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Mini-Project #1
September 21st, 2020

EXECUTIVE SUMMARY

Accident at Belle, West Virginia DuPont facility on January 23rd, 2010 involved the release of toxic phosgene gas to the atmosphere, which was fatal to people, leading to one worker's death from direct exposure. Ruptured transfer hose from the tank was due to the poor management and maintenance of the company, and irresponsibility of workers on site. Two different scenarios in determining the time taken to transfer the phosgene gas to DuPont's own units were analyzed, where scenario I involved the purging of nitrogen gas to remove phosgene out of the tank horizontally, and scenario II meanwhile opened the tank's inlet to the atmosphere and emptied the contents vertically. It was found that it was faster to drain the phosgene with the presence of nitrogen gas at the inlet, in which it only took 79.3 s and 794 s for both scenarios respectively. Plus, the closer the discharge coefficient at the outlet to 1, the quicker the phosgene gas could be drained out of the tank, to prevent pressure built up in the hose due to surrounding temperature, which was the main cause to the sudden rupture in the first place. Application of energy and mass balance was used to analyze the two different scenarios. To minimize the risk of direct exposure, personal protective equipment should be worn all the time when handling toxic chemicals and enclosure units should be built around the working site to prevent atmospheric release which would endanger everyone else.

SAFETY ANALYSIS

Activity

DuPont at Belle, West Virginia used phosgene gas to manufacture five different pesticides intermediates. One ton of phosgene in cylindrical tanks were purchased from one outside company and received on the morning of January 23rd, 2010. The tanks were lifted from the carrier to the weighing scales before they were connected to the stainless steel hoses coated with PTFE to transfer the phosgene to DuPont's own units. The weighing scale and phosgene tanks were exposed to the atmosphere when the process was done. One hose carrying nitrogen gas was attached to the tank to push the phosgene out of another hose. On a daily basis, when one of the tanks was nearly empty, an alarm would go off in the control room, which would alert the workers to close the valve on the empty tank and repeat the process on another tank. The remaining phosgene in the hose would be purged further by nitrogen gas to ensure no remainder left in the hose. Workers were regularly inspecting the process to ensure that everything went smoothly.

Hazard

Phosgene will be compressed when it is put under pressure and it may explode if heated. With acute toxicity of category 1, it is fatal to humans if the gas is inhaled. Fluid will build up in the lungs which can only be discovered a few hours later and if it exceeds lethal doses to humans, it can lead to their deaths. It also can cause skin corrosion and serious eye damage [1]. Based on National Institute for Occupational Safety and Health (NIOSH) recommended exposure limit data, the highest concentration of phosgene gas humans can be exposed to without incurring any adverse health effects within 10 hours of exposure is 0.1 ppm (0.4 $\frac{mg}{m^3}$) [2]. A National Fire Protection Association (NFPA) Diamond of phosgene gas is as shown in **Figure 1** below.

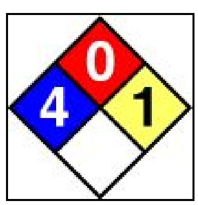


Figure 1: NFPA Diamond of Phosgene Gas (Blue - Health Hazard; Red - Flammability Hazard; Yellow - Instability Hazard; White - Specific Hazard) [3]

In reference to **Figure 1**, phosgene has a level 4 health hazard, indicating extremely high toxic chemicals which are fatal on short-term exposure. With level 1 instability hazard, there may be reactions happening if it is heated or mixed with water. On top of that, with level 0 flammability hazard, it will not burn under normal room conditions [2]. Overall, phosgene is labelled as corrosive and dangerous compressed gas.

Incident

The transfer of phosgene from the tank experienced a flow problem. The hose was not purged with nitrogen gas completely, leading to pressure built up in the hose from warming up around 1.45 pm - 3.00 pm on the same day. When a worker was inspecting the hose, it suddenly exploded, spraying the phosgene gas upto his chest. The leakage was detected by the monitor and he was immediately rushed to the nearby hospital. Unfortunately, he died less than 36 hours later. Two other workers were indirectly exposed to the gas and showed no severe symptoms. The gas was detected on the Kanawha River next to the plant, shortly after the release, and it could have travelled across the river.

Initiating Event

It was found that the PTFE coating the stainless steel hose was susceptible to phosgene, which made it permeable enough to escape and corrode the steel. Based on the DuPont official statement release, a recommendation was made to use Monel, which was a strong metal alloy used in highly corrosive condition, instead of PTFE coating. However, the recommendation was never considered and no actions were done to change the PTFE-coated hose. Moreover, the standard of care was to replace the hose every 30 days of usage. On the day of the accident, the hose had not been replaced for over seven months. On top of that, regular software used for maintenance had been modified for no longer informing the workers to change the hose. The working environment itself was exposed to people and the environment. In 2004, it was suggested to build enclosure units around the phosgene working site, and it was expected to be completed by December 2005. Nonetheless, the deadlines were extended for over many times and still could not be met up to January 2010.

Preventative Actions

DuPont should immediately change the coating of the stainless steel hose to Monel. Although it has a higher cost than PTFE, it has a longer useful life of three months, in which in the long run, the cost will be much lower and improve the safety overall. Furthermore, the management of the control room should improve the maintenance system to regularly inform the workers to change the hose on a monthly basis. Automated audible alarms could be used in place to automatically inform the workers without the control manager to work on it manually. Moreover, secondary enclosure units for phosgene should be built in order to prevent any phosgene leak to the atmosphere, including the installation of mechanical ventilation systems and emergency phosgene scrubbers. Specifically to workers who work in the enclosure units, personal protective equipment should be worn all the time to avoid any contact with the phosgene gas in case of sudden release of gas.

