line, went smoothly and the results in the previous report are complete. However, for the third scenario, a mechanical failure of a thermally activated pressure relief device (PRD), there were some problems. The boundary conditions for the leak went into a low temperature regime where there was a previously undiscovered error in the software. The first two scenarios did not reach this temperature, so there is no issue with the results. In re-examining the case in more detail, the error was found and corrected. We present the differences in the leak conditions after the correction as well as the new CFD results that incorporate the corrections.

The maintenance garage is of typical size, has a pitched roof with cross beams, and ventilation system. This case involves the complete venting, or blowdown, of a cylinder that is 150% of the size of the maximum cylinders used on vehicles. We are not addressing the question of whether this is a likely scenario, and in fact with new safeguards there are reason to believe that it that it might not be, as discussed in SAND2014-2342 [1]. It is presented here for completeness of that report as a worst-case hazard used by code development committees.

2. METHOD

2.1 Mechanical Failure of a Thermally Activated PRD

In the event a CNG cylinder becomes engulfed in a flame, the onboard storage cylinders are protected against excessive pressure buildup by a thermally triggered PRD, designed to fully open without the possibility of reseating in the event of activation. Accordingly, inadvertent actuation due to some mechanical failure would result in a rapid and uncontrollable decompression of all cylinder contents. Advances such as the use of dual activated valves have been implemented to reduce the likelihood of unintended release, although there remains some nominal risk. The Standards Development Organizations view such a release as a bounding event for hazard potential. For this scenario, the entire contents of a 700 L, fully pressurized (250 bar) CNG cylinder at room temperature (294 K) was released into the NGV maintenance facility. The specified release point was identical to the LNG blow-off scenario [1], which is located at the top of the vehicle. The PRD orifice diameter was set to 6.2 mm (0.24”) based on the flow rate specifications of typical commercially available PRDs. At the start of the release, the valve was assumed to immediately transition to a fully open position and remain that way for the duration of the release. While keeping the mass flow rate consistent, the initial leak area was increased to10 cm^2 (1.55 in^2) due to the gridding constraints, and Netflow was used to model the transient blow-down. In the initial report [1] accurate results for this scenario were hampered by a mistake in the Netflow code (described in detail below). That mistake has been corrected for this report.

2.2 PRD Leak Calculation

Netflow is a network flow simulator developed by Sandia. It was originally developed to model low speed airflows and contaminant transport in buildings. It has since been adapted to model high Mach number fully compressible transonic flows in piping networks [2]. A typographical error was found in the thermal conductivity value for methane in Netflow [2, 3]. At standard temperature and pressure methane has a thermal conductivity of 3.5e-2 W/m-k. The value used in Netflow was three orders of magnitude smaller which caused the heat transfer coefficient between the gas and the tank wall to be three orders of magnitude too small. The Netflow analysis was rerun with the corrected thermal conductivity using the ideal gas equation of state (EOS). Once a correct velocity and temperature profile of the leak was established, the entire leak scenario simulation was rerun.

2.3 Garage Description

The maintenance garage was modeled as a pitched roof building (1:6 pitch) that was 30.5 m long (100’), 15.2 m wide (50’) and 6.1 m tall (20’), with the roof peak located at the center and 127 cm (50”) higher than the corresponding eaves (see schematic in Figure 1). Note that although the roof and main building are shown with different colors to emphasize the pitch, the enclosure was treated as a single volume. A roof layout with horizontally orientated support beams was investigated to see if the supports would cause the accumulation of flammable mixture in discrete pockets. Nine beams that were 15.2 cm wide (6”) and 107 cm tall (42”) were spaced 3.05 m apart (10’) and ran parallel to the roof pitch. The garage contained two vents that were used for air circulation; one near the floor along one of the smaller building side-walls, with the second placed on the opposite side wall near the roof. Each vent was 0.645 m tall (25”) and 3.42 m wide (131”). The NGV was modeled as a cuboid with a height and width of 2.44 m (8’) and a length of 7.31 m (24’). The vehicle was centered on the building floor with the major axis aligned to the building minor axis. There was no fluid flow through the volume representing the vehicle.

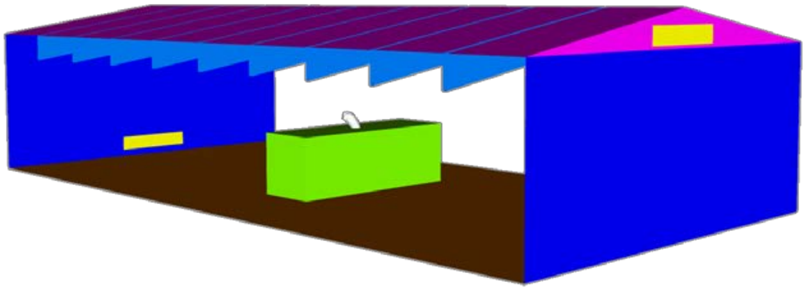

Figure 1. Schematic of the NGV maintenance facility used for the simulations. The roof had a 1:6 pitch and had layouts with and without 9 evenly spaced, horizontal supports. Two circulation vents were located on the smaller building side-walls (shown in yellow), with one placed low and the other high to maximize room currents.

