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# Computational Risk Analysis of Propane Releases in Maintenance Facilities

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# ABSTRACT

Liquefied petroleum gas (LPG) is a viable, cleaner alternative to traditional diesel fuel used in busses and other heavy-duty vehicles and could play a role in helping the US meet its lower emission goals. While the LPG industry has focused efforts on developing vehicles and fueling infrastructure, we must also establish safe parameters for maintenance facilities which are servicing LPG fueled vehicles. Current safety standards aid in the design of maintenance facilities, but additional quantitative analysis is needed to prove safeguards are adequate and suggest improvements where needed. In this report we aim to quantify the amount of flammable mass associated with propane releases from vehicle mounted fuel vessels within enclosed garages. Furthermore, we seek to qualify harm mitigation with variable ventilations and facility layout. To accomplish this we leverage validated computational resources at Sandia National Laboratories to simulate various release scenarios representative of real world vehicles and maintenance facilities. Flow solvers are used to predict the dynamics of fuel systems as well as the evolution of propane during release events. From our simulated results we observe that both inflow and outflow ventilation locations play a critical role in reducing flammable cloud size and potential overpressure values during a possible combustion event.

# ACKNOWLEDGEMENTS

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# ACRONYMS AND DEFINITIONS

| Abbreviation | Definition |
| --- | --- |
| ASI | Alternative subsonic inlet |
| ACH | Air changes per hour |
| CFD | Computational fluid dynamics |
| LFL | Lower flammability limit |
| LPG | Liquefied petroleum gas |
| NFPA | National Fire Protection Agency |
| PRV | Pressure relief valve |
| UFL | Upper flammability limit |

# 1. INTRODUCTION

The U.S. has pledged to cut its greenhouse emissions to below 52% from 2005 levels and alternative fuels have been identified as a potential means of reaching this goal. Propane or liquefied petroleum gas (LPG) is considered an alternative fuel under Energy Policy Act of 1992 [1] and is a cleaner burning fuel source for busses and other heavy-duty vehicles. Per the U.S. Energy Information Administration [2], propane releases ~14% $CO_2$, ~20% NO, and ~60% less CO emissions per million Btu of energy compared to diesel as shown in Figure 1.

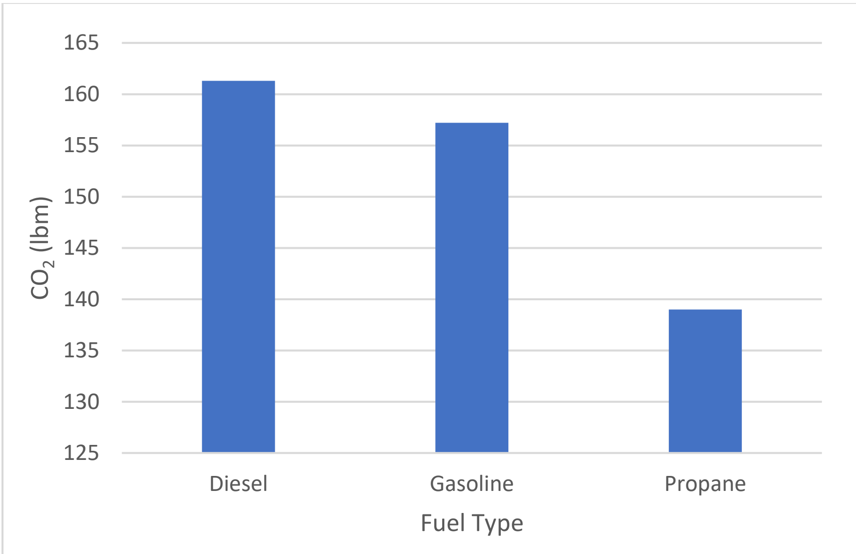



**Figure 1:** Pound of $CO_2$ emitted per million Btu of energy

According to the Propane Education & Research Council, there are nearly 200,000 on-road propane vehicles with certified fuel systems in the United States [1]. As this number continues to rise, so does the need for supportive infrastructure. While significant effort has been devoted to the development of vehicles and fueling technology we must also establish safe parameters for maintenance facilities which service LPG vehicles. As safety standards aid in the design of maintenance facilities, additional quantitative analysis is needed to provide adequate safeguards. This report aims to quantify the amount of flammable mass associated with propane releases from vehicle mounted fuel vessel within maintenance facilities. Through simulation we wish to understand the effectiveness of ventilations and facility layout for risk reduction.

# 2. SCENARIO DESCRIPTION

Our first step for computational propane leak analysis was defining a scenario representative of real world applications. A large portion of the LPG (or AutoGas) vehicle fleet is comprised of heavy-duty vehicles, with over 15,200 autogas school buses in operation within the U.S. [3], thus we focused our analysis on a model representation of a propane fueled bus. Determination of the facility dimensions and layout was based on communications with subject experts and facility owners. Our simulations represents a mid-ship tank capacity Blue Bird Propane bus in a representative single vehicle maintenance facility. An in depth description of both the selected vehicle and maintenance garage follows.

## 2.1. Vehicle and Maintenance Facility Specifications

In the following subsections we review detailed specifications for the simulated LPG vehicle, a typical maintenance facility where one of these busses might be serviced, as well as various ventilation rates and inflow/outflow configurations.

### *2.1.1. Vehicle Description*

LPG fueled bus manufactures such as Blue Bird, Collins Bus Corporation, IC Bus, and Thomas Built Buses offer a wide range of vehicle configurations. Bus sizes vary from 12 up to 80 passenger capacity and as capacity increases so does the vehicles fuel tank size. Typical fuel tanks ranged from 40 to 100 gals with 67 gals representing a mid-ship tank size. The 67 gallon fuel tank was selected as this size represented a common configuration used amongst several manufactures [4] [5] [6] [7].

#### 2.1.1.1. Vehicle Fuel Tank Assembly

Propane fuel tanks are typically manufactured from an ASME certified ductile steel. In addition to fuel delivery components regulations require that the fuel tank is connected to a safety release system. From conversation with fuel tank manufactures, a release system consists of a pressure relief valve (PRV) calibrated to vent fuel if the tank pressure exceeds 312 psi, per NFPA 58 [8], through a valve with a diameter of 1.25”. Generally the PRV is plumbed to the skirt of the bus behind the rear axle, street side, and points directly down, to avoid releasing fuel to a potential ignition source.