Contingency Plan

The management should always take serious consideration to any situation where the alarm went off. They should not completely dismiss the alarm just basing the decision from the fact of the previous incidents with false alarms, unless further inspections were made to prove that there is no emergent hazard to be taken care of. Also, workers should be given proper training in handling such emergencies in order to be fully equipped and prepared if similar incidents happen in the future. Plus, DuPont should revise its near-miss reporting and investigation policy to emphasize anonymous participation by all employees, including addressing all minor problems before they become serious. Besides, the industry organizations should adopt more stringent guidelines of the NFPA for the safe handling of phosgene and other highly toxic gases and referring to Occupational Safety and Health Administration (OSHA) to keep updated with its compressed gas safety standard, including the modern safeguards for toxic gases.

Lessons Learned

The main lesson that can be learnt from the incident is definitely on how the company should perform its maintenance on the working site. It is essential that safety precautions be established on any site, even though it can incur high cost to the company. One cannot predict what might happen in the long run, where investing on safety now is important. Organizational behavior and working environment are also other important factors to take into account for a big company. Low conscientiousness and agreeableness level on employees are not going to contribute to a healthy environment to work at. Employees should be more responsible for their work and cooperate with others in making sure things align and by the way things are supposed to be done. Plus, the Chemical Safety and Hazard Investigation Board (CSB) learnt that the general guidelines published for handling toxic gases are not always suitable for all gases. It is advised to always refer to the NFPA for the safest and updated ways in handling these toxic gases. A BowTie diagram summarizing the incident is as shown in **Figure 2**, followed by the descriptions of the accident.

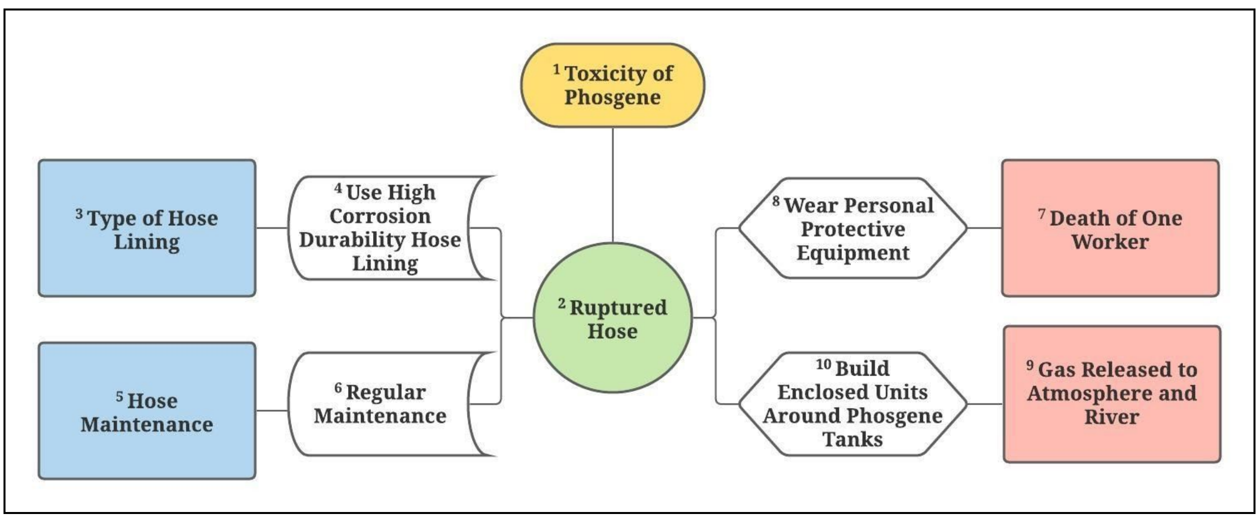


Figure 2: BowTie Diagram [4] of The DuPont Accident

Based on **Figure 2**, the diagram labelled as 1 represents the hazard associated with the accident. Point 2 represents the initiating event which was due to point 3 and 5, which are the potential problems. 4 and 6 are preventative actions to the problems for 3 and 5 respectively. 7 and 9 represent the consequences of the accident, which can be mitigated by appropriate actions listed as 8 and 10 respectively.

SCENARIO ANALYSIS

There are two different scenarios analyzed in these problems. Scenario I involves the removal of phosgene gas out of the bottom valve of the cylindrical tank horizontally, with the aid of nitrogen gas with a constant pressure of 70 psig from the top inlet. Meanwhile, scenario II utilizes the effect of gravity and empties the contents vertically out of the outlet, where the top inlet is exposed to the atmosphere. Same amount of phosgene gas originally in the tank for both scenarios.

Height of Fluid in Tank Over Time

Figure 3 below shows a graphical representation of the relationship between height of fluid with time for scenario II with varying C_V. The data points were plotted by using **Eq. 1**, which was derived as shown in **Appendix A**.