2.4 Flow Solver

To perform the analyses, a numerical modeling, previously validated for large-scale indoor hydrogen releases scenarios [4, 5], was adopted. The CFD solver, Fuego [6], was used to perform the natural gas release simulations from a representative NGV inside the scaled warehouse. Fuego is a Sandia National Laboratories' developed code designed to simulate turbulent reacting flow and heat transfer [6] on massively parallel computers, with a primary focus on heat transfer to objects in pool fires. The code was adapted for compressible flow and combustion, and is well suited for low Mach number flows. The discretization scheme used in Fuego is based on the control volume finite element method [7], where the partial differential equations of mass, momentum, and energy are integrated over unstructured control volumes. The turbulence model was a standard two equation (k-ε) turbulence model [8] with transport equations solved for the mass fractions each chemical species, except for nitrogen which was modeled as the balance. For the calculations reported here, the first order upwind scheme was used for the convective terms. Note that methane was used as a proxy for natural gas in this simulation.

The Fuego code solved the conservation equations in a time-dependent manner with both gravity and buoyancy effects accounted for. A slip wall boundary condition with a constant temperature (294 K) was used for all surfaces. The simulations were performed with mechanical ventilation with a uniform air flow velocity of 2.0 m/s (6.56 ft/s) which was forced through the floor vent into the enclosure, producing 5 air changes per hour (ACH) for the enclosure. The upper enclosure exhaust vent was assigned an open boundary condition with a total pressure of 1 atm and a temperature of 294 K. For all scenarios, the initial turbulence was negligible ($k = 0.11\ \mathrm{cm}^2/\mathrm{s}$, $\varepsilon = 1.51\times10^{-4}\ \mathrm{cm}^2/\mathrm{s}^3$). For the mechanical ventilation, air was forced into the enclosure at the prescribed flow rate for 720 seconds prior to the start of the release to ensure the enclosure airflow was nominally steady.

3. RESULTS

3.1 Corrected Netflow Results

To velocity and temperature of a leak caused by the failure of a PRD was calculated by simulating the entire contents of a 700 L, fully pressurized (250 bar) CNG cylinder at room temperature (294 K) being released into normal atmospheric conditions. The PRD orifice diameter was set to 6.2 mm (0.24") based on the flow rate specifications of typical commercially available PRDs. At the start of the release, the valve was assumed to immediately transition to a fully open position and remain that way for the duration of the release.

The figure below shows a comparison of the exit velocity profiles for the original and new simulation with the corrected thermal conductivity. There is a small deviation between 80 and 300 seconds of the tank blowdown.

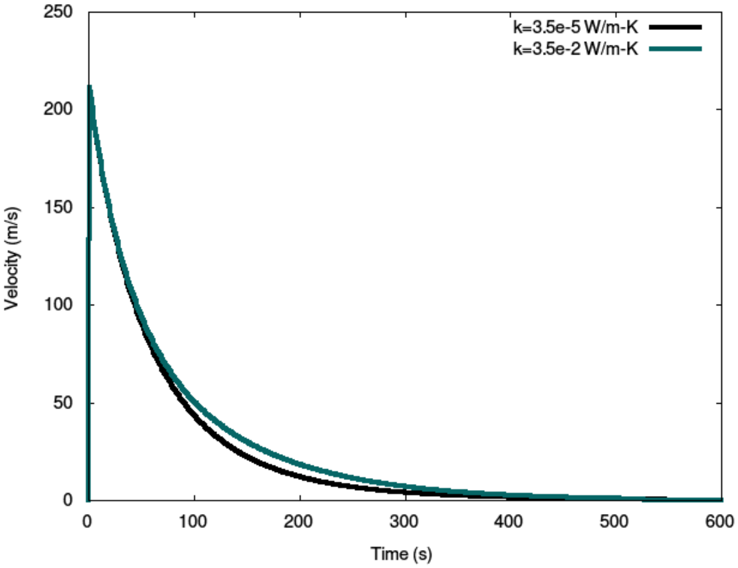

Figure 2. Leak exit velocity for simulation with incorrect thermal conductivity, 3.5e-5 W/m-K, and correct thermal conductivity, 3.5e-2 W/m-k.

While the velocity profile is relatively unchanged with the correction (Figure 2), a larger difference between the two simulations can be seen below in the tank temperature history (Figure 3). With the corrected thermal conductivity, the minimum temperature reached in the tank was approximately 240 K, while a value of 100 K was obtained in the original simulation. This higher, more consistent temperature is also within the valid temperature range of the software used for the CFD simulation, while the previous lower, incorrect temperature was not. This results in much more trustworthy results from the simulated leak scenario.