### *2.1.2. Facility Specifics*

The dimensions of the simulated facility are a representation of a typical garage layout, based off communications with subject-matter experts and facility owners. We elect to simulate a single vehicle garage as the reduced internal volume would provide more conservative assessments. The internal volume of our simulated garage is 2,147 $m^3$ with a floor area of roughly 223 $m^2$. As outlined in safety standard National Fire Protection Agency (NFPA) 30A [9]– Code for Motor Fuel Dispensing Facilities and Repair Garages, facilities servicing LPG or autogas vehicles shall meet the requirements outlined in NFPA 58: Liquefied Petroleum Gas Code [8]. NFPA 58 states mechanically driven ventilation systems must provide 1 $ft^3$ of air flow per $ft^2$ of working floor surface area per minute. To meet this, for vents with a cross-sectional area of 0.5 x 1.887 m (a size based on subject-matter expert opinion) it was determined that the vent flow speeds should be either 1.2 m/s for a single vent configuration, or 0.6 m/s per vent for two. At these speeds the required 67.96 $m^3$/min flow rate is recovered representing 1.89 air changes per hour (ACH). Note this rate is far less than that required in NFPA 30A, which requires 6 ACH for a garage of this size servicing other liquefied alternative fuels. Additional assumptions regarding the maintenance facility were made on the configuration of the garage doors. It was assumed that the maintenance facility was a drive through building, with bay doors located on both sides of the garage. Additionally, the garage doors were only partially open to a height of ~0.2 m representative of working conditions in winter conditions where wide open doors would render the garage too cold for workers. More details on the simulated ventilation and garage configurations are covered in more detail in Section 3.2.1.

# 3. SIMULATION METHODS

In this study we use Sandia's in house flow solvers to simulate LPG releases within the simulated single vehicle garage. A model of the fuel systems release was developed using MassTran, a one-dimensional internal flow solver [10]. MassTran leverages the property database CoolProp [11] to inform a set of empirically derived equations which describe the thermodynamic state of fluid at a components level within the fuel system. In this case, MassTran was used to calculate the flow of propane from the pressurized fuel tank, through the PRV, and into the surrounding environment. The modeled fuel system only contains two components, the pressurized fuel vessel and the attached pressure release valve. Because the propane changes phases from its initial state of compressed liquid to vapor as the pressure drops over the duration of the release, multiphase flow modeling was required. Equilibrium of the propane at all times was assumed.

From this component level simulation, we captured valve outflow profiles for use as a release inflow profiles into the garage. We then simulated the full release within the maintenance facility with Fuego [12], a fully three-dimensional computational fluid dynamics (CFD) solver. Fuego is Sandia's low Mach number, turbulent incompressible flow solver. Specifics of the setup and execution of each flow solver is discussed in the following subsections.

## 3.1. Fuel Tank Simulation – MassTran

To begin our simulations we first estimated the initial conditions of the LPG tank prior to release. LPG fuel tanks are typically only filled to 80% volumetric capacity. Propane expands approximately 1% volumetrically per 6°F increase in temperature [13]; filling to 80% allows the propane to expand to its vapor phase if the ambient temperature rises without driving the internal pressure of the tank above its limits. The nominal working pressure (NP) of vehicle LPG tanks is 10-14 bar [13]. The liquefied propane density does not vary significantly within this pressure range at a fixed temperature 294 K, as shown in Figure 2.

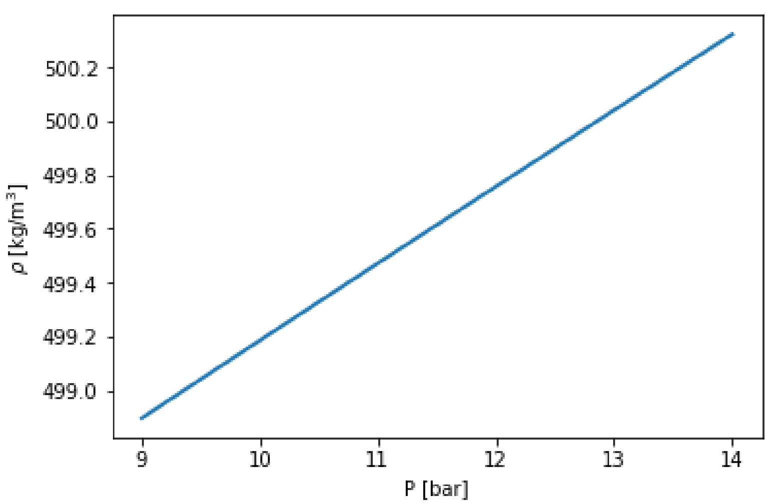



**Figure 2:** Density of propane versus pressure over nominal working pressure range at 294° K

With density of 500 kg/m$^3$, the mass of LPG within 80% of the tank volume ($0.8 \cdot 67$ gal) will be 101 kg. With this mass of propane in the entire tank volume (67 gal), the average fluid density within the tank will be 400 kg/m$^3$. At this density, the pressure and vapor quality at equilibrium can be calculated using CoolProp. Equilibrium conditions for a typical tank temperature, stored at NP and high pressure (HP) condition were obtained, where HP conditions may be caused by a high temperature (such as an adjoining fire). The high pressure (HP) state is at a pressure of 312 psi (21.5 bar), which is the set-pressure of the PRV (the tank contents will be released if the pressure exceeds this value). Table 2 displays the thermodynamic state for both configurations.

**Table 1:** Thermodynamic State of LPG for nominal and high pressure conditions

| Thermodynamic Properties | Nominal Pressure (NP) | High Pressure (HP) |
|---|---|---|
| Temperature | 294 K | 334 K |
| Equilibrium Pressure | 0.855 MPa | 2.15 MPa |
| Vapor Quality ($M_{gas}$ / $M_{mixture}$) | $9.50 \times 10^{-3}$ | $8.80 \times 10^{-3}$ |

The initial tank conditions were used to simulate a full blow down simulation via MassTran. The evolution of various thermal states for both nominal and high pressure conditions are shown in Figures 3a-c.