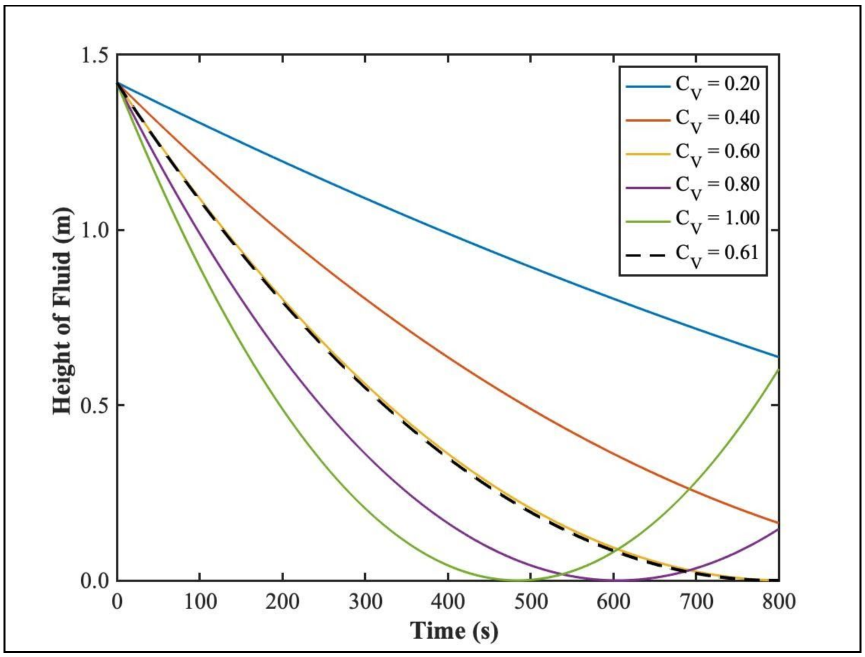


Figure 3: Graph of Fluid Height vs. Time of Varying C_V with Inlet Opened to Atmosphere

$$z(t) = \left(\sqrt{z_0} - \frac{C_V A_{Outlet}\sqrt{2g}}{2A_{Inlet}} t\right)^2 \quad \textbf{(Eq. 1)}$$

$$z_0 = 1.421m; \ \frac{A_{Outlet}}{A_{Inlet}} = \frac{1}{900}; \ g = 9.81\frac{m}{s^2}$$

As depicted in **Figure 3**, as time progresses, the height of phosgene gas in the tank decreases. Looking at specifically discharge coefficient, C_V of 0.61 from the figure above, the tank is fully emptied after approximately 800 s. To be exact, the tank is emptied after 794 s. The calculation is as shown in **Appendix A**. By varying the value of C_V, the tank can be emptied either faster or slower than C_V of 0.61. As shown in the same figure, the closer the value of C_V to 1, the faster the tank can be emptied completely. C_V took into account the friction losses that the fluid experienced. When C_V is equal to 1, it represents a non-friction ideal situation, and provides the minimum amount of time the fluid can be removed from the tank. The problem is further analyzed with a constant C_V of 0.61 by changing the inlet condition, where the tank is then exposed to varying pressure of nitrogen gas. **Figure 4** shows the relationship between height of fluid with time for scenario II of varying inlet pressure. The graph is plotted by using **Eq. 2** as derived in **Appendix B**.

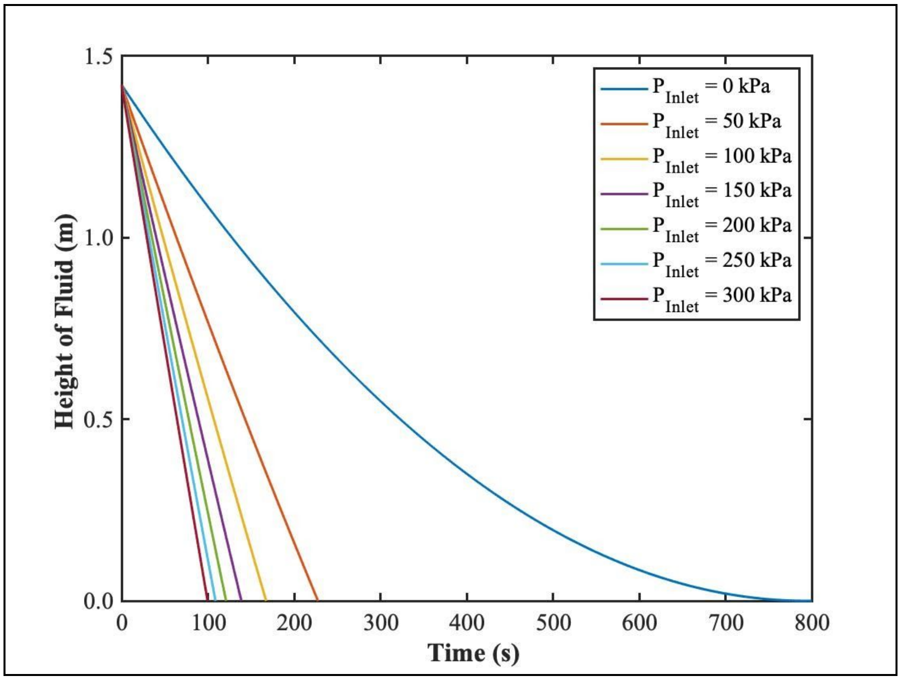


Figure 4: Graph of Fluid Height vs. Time of Varying Inlet Pressure of C_V = 0.61

$$z(t) = \frac{1}{g}\left[\left(\sqrt{\frac{P_{Inlet}}{\rho} + z_0 g} - \frac{C_V A_{Outlet}\sqrt{2g}}{2A_{Inlet}}t\right)^2 - \frac{P_{Inlet}}{\rho}\right] \textbf{(Eq. 2)}$$

$$z_0 = 1.421m;\ \frac{A_{Outlet}}{A_{Inlet}} = \frac{1}{900};\ g = 9.81\frac{m}{s^2};\ \rho = 1400\frac{kg}{m^3}$$

As depicted in **Figure 4** above, varying the inlet pressure of nitrogen gas has a significant impact in the time taken to completely withdraw the phosgene gas out of the tank. When the inlet pressure is 0 kPa, the condition is exactly the same as shown in **Figure 3**, with the same C_V of 0.61. As the inlet pressure increases, assuming constant flow of nitrogen gas into the tank, the time taken to empty the tank decreases. This is the case because higher pressure of nitrogen gas will push the phosgene gas out quicker and more efficiently, despite the diameter of the outlet. In scenario I, it takes 79.3 s to completely drain the contents, but it takes 10 times longer in scenario II, which is 794 s. The calculation is as shown in **Appendix A** and **C**.