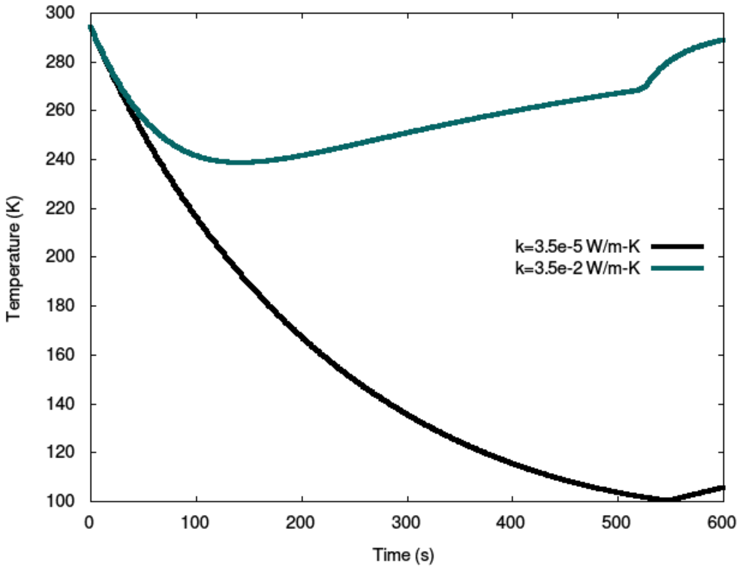

Figure 3. CNG tank temperature history comparison between incorrect and corrected thermal conductivity.

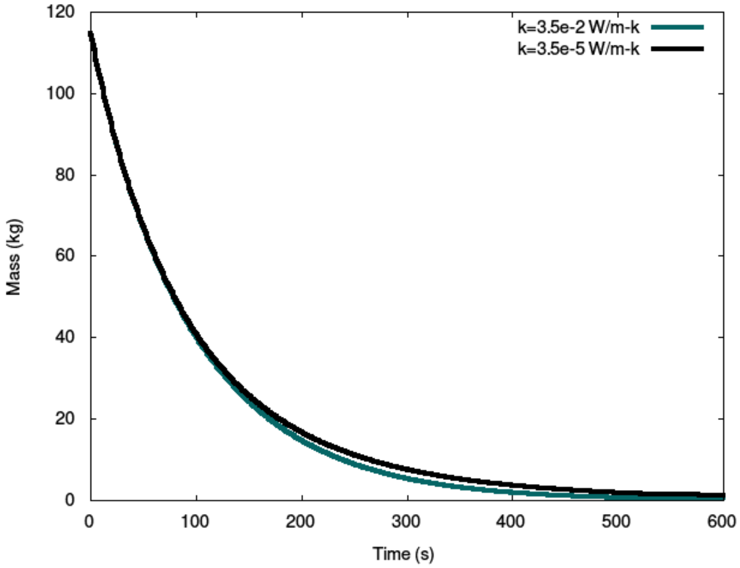

Figure 4. The CNG tank mass inventory remains fairly consistent with the correction of the thermal conductivity.

3.3 CFD Results

For this scenario, a plume of flammable gas formed between the leak location at the top of the vehicle and the ceiling of the garage. The region with flammable gas concentrations then spread outward across the ceiling and filled a region up to approximately 80” thick while the leak was occurring. It should be noted that during the initial phases of the blowdown, flow patterns allowed the flammable mass region to completely fill the space between the vehicle and the ceiling (see Figure 5 through Figure 7). As can be seen in Figure 2, the entire blowdown lasts approximately 10 minutes, and most of the mass has emptied the tank in less than 5 minutes (see

Figure 4). The flammable mass dissipates from the ceiling within 15 minutes of the start of the blowdown. A more complete time lapse of the leak is presented in Appendix A. Flammable volumes in the figures are in units of cm^3.

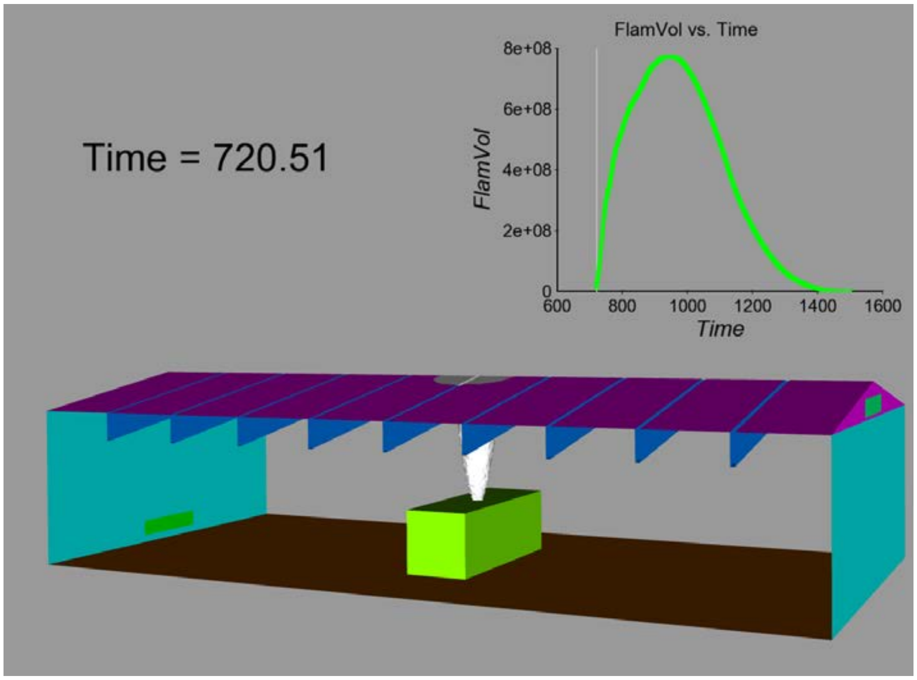

Figure 5. The ventilation was run for 720 seconds before the leak was started, so this image shows what happens within the first second of the leak. The boundary of flammable mass is shown in white. A plume has already reached between the leak location at the top of the vehicle and the ceiling of the garage.