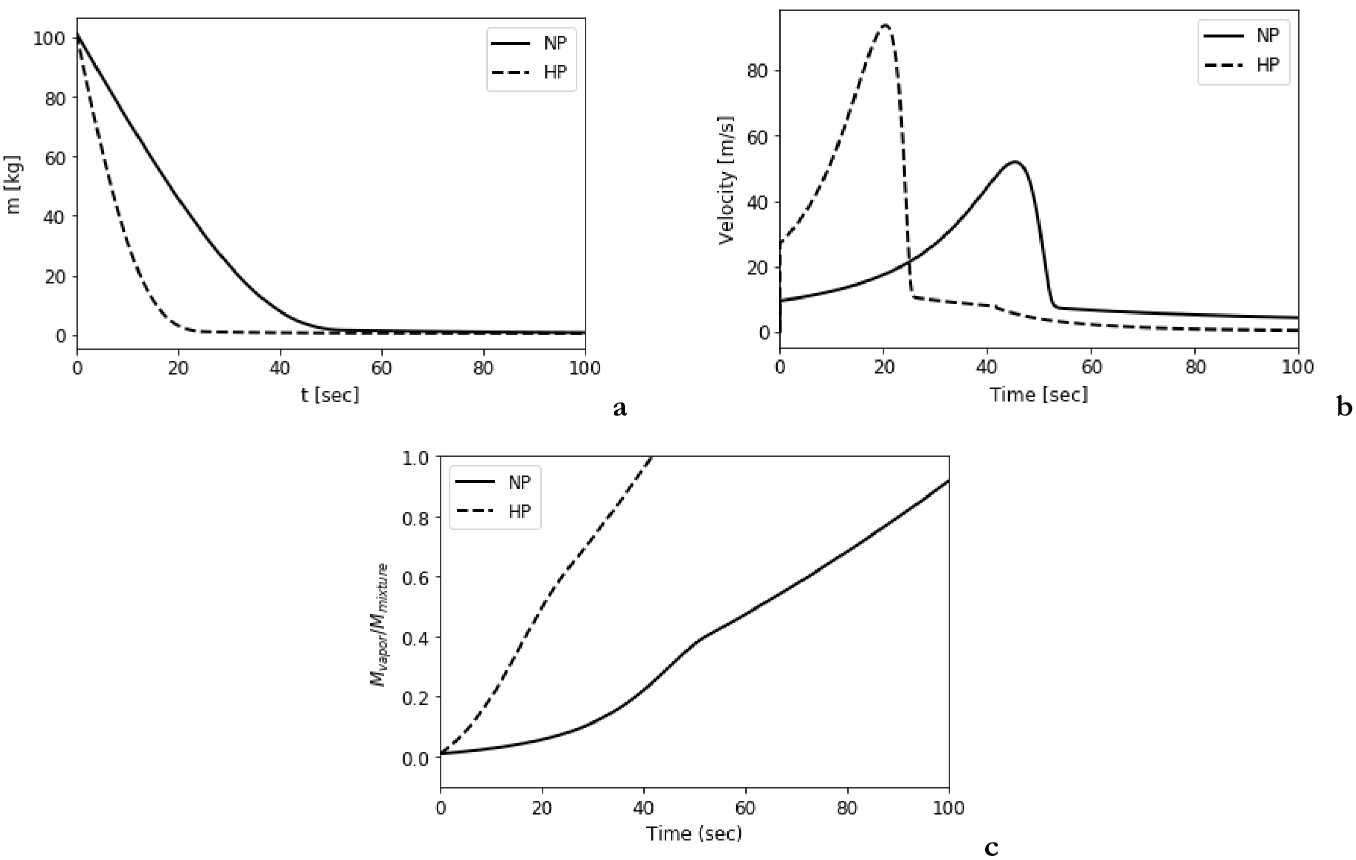



**Figure 3a-c:** Blow down profiles for tank mass (a), valve velocity (b), and tank quality (c) from MassTran simulation NP – nominal pressure, HP – high pressure

As expected, Figure 3b shows HP releasing propane at a much faster rate. The increase in valve velocity to a peak and strange curvature/lack of a steady or choked velocity is attributed to the ongoing phase change during release depicted in Figure 3c. The bottom Figure shows LPG changing from primarily a compressed liquid to a liquid-vapor mixture and finally to pure vapor phase. During this the specific heats vary, changing the local speed of sound at the valve which varies the observed release velocity significantly.

Fuego can only simulate fluid flows for a single phase at a subsonic velocity. The multi-phase, (mostly) sonic MassTran profiles were converted to a mass flow equivalent single phase vapor release, or artificial subsonic inlet (ASI) boundary condition. The ASI boundary condition preserves mass flow rate, but increases the release cross sectional area such that the flow is subsonic and in this case single phase (vapor). The artificial diameter increase does not significantly impact the critical metrics for risks assessment such as flammable mass, maximum cloud size, and peak overpressure values in case of combustion. A sensitivity study was carried out for the nominal pressure case to confirm this assumption. When the artificial diameter was increased by a factor of 2, only a 2% increase in peak flammable mass occurred.

Figure 4 displays the equivalent ASI velocity profiles over the originals for both pressure configurations. The nominal pressure (NP) case had an artificial diameter of 10 cm, and 20 cm was assumed for the high pressure (HP) case. As shown, each artificial diameter preserves subsonic speeds, while peak velocity never exceeds 258 m/s, the sound speed of propane in vapor phase.