Escaping Volumetric Flow Rate Over Time

Figure 5 below shows the plot of volumetric flow rate of phosgene gas exiting the outlet against time for scenario II with varying C_V values. The graph is plotted by using **Eq. 3**, derived as shown in **Appendix B**.

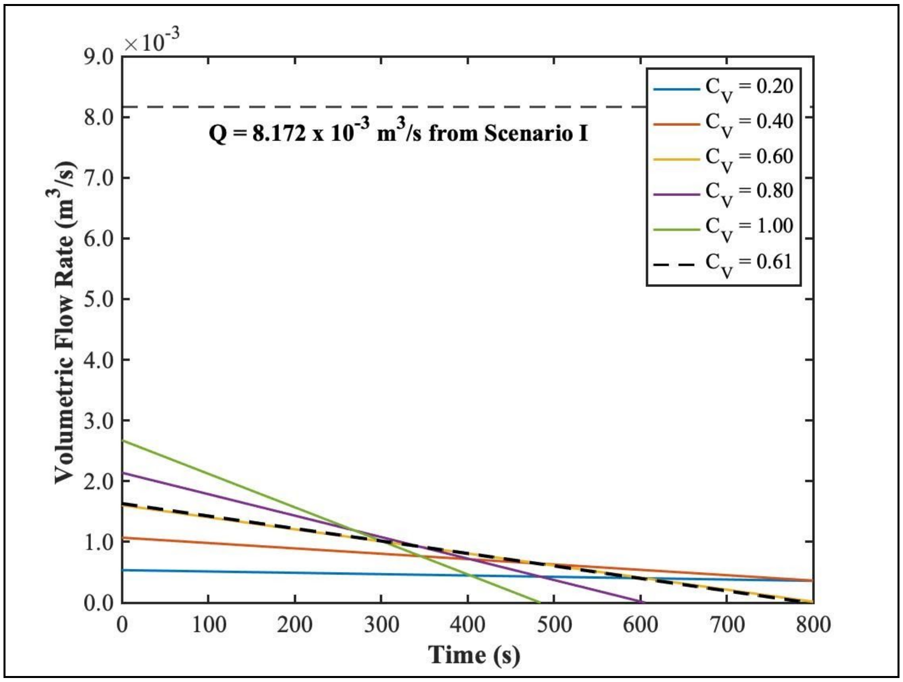


Figure 5: Graph of Volumetric Flow Rate vs. Time of Varying C_V with Tank Opened to Atmosphere

$$Q(t) = C_V A_{Outlet}\sqrt{2g}\left(\sqrt{z_0} - \frac{C_V A_{Outlet}\sqrt{2g}}{2A_{Inlet}}t\right) \quad \textbf{(Eq. 3)}$$

$$z_0 = 1.421m;\ \frac{A_{Outlet}}{A_{Inlet}} = \frac{1}{900};\ g = 9.81\frac{m}{s^2};\ A_{Outlet} = 5.067 \times 10^{-4}m^2$$

As illustrated in **Figure 5** above, the volumetric flow rate decreases as time progresses. The magnitude of change in volumetric flow rate with time depends on the value of C_V. It could be observed that the volumetric flow rate starts at a higher rate as C_V approaches 1, and completely drains the tank quicker. The dashed line shown above represents the volumetric flow rate of Cv = 0.61. In scenario I, the flow rate is assumed to be constant. Scenario II has the rate to be changing with time and has an overall rate of lower than scenario I. From the observation, it makes sense to have the gas drained quicker in scenario I than II because it has much greater flow rate. Assuming now the inlet tank is opened to varying pressure of nitrogen gas, at the same C_V of 0.61 the volumetric flow rate changes with time are as demonstrated in **Figure 6** for scenario II. The graph is plotted by using **Eq. 4** as derived in **Appendix B**.

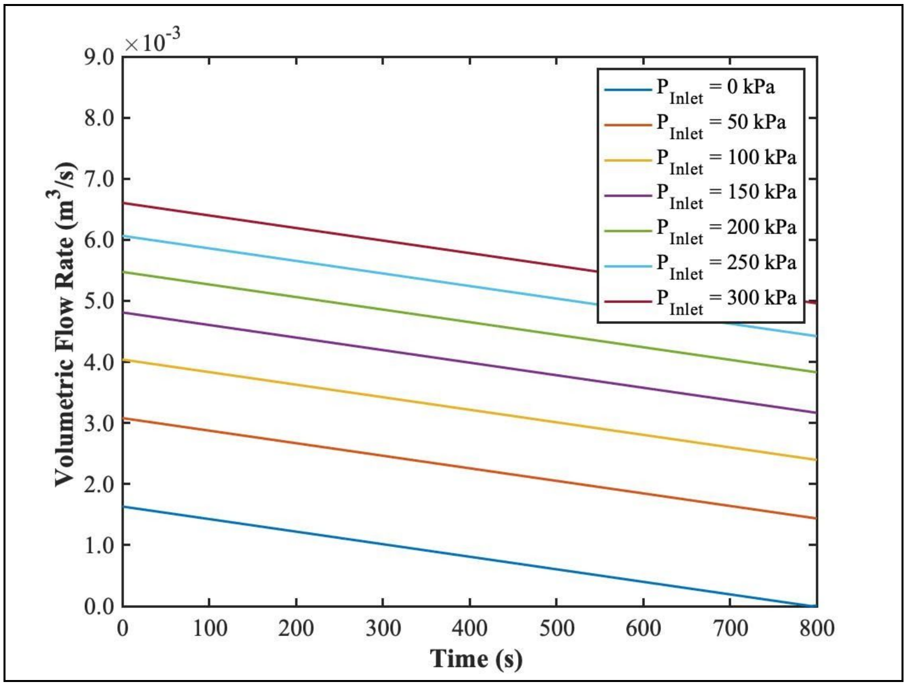


Figure 6: Graph of Volumetric Flow Rate vs. Time of Varying Inlet Pressure of C_V = 0.61