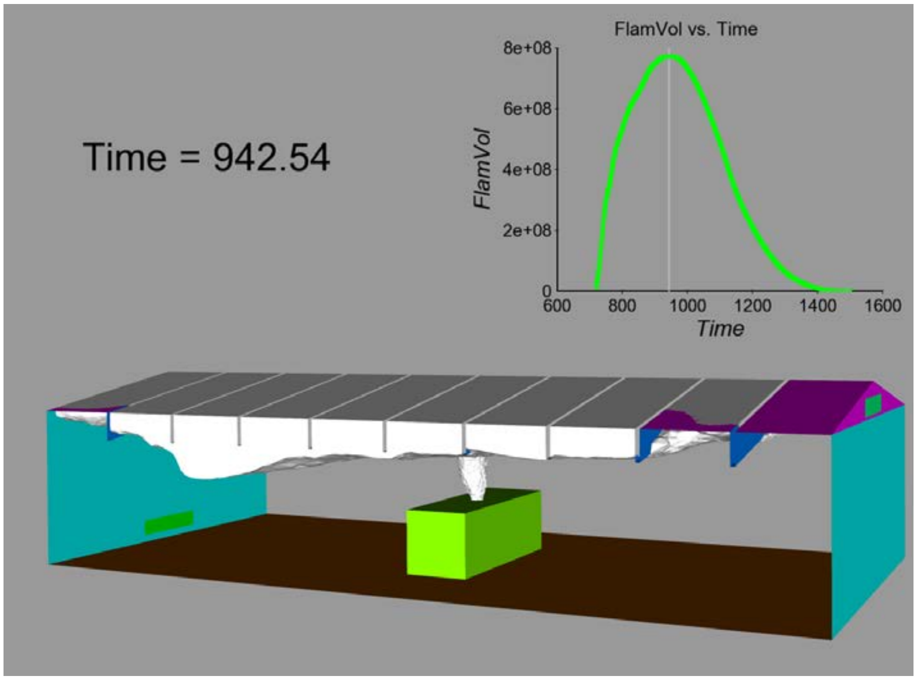

Figure 6. The maximum flammable volume of natural gas in the garage is reached ~220 seconds after the start of the leak. At this point, most of the mass has left the tank. The gas dispersing out of the ventilation and throughout the garage starts to bring the concentration back below the flammable limit of 15%. The flammable mass is still in the plume above the leak and has spread to cover most of the ceiling. In places it is more than 80 inches thick.

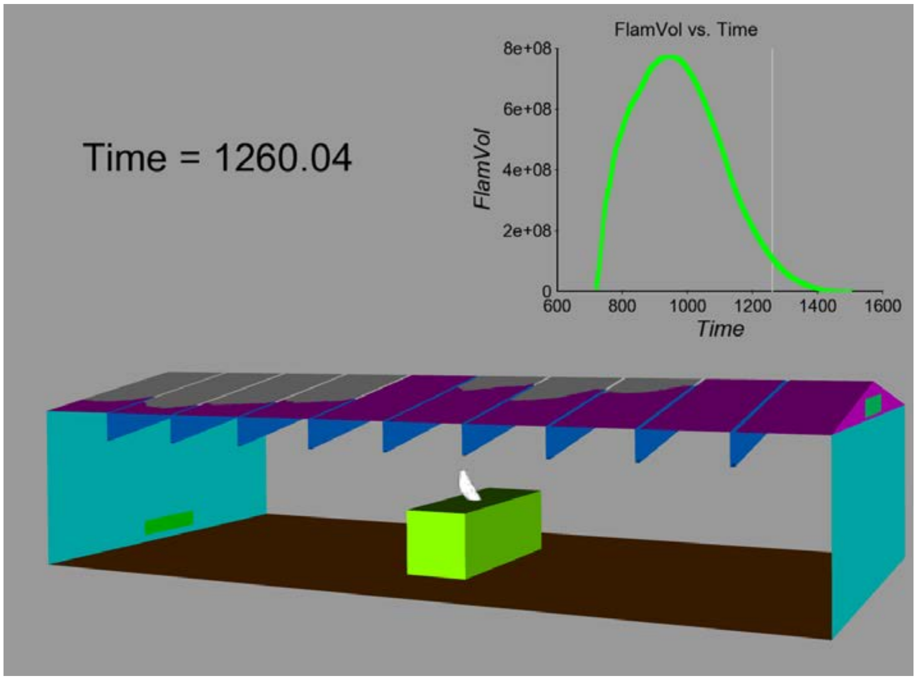

Figure 7. As the tank empties, the flammable mass clears from the garage and has completely dispersed by 680 seconds.