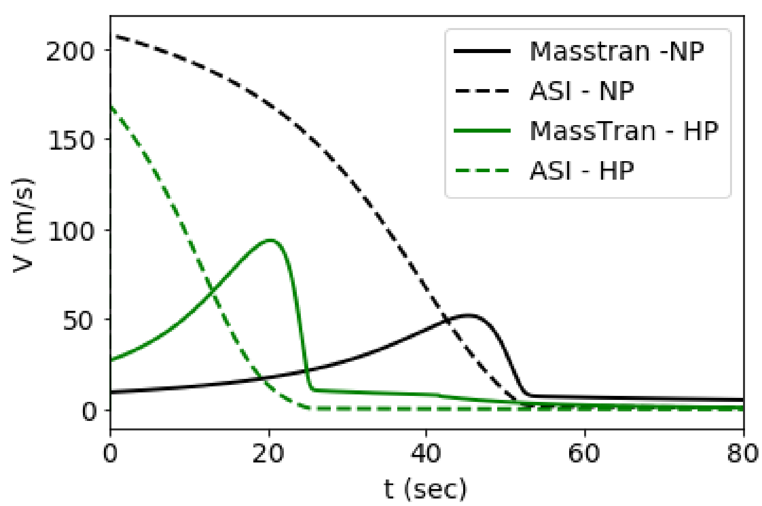



**Figure 4:** Velocity profiles for multi-phase and equivalent single phase ASI release per pressure condition

## 3.2. Maintenance Facility Release Simulation - Fuego

To simulate the fuel tank release within the garage we used Fuego, Sandia's low Mach turbulent flow CFD software package. The turbulence model was a standard two equation (k-ε) turbulence model [14] with transport equations solved for the mass fractions of each chemical species, except for nitrogen which was modeled as the balance. For the calculations reported here, a first order upwind scheme was used for convective terms.

A three dimensional unstructured computational domain was generated using Cubit, Sandia's in house meshing software [15]. Figure 5 displays the computational domain with the mesh elements hidden for clarity. The mesh is made up of 1,125,622 tetrahedral elements, and the minimum Jacobian was reported greater than 0.5 showing a good match between physical space and computational space. The yellow rectangle in the center of Figure 5 is a volumetric accurate representation of the 67 gal mid-ship Vision school bus. The rectangle is located 52.7 cm above the floor representative of tire radius plus suspension height.

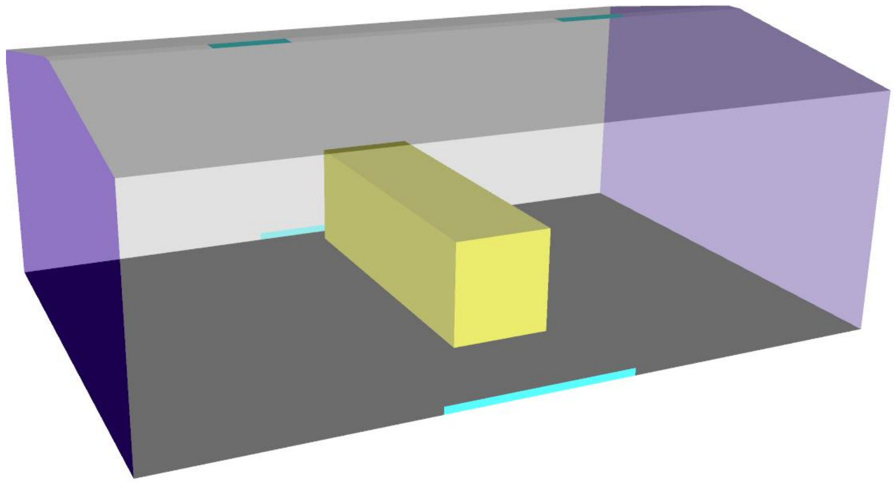


**Figure 5:** Simulated Garage and Bus Volume

### *3.2.1. Ventilation and Boundary Conditions*

All physical walls (both garage and bus) shown in Figure 5 were assigned a no-slip boundary condition and an equilibrium heat transfer model with constant wall temperature of 294 k. The light blue rectangles on the front and back walls, as well as the top of the roof represent the open garage doors and ventilation ducts. The garage doors are only partially open (~19 cm) to represent a cold day when the doors are partially closed to retain heat. This choice was made to obtain more conservative estimates. Underneath the bus, on the front left corner is the location of the leak, represented by the ASI boundary condition.

To fully assess potential risks of the release, we performed a parametric study of multiple ventilation configurations. The vent location, number, and garage door openings were all varied to capture a wide breath of layouts and situations. Table 2 displays the full list of evaluated configurations, where simulated cases are marked with an (X). For the single vent cases, a vent the same size as the two shown in 5 was centered above the bus. When only one door was open, it was the furthest from the release point.

**Table 2:** Simulated Garage Ventilation Configurations

| Vent Configuration | Nominal Pressure (NP) | High Pressure (HP) |
|---|---|---|
| Vents: 2 Doors: 2 | X | X |
| Vents: 1 Doors: 2 | X | |
| Vents: 0 Doors: 2 | X | |
| Vents: 2 Doors: 1 | X | |
| Vents: 0 Doors: 0 | X | X |