$$Q(t) = C_V A_{Outlet}\sqrt{2}\left(\sqrt{\frac{P_{Inlet}}{\rho} + z_0 g} - \frac{C_V A_{Outlet}\sqrt{2}g}{2A_{Inlet}}t\right) \quad \textbf{(Eq. 4)}$$

$$z_0 = 1.421m;\ \frac{A_{Outlet}}{A_{Inlet}} = \frac{1}{900};\ g = 9.81\frac{m}{s^2};\ \rho = 1400\frac{kg}{m^3};\ A_{Outlet} = 5.067 \times 10^{-4}m^2$$

From **Figure 6** shown above, the lines of volumetric flow rate have the same gradients but different intercepts. The initial flow rate is greater as the pressure of nitrogen gas increases. 0 kPa of nitrogen gas above represents the same condition as the prompt initially, which was the inlet exposed to the atmosphere. The intersection of lines at the x-axis in the figure does not represent the time taken for the tank to be completely empty. From the equation itself, the pressure does not affect the gradient of the line, but only the intercept. Constant flow of nitrogen gas from the inlet out causing the volumetric flow rate to be beyond the range shown above. The key finding from the graph shown above is as the pressure increases, the greater the volumetric flow rate is, thus the quicker to empty the tank. **Figure 3 - 6** were plotted using MATLAB and the codes are as provided in **Appendix D-I** and **D-II**.

Significance of These Estimations

Based on the given two scenarios, the time taken to completely remove the phosgene gas out of the tank for scenario I is shorter than scenario II, which are 79.3 s and 794 s respectively. It is important to acknowledge the transfer time of phosgene gas in order to figure out how long the gas is flowing through the transfer hose to avoid pressure built up due to the rise of surrounding temperature. Despite the different tank position in both scenarios, one might think transferring vertically would be faster due to the effect of gravity. However, the key takeaway from both scenarios is the presence of nitrogen gas to purge the phosgene gas out. Scenario I has a more challenging analytical solution than scenario II because the surface area of phosgene (the interface between phosgene and nitrogen) is constantly changing as the height of phosgene decreases. For the ease of calculation, volumetric flow rate is assumed to be constant instead. It is necessary to know the volumetric outflow rate in designing the safeguards around the tank due to the main reason previously mentioned, which is to avoid built-up pressure in the hose. Moreover, the quicker the gas transfer is, the lower the probability of the hose to rupture during the regular inspection by the workers, if the ruptures were to happen. On top of that, the tank height also has a significant factor in designing tanks' safeguards. Much lower tank height that still can accommodate the same volume of phosgene, can lower its center of gravity. The chances of workers to experience physical injuries due to fallen tanks when working is lowered due to the more stable tanks. The calculations made previously can be used as estimations to inform potential hazard to employees. The company should install a program to constantly monitor the flow rate of phosgene out of the tank. The flow rate calculated can be used as baselines and if there are sudden changes in flow rate, either higher or lower, inspection can be made on the working site, fully equipped with proper protections. The change in flow rate can indicate leakage of gas which can be fatal to everyone.

PERSONAL REFLECTION

The most unsettling thing about the incident to me is the work ethics and responsibility possessed by the workers and management. Looking specifically at the working site for phosgene gas, the maintenance systems to alert every worker to change the transfer hose monthly was turned off. No one ever raised any concern and asked the reasons why no future maintenance was needed to replace the hose regularly. The management wise was short-sighted by the fact that they were only looking at the current costs and profit, but not the future benefits and safety improvement for the company. If they were to follow the recommendations made to use Monel to replace PTFE coating on the hose and built enclosure units around phosgene tanks, the incident could be prevented from happening in the first place. My knowledge of fluid dynamics helps me to assess the safety concerns in determining the time taken to discharge the phosgene gas completely out of the tank. The application of mass and energy balance in understanding the volumetric outflow rate a tank can have is used as estimations for designing safeguards in handling toxic phosgene gas. Longer time to transfer the gas may cause pressure built up in the tank and hose, which should raise everyone's concern in potential release of hazardous materials to the surrounding.

The incident taught me to be extra careful in the workplace, especially involving the handling of hazardous chemicals like phosgene. I should strictly follow the RAMP procedure, which includes recognizing the hazard, assessing and minimizing risks, and preparing for any emergencies that may happen [5]. I should practice wearing personal protective equipment everytime working with hazardous and toxic chemicals. Prior to entering any chemical engineering potential jobs in the future, it is important to acquire as much information about the company as possible to avoid lethal safety incidents that may happen to me if I were to work with them. One of the important information includes the incident rates of the company. Both disclosed and concealed reports on any incident related to the company should be obtained, either from online or directly from the company during job interviews. Furthermore, knowing the workers turnover rates is also important to recognize the working environment as teams and organization as a whole. High turnover rates may indicate poor management or lack of work motivation, which shows bad sign for the company to work for.

REFERENCES

[1] VanDeMark. Safety Data Sheets - Phosgene http://vandemark.com/wp-content/uploads/MSDS_Other_Phosgene_Products/PHOSGENE-SDS.pdf (accessed Sep 20, 2020).