4. OVERPRESSURE CALCULATIONS

Using a simple calculation [9] that accounts for the maximum flammable mass in the building, we can estimate the overpressure that would result if the leak were to ignite at that point in time.

$$\Delta p = \left\{\left[\frac{V_T + V_{NG}}{V_T} - \frac{V_T - V_{stoich}(\sigma - 1)}{V_T}\right]^{\gamma} - 1\right\}$$

Where V_T is the volume of the facility, V_{NG} is the volume of flammable methane, V_{stoich} is the stoichiometric consumed methane volume, σ is the stoichiometric methane expansion ratio (7.561), and γ is the specific heat ratio of air (1.4). This overpressure correlation as developed only considers the sudden combustion of all flammable contents, which is unlikely to happen for a volume of flammable gas that is as large as seen in this case. The presence of ventilation, wall heat transfer, and the fact that the mixtures will continually lean out will mean that the actual overpressure will be much lower than is calculated. (If the enclosure was perfectly sealed and there was no heat transfer out of the box, then the Δp calculated would be the same, assuming the flammable volume stayed constant throughout the entire burn.) On the other hand, the flame front might become increasingly turbulent due to obstacles such as the beams, perturbing the flame-front making and making it even more turbulent, which would result in an increase in the turbulent flame speed. It is possible that the burn velocity could become fast enough that it could transition into a detonation, in which case the overpressures will be much greater. This is brought to the attention of the reader so that the assumptions in the calculation are clear, and it is known that the result should be taken as an estimate only.

During this simulation, the maximum flammable volume of 772.7 m^3 occurred at 222.5 seconds from the start of the leak blowdown (942.5 seconds into the simulation). The volume of the garage is 3122 m^3, and the stoichiometric consumed methane volume is 590 m^3. These conditions are estimated to produce a change in pressure, or overpressure, of about 220 kPa. As stated above, as long as there is not enough turbulence to produce a detonation, this is most likely an overestimation of the actual overpressure that would occur for this scenario in this garage. According to [10], this is large enough to collapse unreinforced concrete walls (see Table 1). Even if the calculated overpressure were as much as 50% off, it would still have this same consequence.

Table 1. Consequences of overpressures in an enclosed space [10].

Overpressure (kPa)	Consequence
6.9	Injuries due to projected missiles
13.8	Fatality from projection against obstacles
13.8	Eardrum rupture
15-20	Unreinforced concrete wall collapse

5. CONCLUSIONS AND FUTURE WORK

With the corrected algorithms for the Netflow calculation of a blowdown of a CNG tank, we were able to successfully simulate the leak flow of a NGV inside of a garage using CFD. For this extremely large but unlikely event, the flammable mass region was able to completely fill the ceiling area of a “typical” garage.

While this is a somewhat short lived event, with ventilation all of the flammable gas dissipates within 15 minutes, the possible consequences if there is an ignition source in contact with the flammable mass region are quite severe. The maximum overpressure, which would occur around 200 seconds into the blowdown, would be most likely be large enough to collapse unreinforced concrete walls.

In the Netflow analysis of the storage tank, the ideal gas equation of state was used to model the thermodynamic properties of the fuel. The main assumption here is that the compressibility effects are small. To help qualify this assumption, REFPROP [11] real gas equations were used to calculate the thermodynamic properties in the storage tank during a transient blowdown. The result of this analysis was a higher predicted mass flow rate. However, for the full CNG tank Feugo analysis, a severe overpressure was already predicted when using the ideal gas equation and using the higher mass flow rates will not change this outcome. The use of the real versus ideal gas equations should, however, be studied further for future transient analysis.

We should also note that all the simulations performed used Methane as a proxy for the Natural Gas mixture that is found in these types of systems. It is currently unknown how much of an effect using a proxy for the fuel has on the mass flow rates and is worth investigating in the future.

6. RECOMMENDATIONS

We recommend that any codes and standards committees using this report as a reference consider whether or not they think that this is a credible release (none have occurred since 2002) which needs to be considered when updating fire code restrictions. If it is considered to be a credible release, it is clear that sever results could occur if this large of a release were to ignite, so precautions to prevent that ignition should be put in place. If not, then the modeling done for the Phase I report [1] shows that the most likely release scenarios do not result in hazardous concentrations in the beam pockets, within 18 inches of the ceiling, with or without ventilation.