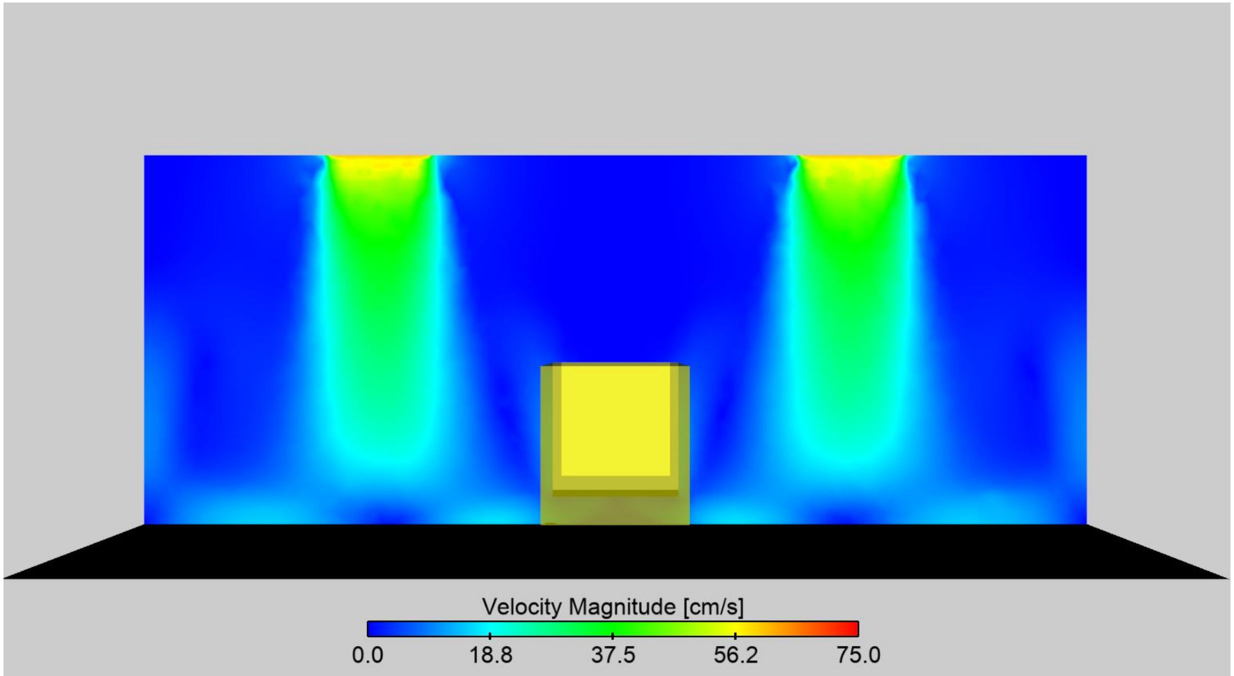
The turbulence kinetic energy $k$ and turbulent dissipation rate $\epsilon$ was calculated for the inlet ventilation assuming a fully developed non-circular pipe, as done in previous ventilation risk assessment studies [16]. Thus, the following equations were used to calculate the turbulence parameters for jet inflow and the ventilation.

$$\mathrm{Re}_{\mathrm{d}_h} = \frac{\rho U d_h}{\mu}$$
$$l = 0.07\, d_h$$
$$I = 0.16\, Re_{d_h}^{-\frac{1}{8}}$$
$$k = \frac{3}{2}(UI)^2$$
$$\epsilon = C_\mu^{\frac{3}{4}} \frac{k^{\frac{3}{2}}}{l}$$

Where:

- $C_\mu \approx 0.09$ is an empiracle constant defined in the $k - \epsilon$ turbulence model
- $U$ is the inlet (maximum jet and bulk ventilation) velocity
- $I$ is the turbulence intensity
- $\mu$ is the dynamic viscosity
- $d_h = \frac{2ab}{a+b}$ is the hydraulic diameter of the rectangular pipe (sides of length $a$ and $b$)
- $l$ is the turbulent length scale
- $k$ is the turbulent kinetic energy
- $\epsilon$ is the dissipation rate

The turbulence intensity was taken to be 1% given the initial conditions of the garage. Both the single and two vent configurations met the ~2 ACH per NFPA 58. Steady state velocity profiles taken from center line slices of the garage are shown in Figures 6a-b. From the sliced profiles a higher velocity magnitude under the bus can be observed in the two vents configuration. More on this will be discussed in Section 4.



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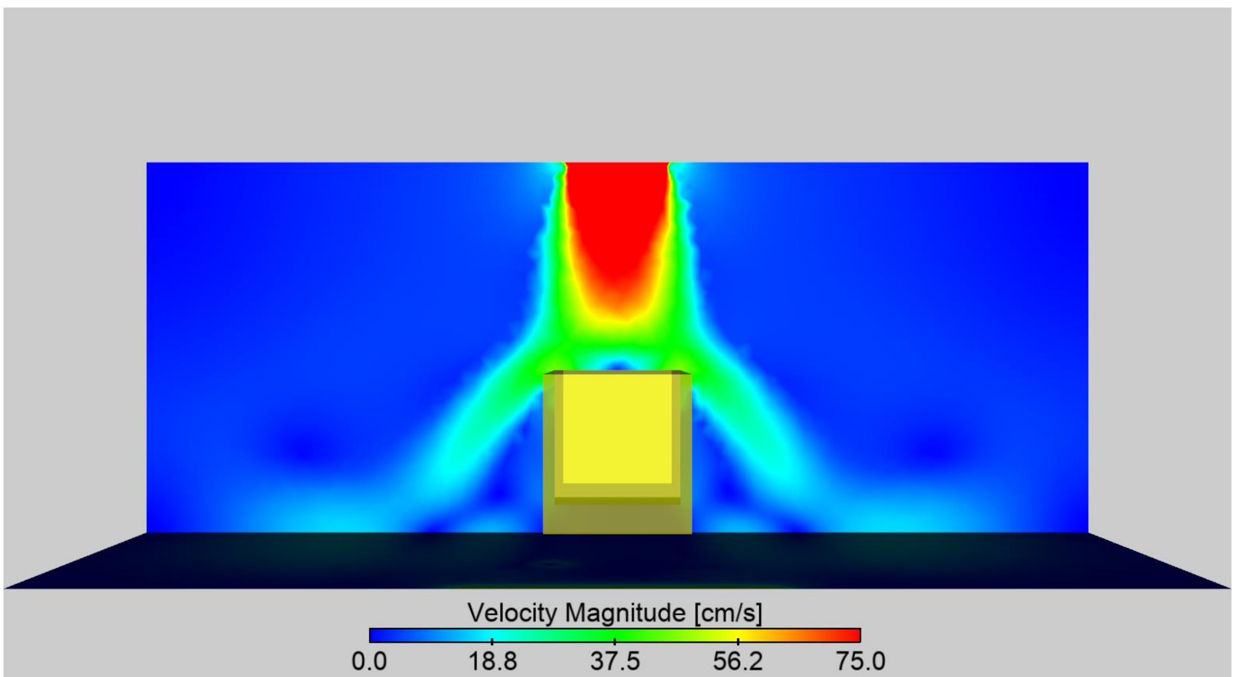
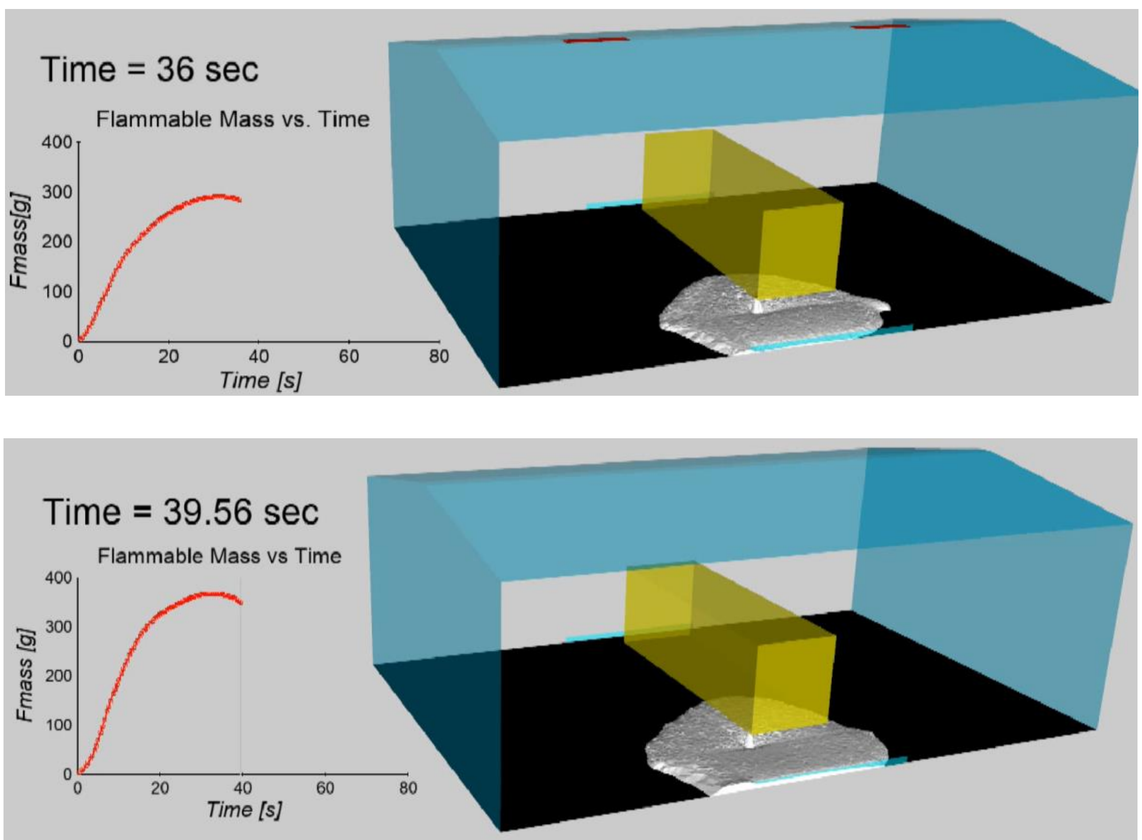