[2] CDC - The Emergency Response Safety and Health Database: Lung Damaging Agent: PHOSGENE (CG) - NIOSH https://www.cdc.gov/niosh/ershdb/emergencyresponsecard_29750023.html (accessed Sep 20, 2020).

[3] National Fire Protection Association Hazard Identification System https://www.acs.org/content/acs/en/chemical-safety/basics/nfpa-hazard-identification.html (accessed Sep 20, 2020).

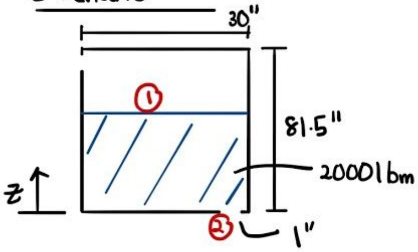
[4] BowTie Diagram http://umich.edu/~safeche/bowtie.html (accessed Sep 20, 2020).

[5] Safety, L. RAMP: Recognize, Assess, Minimize, Prepare https://wp.stolaf.edu/chemical-hygiene/ramp-recognize-assess-minimize-prepare/ (accessed Sep 20, 2020).

APPENDIX

Appendix A

Scenario II



$$2000\ \cancel{lbm}\left(\frac{0.4536\ \cancel{kg}}{\cancel{lbm}}\right)\left(\frac{m^3}{1400\ \cancel{kg}}\right) = 0.648\ m^3$$

$$\frac{\pi}{4}D^2 H = 0.648\ m^3$$

$$D = 30\ \cancel{in}\left(\frac{1\ \cancel{ft}}{12\ \cancel{in}}\right)\left(\frac{0.3048\ m}{1\ \cancel{ft}}\right) = 0.762\ m$$

(iii) $H = \dfrac{4(0.648\ m^3)}{\pi\ (0.762\ m)^2} = 1.421\ m$ (initial height of fluid)

system: phosgene gas in the tank

$\Rightarrow$ Again, $A_1 \ggg A_2$, system in steady state!

1 in/out, incompressible, $W_s = 0$, $\mathcal{F} = 0$ (for now, C_v will incorporate it!)

$$\cancel{\frac{P_1}{\rho}} + \cancel{\frac{V_1^2}{2}} + z_1 g = \cancel{\frac{P_2}{\rho}} + \frac{V_2^2}{2} + \cancel{z_2 g}$$

$P_1 = P_2 = P_{atm} = 0$ (gauge), $V_1 = 0$, $z_2 = 0$

$$V_2 = \sqrt{2 z_1 g} = \sqrt{2 z g}$$

$$\frac{dm}{dt} = -\dot{m}_{out}$$

$$\cancel{\rho} A_1 \frac{dz}{dt} = -\rho Q = -\cancel{\rho} C_D V_2 A_2$$

$$\frac{dz}{dt} = -\frac{C_v A_2}{A_1}\sqrt{2 z g}$$

$$\int_{z_0}^{z(t)} \frac{dz}{\sqrt{z}} = -\frac{C_v A_2 \sqrt{2g}}{A_1}\int_0^t dt$$

$$2\left[\sqrt{z}\,\right]_{z_0}^{z(t)} = -\frac{C_v A_2 \sqrt{2g}\ t}{A_1}$$

$$\sqrt{z(t)} - \sqrt{z_0} = -\frac{C_v A_2 \sqrt{2g}\ t}{2 A_1}$$

$$\boxed{z(t) = \left(\sqrt{z_0} - \frac{C_v A_2 \sqrt{2g}\ t}{2 A_1}\right)^2}$$

$$\frac{C_v A_2 \sqrt{2g}}{2 A_1} = \frac{0.61 \cdot (1\ \cancel{in})^2 \sqrt{2(9.81\ \frac{m}{s^2})}}{2\ (30\ \cancel{in})^2} = 1.501 \times 10^{-3}\ m^{1/2}/s$$

$$\sqrt{z_0} = 1.192\ m^{1/2}$$

$$\boxed{z(t) = (1.192 - 1.501 \times 10^{-3} t)^2}$$

empty tank, $z(t) = 0$

$$1.501 \times 10^{-3} t = 1.192$$

$$t = \frac{1.192\ \cancel{m^{1/2}}}{1.501 \times 10^{-3}\ \cancel{m^{1/2}}/s}$$

$$\boxed{t = 794\ s}$$

Appendix B

(iv) $$z(t) = \left(\sqrt{z_0} - \frac{C_v A_2 \sqrt{2g}}{2A_1} t\right)^2$$

$$Q(t) = C_v A_2 v(t)$$

$$v(t) = \sqrt{2 g z(t)}$$ ⇒ same condition as before.

$$Q(t) = C_v \cdot A_2 \sqrt{2g\left(\sqrt{z_0} - \frac{C_v A_2 \sqrt{2g}}{2A_1} t\right)^2}$$

$$\boxed{Q(t) = C_v A_2 \sqrt{2g} \cdot \left(\sqrt{z_0} - \frac{C_v A_2 \sqrt{2g}}{2A_1} t\right)}$$

* If there were still N_2 pressure in the tank

$$\frac{P_1}{\rho} + \cancel{\frac{V_1^2}{2}} + z_1 g = \cancel{\frac{P_2}{\rho}} + \frac{V_2^2}{2} + \cancel{z_2 g}$$

$V_1 = 0$, $z_2 = 0$, $P_2 = P_{atm} = 0$ (gauge), $P_1 = P_{N_2}$

$$V_2 = \sqrt{2\left(\frac{P_1}{\rho} + z_1 g\right)} = \sqrt{2\left(\frac{P_1}{\rho} + zg\right)}$$

system : phosgene gas in the tank.

$$\frac{dm}{dt} = -\dot{m}_{out}$$

$$\cancel{\rho} A_1 \frac{dz}{dt} = -\rho C_v A_2 V_2 = -\cancel{\rho} C_v A_2 \sqrt{2\left(\frac{P_1}{\rho} + zg\right)}$$

$$\int_{z_0}^{z(t)} \frac{dz}{\sqrt{\frac{P_1}{\rho} + zg}} = -\frac{\sqrt{2}\, C_v A_2}{A_1} \int_0^t dt$$

$u = \frac{P_1}{\rho} + zg$.