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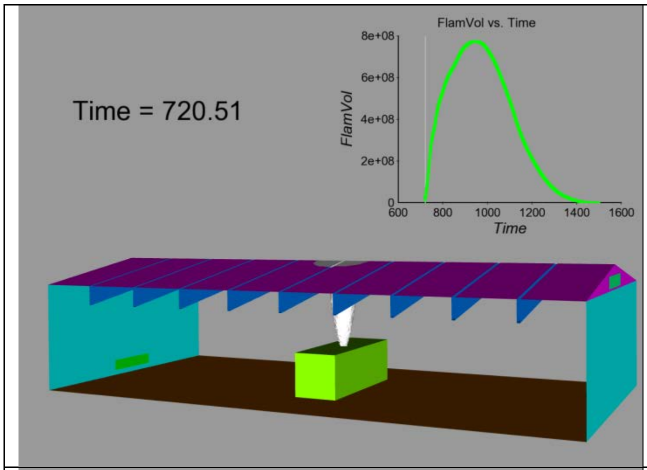
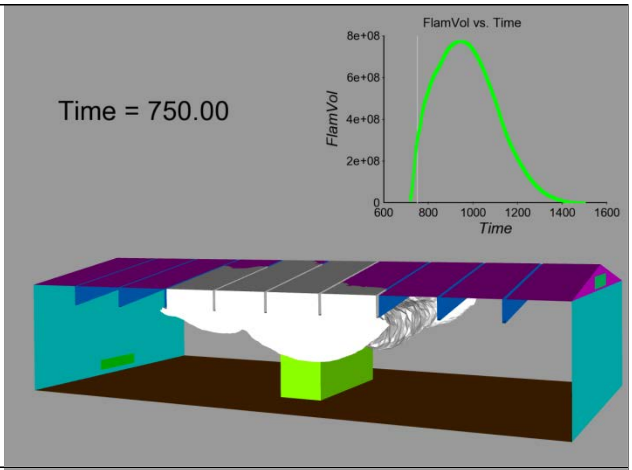
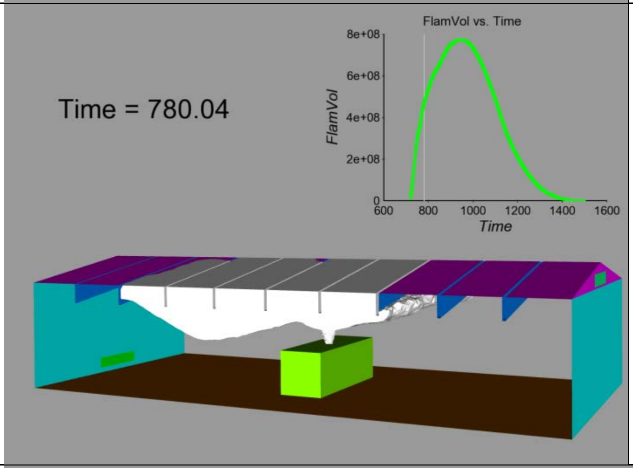
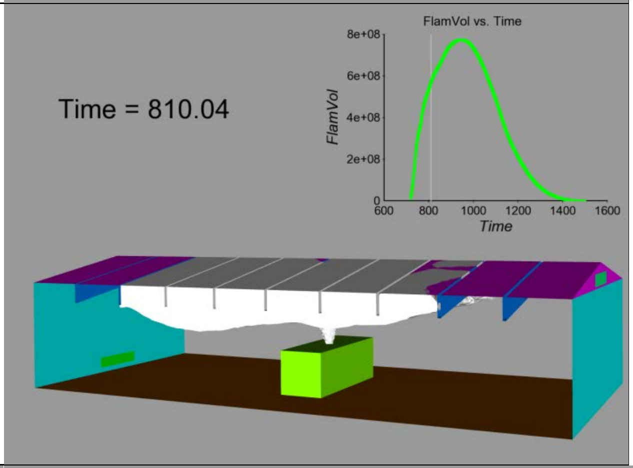
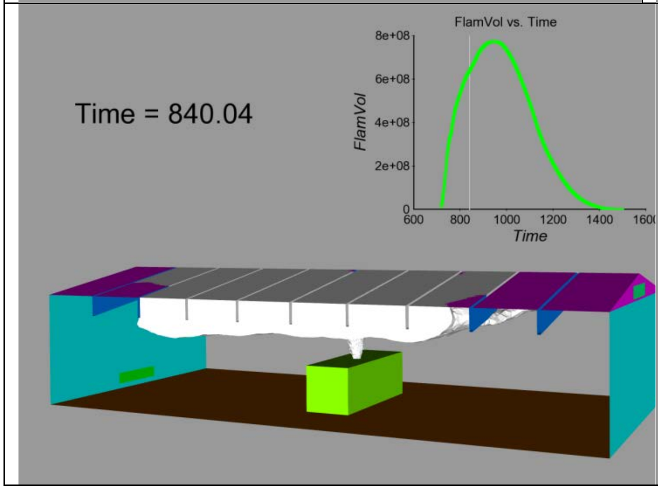
APPENDIX A: TIME LAPS OF LEAK