b

**Figures 6a-b:** Steady state ventilation velocity magnitude of both two (a) and one (b) vent configurations

# 4. RESULTS AND DISCUSSION

With the domain discretized, boundary conditions in place, and leak inflow profile modeled, the fully three-dimensional CFD simulation was carried out as described. First we established the steady state velocity profile of the ventilation, as shown in Figures 6a-b. Next we introduce the ASI inflow profile and sustained the inflow boundary condition until the mass left in the tank was less than 1% of the initial mass. Our final step was to swap the leak inflow boundary condition to that of an isothermal closed wall and run the simulation till final traces of flammable propane dissipated. Figures 7a-b display an approximate max flammable cloud size for the two vent and no vent release, both configurations had open garage doors.




**Figures 7a-b**: Max flammable mass during release for two vent two open doors (a) and no vents two open doors (b) configurations

The flammable region was identified as follows, first we extract the mole fraction from the mass fraction obtained from species conservation equations. Mole fraction is computed with

$$x_{C_3H_8} = \frac{Y_{C_3H_8}}{M_{C_3H_8}8} M_{mixture}$$

Where $x_{C3H8}$ represents the molar fraction of propane, $Y_{C3H8}$ the mass fraction, and M the molecular weight of the air plus the fuel mixture. With molar fraction we isolate volumes of gas that fall within the flammable limits of propane. Per [13] the upper and lower flammability limits (UFL & LFL) are

$$UFL_{C_3H_8} = 10.1\%$$
$$LFL_{C_3H_8} = 2.1\%$$

The white cloud within the garage in Figures 7a-b represents the volume occupied by a propane-air mixture which falls within said limits.

Integrating the density of propane over the flammable gas volume we obtain the total flammable mass within the garage over time. Between the two cases Figure 7 shows that a larger foot print is occupied by flammable gas in the no ventilation case. The scatter plots on the left side of Figure 7 also indicate the maximum flammable mass is significantly larger when ventilation is not active.

Additional images, from above the garage facing down, were extracted per the configurations described in Table 2 for the nominal pressure configurations. Similar to Figures 7a-b, the white clouds represent the flammable gas volumes. Additionally velocity magnitude contours are shown along the garage floor. The snap shots were taken during release, at the time of maximum flammable mass occurrence.