$du = g\,dz \Rightarrow dz = \frac{1}{g} du$.

$$\int \frac{du}{\sqrt{u}} = -\frac{\sqrt{2}\, g\, C_v A_2 t}{A_1}$$

$$\left[\sqrt{\frac{P_1}{\rho} + zg}\right]_{z_0}^{z(t)} = \frac{-\sqrt{2}\, g\, C_v A_2 t}{2A_1}$$

$$\sqrt{\frac{P_1}{\rho} + z(t) g} - \sqrt{\frac{P_1}{\rho} + z_0 g} = \frac{-\sqrt{2}\, g\, C_v A_2 t}{2A_1}$$

$$\sqrt{\frac{P_1}{\rho} + z(t) g} = \sqrt{\frac{P_1}{\rho} + z_0 g} - \frac{\sqrt{2}\, g\, C_v A_2}{2A_1} t$$

$$\boxed{z(t) = \frac{1}{g}\left[\left(\sqrt{\frac{P_1}{\rho} + z_0 g} - \frac{\sqrt{2}\, g\, C_v A_2}{2A_1} t\right)^2 - \frac{P_1}{\rho}\right]}$$

$$Q(t) = C_v A_2 V(t)$$

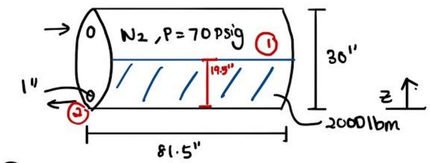
$$Q(t) = C_v A_2 \sqrt{2\left(\frac{P_1}{\rho} + z(t) g\right)}$$

$$Q(t) = C_v A_2 \sqrt{2\left[\cancel{\frac{P_1}{\rho}} + \left(\sqrt{\frac{P_1}{\rho} + z_0 g} - \frac{\sqrt{2}\, g\, C_v A_2}{2A_1} t\right)^2 - \cancel{\frac{P_1}{\rho}}\right]}$$

$$\boxed{Q(t) = C_v A_2 \sqrt{2}\left(\sqrt{\frac{P_1}{\rho} + z_0 g} - \frac{\sqrt{2}\, g\, C_v A_2}{2A_1} t\right)}$$

Appendix C

Scenario I



$C_v = 0.61$

$\rho = 1.4 \frac{g}{cm^3}$ (constant)

T = 55°F, $T_{bp} = 47$°F (gas @ STP)

(i) Since $A_1 >>> A_2$, we can assume steady state!

1 in/out, incompressible fluid, $W_s = 0$, $\cancel{q} = 0$ for now (incorporate w/ C_v)

$$\frac{P_1}{\rho} + \cancel{\frac{V_1^2}{2}} + z_1 g = \cancel{\frac{P_2}{\rho}} + \frac{V_2^2}{2} + \cancel{z_2 g}$$

$V_1 = 0$, $P_2 = P_{atm} = 0$ (gauge), $P_1 = P_{N_2} = 70$ psig, $z_2 = 0$, $z_1 = 19.5$ in

$$V_2 = \sqrt{2\left(\frac{P_1}{\rho} + z_1 g\right)}$$

$$P_1 = 70\,\cancel{psig}\left(\frac{144\,\cancel{lbf}}{1\,\cancel{psig}\cdot\cancel{ft^2}}\right)\left(\frac{32.17\,(\cancel{lbm}\cdot\cancel{ft})}{1\,\cancel{lbf}\cdot s^2}\right)\left(\frac{0.4536\,kg}{1\,\cancel{lbm}}\right)\left(\frac{1\,\cancel{ft}}{0.3048\,m}\right)$$

$$= 482\,580.40\ \frac{kg}{m\cdot s^2} = 482\,580.40\ Pa$$

$$z_1 = 19.5\,\cancel{in}\left(\frac{1\,\cancel{ft}}{12\,\cancel{in}}\right)\left(\frac{0.3048\,m}{\cancel{ft}}\right) = 0.4953\ m$$

$$\rho = 1.4\,\frac{\cancel{g}}{\cancel{cm^3}}\left(\frac{1\,kg}{1000\,\cancel{g}}\right)\left(\frac{10^2\,\cancel{cm}}{1\,m}\right)^3 = 1400\ \frac{kg}{m^3}$$

$$V_2 = \sqrt{2\left[\frac{482\,580.40\ \frac{kg}{m\cdot s^2}}{1400\ kg/m^3} + 0.4953\,m\left(9.81\,\frac{m}{s^2}\right)\right]}$$

$V_2 = 26.44$ m/s

@ t = 0, $Q_2 = C_v V_2 A_2$

$$A_2 = \frac{\pi}{4}(1\,\cancel{in})^2\left(\frac{1\,\cancel{ft}}{12\,\cancel{in}}\right)^2\left(\frac{0.3048\,m}{1\,\cancel{ft}}\right)^2 = 5.067\times10^{-4}\ m^2$$

$$\boxed{Q_2 = 0.61\left(26.44\,\frac{m}{s}\right)\left(5.067\times10^{-4}\,m^2\right) = 8.172\times10^{-3}\ m^3/s}$$