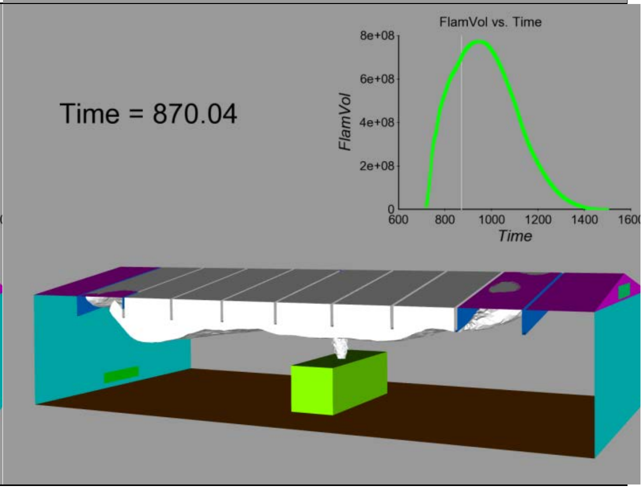


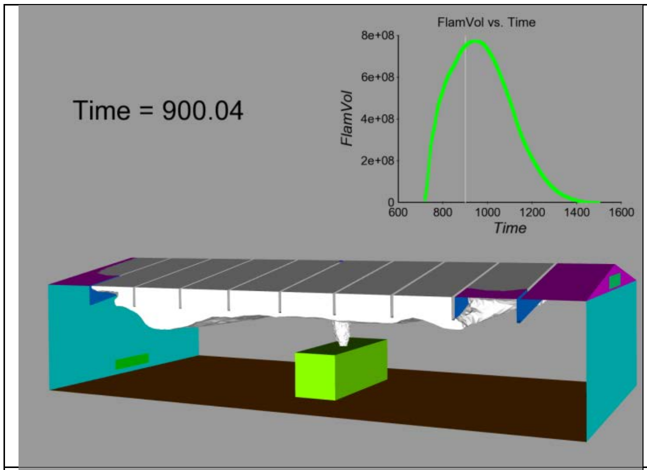








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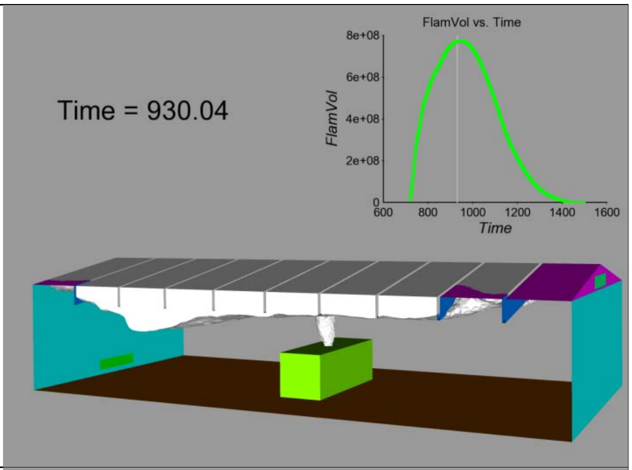
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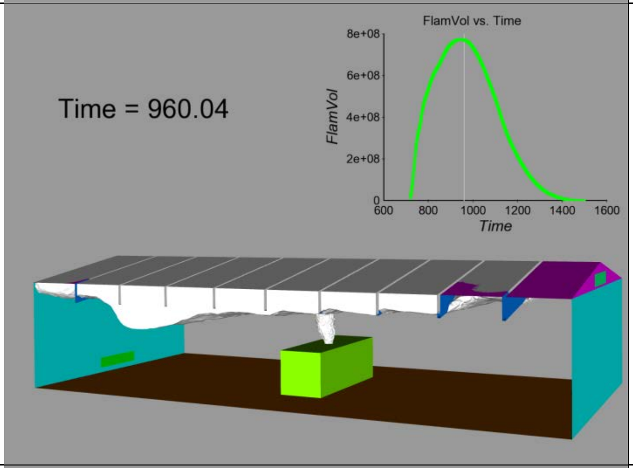
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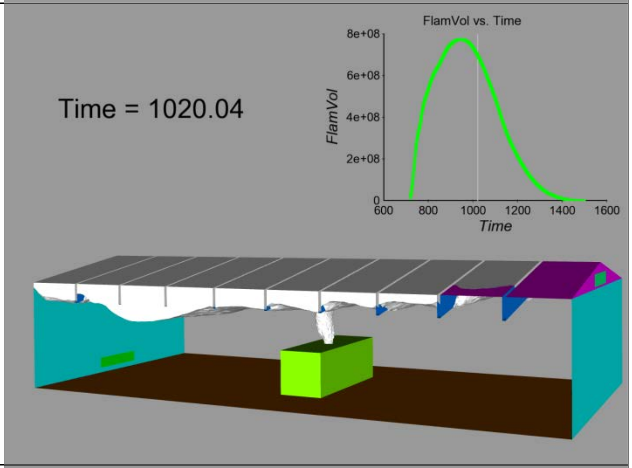
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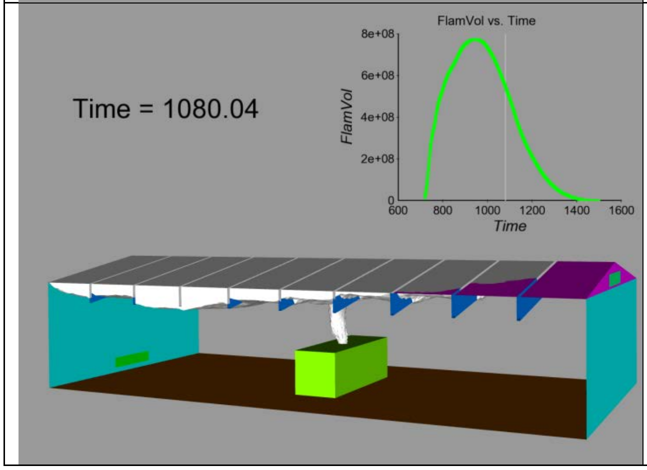
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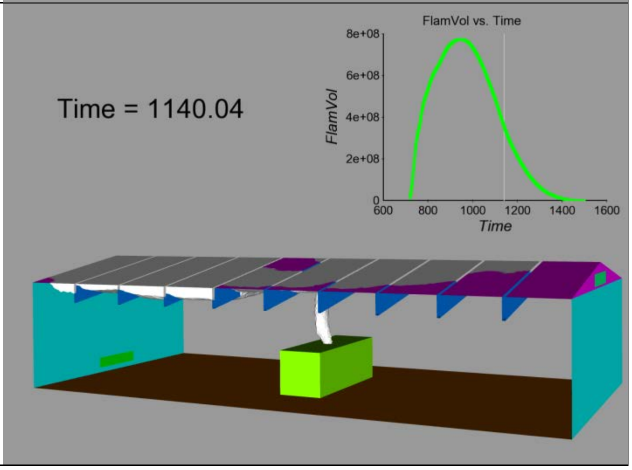