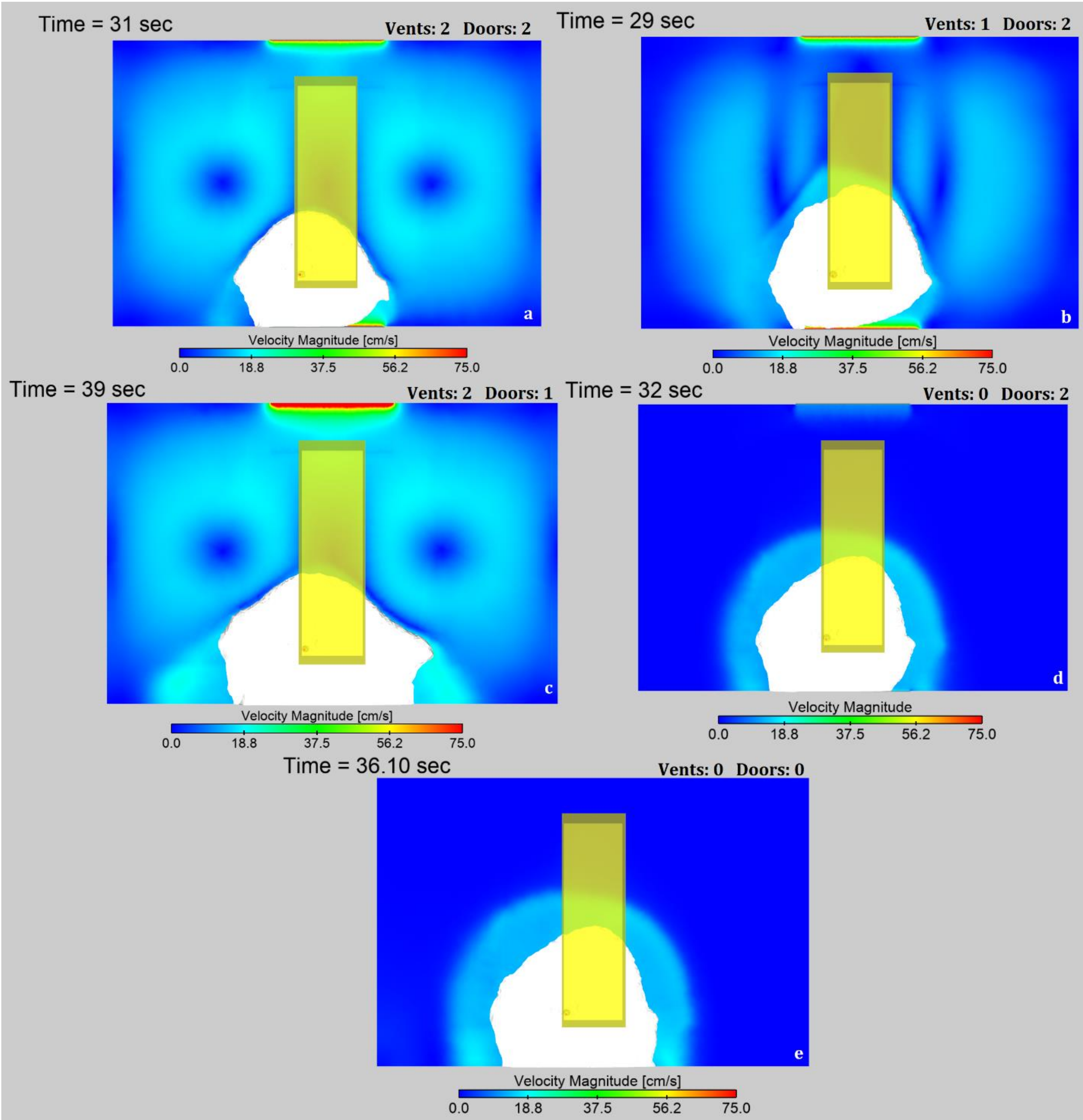



**Figure 8a-e:** Velocity magnitude contour and flammable gas clouds for nominal pressure configurations

The configuration of each release is labeled in the top right corner of each image. Figure 8c shows having the leak side door closed produces the largest flammable cloud size. Another interesting observation is the no vent (Figure 8d) and single vent (Figure 8b) case had similar max cloud sizes. This may be attributed to significant blockage of ventilation flow by the bus as shown in Figure 6b. The maximum flammable cloud lengths (z-coordinate, along the bus length), widths (x-coordinate, along the bus width) are shown in Table 3 along with estimated cloud area assuming an ellipsoid shape and peak flammable mass.

**Table 3:** Flammable cloud dimensions at peak flammable mass per simulated case

| Garage Configuration | Width in X [cm] | Length in Z [cm] | Area [$cm^2$] | Flammable Mass [kg] | Largest/ Smallest |
|---|---|---|---|---|---|
| 2 Vents – 1 Open Doors | 874.2 | 531.1 | 1458601 | 0.515 | 1 |
| 0 Vents – Closed Doors | 715.2 | 595.5 | 1338008 | 0.432 | 2 |
| 0 Vents – 2 Open Doors | 682.5 | 576.3 | 1235665 | 0.367 | 3 |
| 1 Vent – 2 Open Doors | 686.1 | 603.9 | 1301673 | 0.359 | 4 |
| 2 Vents – 2 Open Doors | 666.1 | 494.5 | 1034797 | 0.291 | 5 |
| 0 Vents – Closed Doors – HP | 643.3 | 727.3 | 1469862 | 0.792 | 1 |
| 2 Vents – 2 Open Doors – HP | 645.4 | 470.0 | 952963 | 0.478 | 2 |

By integrating local propane density over the flammable volumes as described previously (shown as the white mass in Figure 8a-e), we are able to extract the flammable mass per simulation time step. Using the flammable mass, we approximate the overpressure values which may occur in the event of combustion. In order to do this, we first compute the volume the flammable mass would occupy as a cloud of pure propane. Assuming the combustion will occur as a subsonic deflagration without significant blocking, we use Bauwens and Dorofeev [17] expression for overpressure described as

$$\Delta p = p_0 \left\{ \left[ \frac{V_T + V_F}{V_T} \frac{V_T + V_{stoich}(\sigma - 1)}{V_T} \right]^{\gamma} - 1 \right\}$$

$p_0$: Ambient pressure
$V_T$: Facility volume
$V_F$: Expanded volume of pure fuel
$V_{stoich}$: Stoichiometric consumed fuel volume
$\sigma$: Stoichiometric fuel expansion ratio
$\gamma$: Fuel specific heat ratio

The overpressure profiles were extracted for each configuration described in Table 2. Figure 9 displays the overpressure, with flammable mass corresponding to the right y-axis and overpressure to the left y-axis.