(ii) $Q_2 = 8.172\times10^{-3}$ m³/s ⇒ assumed constant

system: the phosgene gas in the tank

$$\frac{dm}{dt} = -\dot{m}_{out} = -\rho Q$$

$$\int_{m_0}^{m(t)} dm = -\rho Q \int_0^t dt$$

$$m(t) - m_0 = -\rho Q t$$

$$t = \frac{m_0 - m(t)}{\rho Q}$$

$$m_0 = 2000\ lbm\left(\frac{0.4536\,kg}{1\,lbm}\right) = 907.2\ kg$$

$m(t) = 0$, $\rho = 1400\ \frac{kg}{m^3}$

$$t = \frac{907.2\,\cancel{kg}}{1400\,\frac{\cancel{kg}}{\cancel{m^3}}\left(8.172\times10^{-3}\,\frac{\cancel{m^3}}{s}\right)}$$

$$\boxed{t = 79.30\ s}$$

Appendix D-I

```
t = linspace(0,1000,1001); % s
cv_fix = 0.61; % fix value of cv
cv = linspace(0.2,1,5);
a2a1 = 1/900; % ratio of outlet area to surface
z0 = 1.421; % initial height, m
g = 9.81; % m/s^2
a2 = 5.067e-4; % area of outlet, m^2

z1 = (sqrt(z0) - cv_fix/2*a2a1*sqrt(2*g).*t).^2;
q1 = cv_fix*a2*sqrt(2*g)*(sqrt(z0) - cv_fix/2*a2a1*sqrt(2*g).*t);
```

<u>Plot of z(t) and Q(t) vs t for many Cv (w/ fixed Cv too)</u>

```
for i = 1:length(cv)
        z2 = (sqrt(z0) - cv(i)/2*a2a1*sqrt(2*g).*t).^2;
        plot(t,z2,'linewidth',1.5)
        hold on
end
plot(t,z1,'color','k','LineWidth',1.5,'LineStyle',"--")
xlabel('\bf \fontname{Times} Time (s)')
ylabel('\bf \fontname{Times} Height of Fluid (m)')
legend('C_V = 0.20','C_V = 0.40','C_V = 0.60','C_V = 0.80','C_V = 1.00','C_V = 0.61')
ax = gca; ax.FontSize = 15; ax.FontName = 'times'; ax.LineWidth = 1.5;
ax.XLim = [0 800];ax.YLim = [0 1.5]; ytickformat('%.1f')
hold off

for i = 1:length(cv)
        q2 = cv(i)*a2*sqrt(2*g)*(sqrt(z0) - cv(i)/2*a2a1*sqrt(2*g).*t);
        plot(t,q2,'linewidth',1.5)
        hold on
end
plot(t,q1,'color','k','LineWidth',1.5,"LineStyle","--")
yline(8.172e-3,'color','k','linewidth',1.5,'linestyle','--');
text(100,7.8e-3,"Q = 8.172 x 10^-^3 m^3/s from Scenario I",'FontName','times', ...
        "FontWeight","bold","FontSize",15)
xlabel('\bf \fontname{Times} Time (s)')
ylabel('\bf \fontname{Times} Volumetric Flow Rate (m^3/s)')
legend('C_V = 0.20','C_V = 0.40','C_V = 0.60','C_V = 0.80','C_V = 1.00','C_V = 0.61')
ax = gca; ax.FontSize = 15; ax.FontName = 'times'; ax.LineWidth = 1.5;
ax.XLim = [0 800];ax.YLim = [0 9e-3];ytickformat('%.1f')
hold off
```

Appendix D-II

Plot of z(t) and Q(t) vs t for Cv = 0.61 with many N2 pressure

```
P1 = linspace(0,3e5,7); % Pa, pressure inlet
rho = 1400; % kg/m^3
for i = 1:length(P1)
    z3 = 1/g*((sqrt(P1(i)/rho + z0*g) - sqrt(2)/2*g*cv_fix*a2a1.*t).^2 - P1(i)/rho);
    plot(t,z3,'linewidth',1.5)
    hold on
end
xlabel('\bf \fontname{Times} Time (s)')
ylabel('\bf \fontname{Times} Height of Fluid (m)')
legend('P_I_n_l_e_t = 0 kPa','P_I_n_l_e_t = 50 kPa','P_I_n_l_e_t = 100 kPa','P_I_n_l_e_t = 150 kPa', ...
    'P_I_n_l_e_t = 200 kPa','P_I_n_l_e_t = 250 kPa','P_I_n_l_e_t = 300 kPa')
ax = gca; ax.FontSize = 15; ax.FontName = 'times'; ax.LineWidth = 1.5;
ax.XLim = [0 800];ax.YLim = [0 1.5];ytickformat('%.1f')
hold off

for i = 1:length(P1)
    q3 = cv_fix*a2*sqrt(2*(sqrt(P1(i)/rho + z0*g) - sqrt(2)/2*g*cv_fix*a2a1.*t).^2);
    plot(t,q3,'linewidth',1.5)
    hold on
end

xlabel('\bf \fontname{Times} Time (s)')
ylabel('\bf \fontname{Times} Volumetric Flow Rate (m^3/s)')
legend('P_I_n_l_e_t = 0 kPa','P_I_n_l_e_t = 50 kPa','P_I_n_l_e_t = 100 kPa','P_I_n_l_e_t = 150 kPa', ...
    'P_I_n_l_e_t = 200 kPa','P_I_n_l_e_t = 250 kPa','P_I_n_l_e_t = 300 kPa')
ax = gca; ax.FontSize = 15; ax.FontName = 'times'; ax.LineWidth = 1.5;
ax.XLim = [0 800];ax.YLim = [0 9e-3];ytickformat('%.1f')
hold off
```