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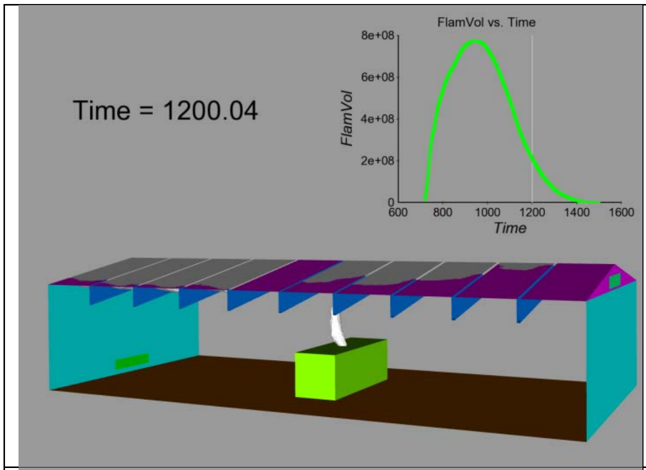
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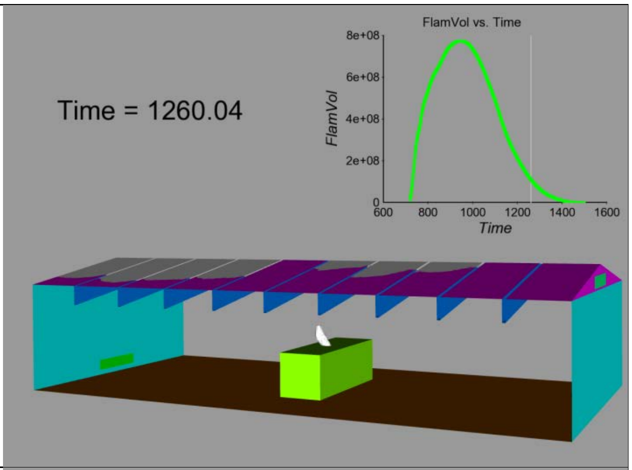
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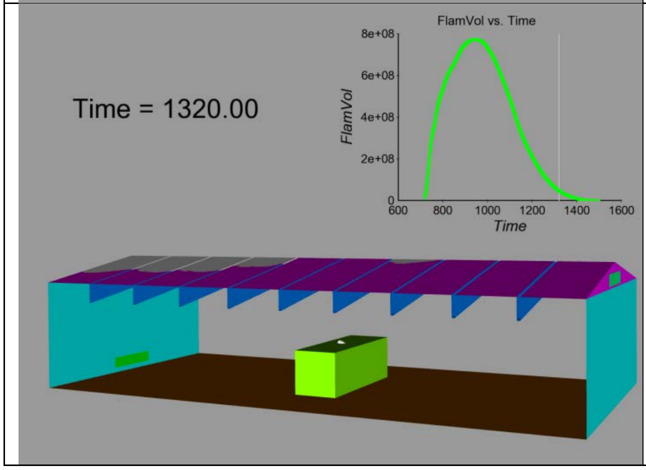
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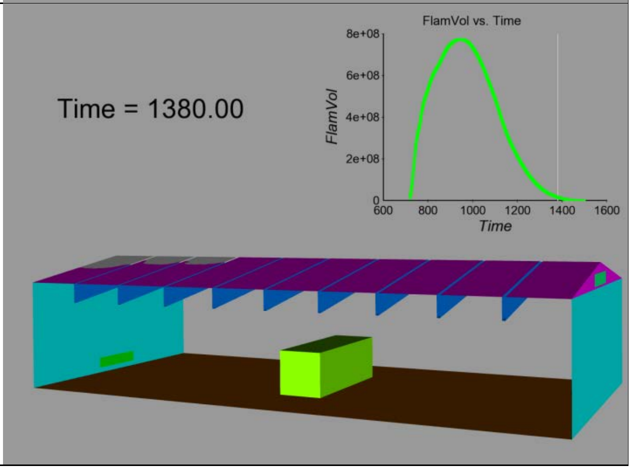
1600
Time


Time = 1380.00
FlamVol vs. Time
FlamVol
8e+08
6e+08
4e+08
2e+08
0
600
800
1000
1200
1400
1600
Time

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