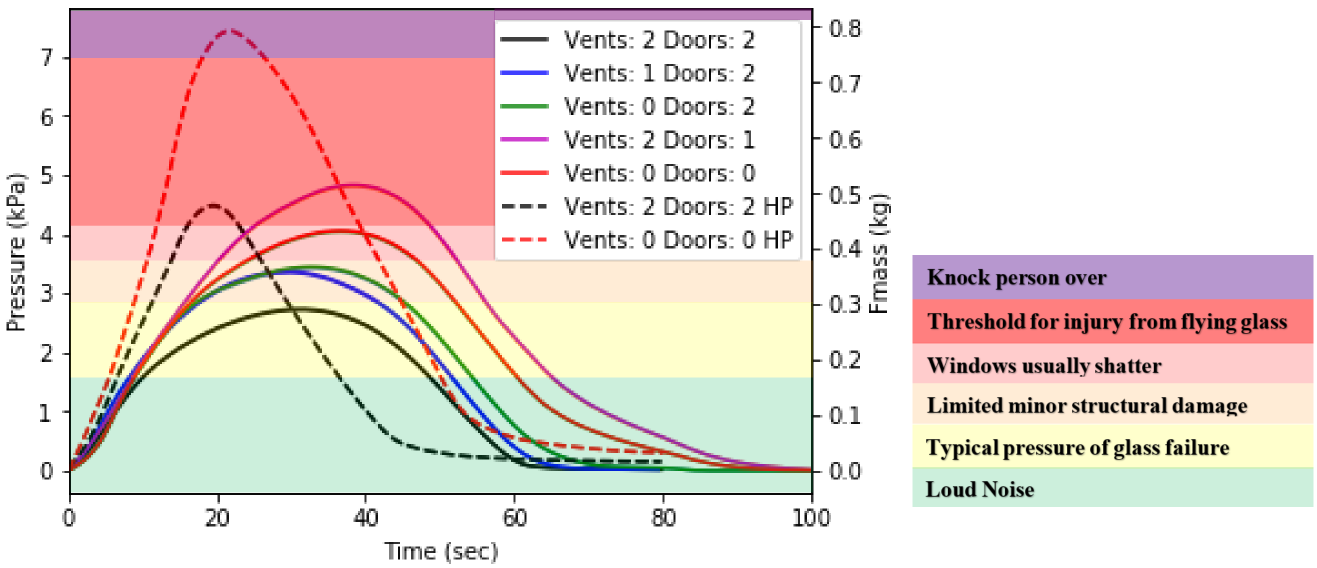



**Figure 9:** Flammable mass and overpressure values per release configuration

The color bands in Figure 9 represent potential harm and damages corresponding to various overpressure levels as described in the key to the right [18]. For the nominal pressure cases, indicated by solid lines, the 2 vents – 1 door configuration results in the largest occurrence of flammable mass and corresponding overpressure. As the closed door was that nearest to the leak, the ventilation actively pushed the expelled vapor to the wall where it coalesced. It is notable that the single vent open garage configuration produced equivalent peak overpressure values as the no vent case. This was attributed to ventilation blockage obstructing air flow beneath the bus, and the formation of eddies along the sides of the bus slowing the spreading of propane gas in that direction. These observations display the importance of both inflow (vent) and outflow (door) locations with respect to the leak.

Comparing the high pressure release to nominal equivalents, a faster blow down is observed as well as a significant increase in peak flammable mass by almost a factor of two. The flammable mass covers significantly larger volume as shown in Table 3, or by comparing Figure 10 to Figure 8.

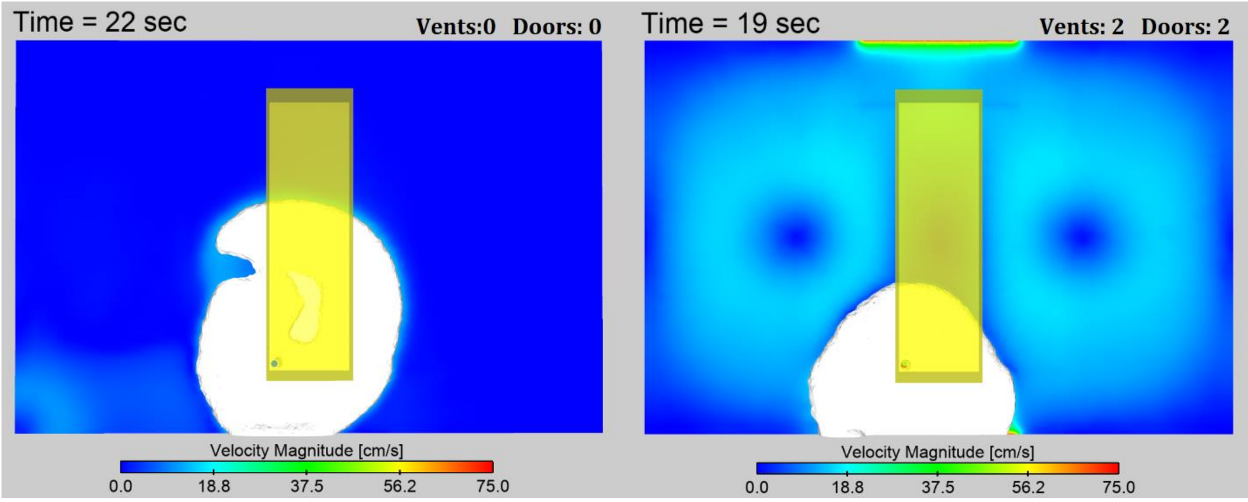



**Figure 10:** Overhead velocity magnitude and flammable gas contour (white) for high pressure configurations

# 5. SUMMARY AND CONCLUSION

In this report we set out to quantify the risk associated with propane releases within maintenance facilities. Our simulation represented a propane bus with a 67 gallon fuel tank in a single vehicle garage with dimensions based off discussions with subject experts. In house CFD software was used to simulate the release of LPG from the pressurized fuel tank into a garage with various configurations. Our results of made clear the importance of ventilation and inflow / outflow location with respect to the fuel release. Ventilation played a critical role in increasing flammable mass dissipation rate and reducing potential peak overpressure in the event of combustion. We also witnessed these positive effects diminishing when the vent location was blocked by the bus or outflow location worked against the ventilation. For the latter, a rather interesting phenomena occurred where the ventilation actually acted against the dissipation of the fuel as it pushed and coalesced the propane gas against the closed garage door and side wall (see Figure 9c for clarification).

Regardless of size and mass of the flammability cloud, using Bauwens and Dorofeev [17] expression for overpressure it was shown peak pressure values only cause minimal structural damage and imposes low probability of harm to humans.

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