

## Simulation Analysis of Air Temperature Effects on Propylene Storage Tank Leaks

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### Abstract

Advance computer simulations can help getting ideas about chemical spills and how to mitigate those critical emergency situations. A propylene ( $C_3H_6$ ) storage tank is considered for this analysis to learn hazard involve from its leaks. The analysis reveals using the software the extent of damage to nearby neighborhoods and surroundings. This analysis also leads to scientific strategies for propylene storage leak safety management. This software is used in the classrooms for this study over the years to teach chemical spill. Students' comments and responses indicate that they like this software as it is easy to use and has very user-friendly Graphical User Interface (GUI). Classroom and training class discussions using this software will save money to do chemical spill mitigation and control in house with expensive devices. Furthermore, to the best of the author knowledge, this is the first reported work where chemical spill hazards related to air temperature using this software is used which is an inexpensive way to prepare and control chemical spills.

### Keywords: Propylene, Chemical Spill, ALOHA, Air Temperature, Computer Simulation.

### **Introduction:**

Everyone's dependence on energy especially fossil fuels production and usage is growing day by day. The petroleum industries face many challenges during drilling, extracting, production, refining, storing, transporting, and usage [1]. Large leak can happen from any stage from drilling to usage due to mismanagement, mishandling, disoperation, material degradation like corrosion etc. which can cause catastrophic consequence. One of the important chemical propylene is among those which can be hazardous during those phases. When leak happen due to corrosion over the years, hit by truck, man-made emergency etc. the place where it occurs to nearby neighborhoods suffer the consequence especially if the chemical is very flammable, explosive, and toxic in nature. Up to now, various researchers have studied the hazardous chemical leak diffusion models which include theoretical analysis, experimental research, and practical application [1, 2]. Compared to other commercial softwares, Environmental Protection Agency (EPA) made Aloha [3] is an opensource and very good software to address this simulation properly.

Among various environmental parameters on dispersion, Temperature plays an important role for dispersion of this chemical leak and spill. In this study, a horizontal propylene tank is considered. The present study aimed to determine how temperature variations or fluctuations from different time and day of the year (summer, fall, winter, and spring seasons) have effects on chemical propylene leak and spreading by using Aloha software.

Chemical leak is a point of interest for various literatures. Yang et al. [2] conducted simulation on propylene leak using Aloha software [3]. Their study specified location on a city in China. There was no discussion about leak scenarios in some other places where temperature varies over the year. Also, their study did not look at temperature effects on propylene chemical leaks. The author has followed Yang et al. [2] for baseline study.

This paper provided information about what has been done with simulations in the past in chemical spill education and how this paper attempts to close a gap. Although, various chemical engineering topics are discussed in the classrooms over the years, however chemical spill discussions with simulation software usage in the classrooms has not been done before according to author's knowledge.

The literature reveals lack of study of temperature effects on dispersion of propylene leak on environment. Therefore, this study focused this issue to find different temperature variations that occurs over the years due to seasons change on chemical leak dispersion.

### **Physicochemical Properties of Propylene:**

Molecular weight of Propylene ( $C_3H_6$ ) is about 42 g/mol which is heavier than air. It is a colorless and slightly sweet gas at room temperature. It is an asphyxiated but mildly anesthetic gas. It has carcinogenic effect, is undissolved in water, however soluble in organic solvents. Its freezing temperature is -185.2°C, boiling temperature is -47.4°C, autoignition temperature of 460°C, and flash point temperature of -108°C. Vapor pressure of this chemical is higher than atmospheric pressure. These data indicate that this chemical will turn to gas instantly as soon as

it is exposed to environment. It is the basic raw material of three major chemicals: mainly used in the production of polypropylene, as well as for acetone and propylene oxide.

### Software Introduction and Features:

Areal Locations of Hazardous Atmospheres (Aloha) software is developed by National Oceanic and Atmospheric Administration (NOAA) and EPA is a hazard modeling software and is widely used to plan and respond to chemical emergencies like leak. This software is used by people who handle chemical spills, prepare emergency solutions and related training, and can observe concentration diffusion, toxicity variation, flammability, heat of toxic gas diffusion, fire and explosion of important hazardous chemicals from a list of chemicals in a certain area.

The level of hazard that may occur after propylene storage tank leaks encompassed human beings, animals, environment, and properties etc. However, the focus of this study is on the damage caused by the explosion due to high pressure, poisoning due to toxicity, heat effects of radiation and convection, and vapor cloud explosion.

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### **Base Study:**

This study considered the site, tank, and environmental parameters used for Propylene chemical spill base study simulation [2]. The volume of the tank is 50m<sup>3</sup>, whereas the design pressure of the storage tank is 2.16 MPa considering the filling factor of 0.9. The diameter of the horizontal aligned cylindrical tank is 2.6 m and length is 9.42 m. The tank chemical phase is liquid, whereas temperature inside and outside the tank is 8.77°C. Ambient Relative humidity is 62%, annual maximum frequency wind speed is 2.4 m/s with SE direction. The tank is in unsheltered single storied condition and open country ground roughness. Cloud cover is 50% with stability class of E. There is no inversion height. The fractured/punctured hole is located at 1.5 m above the ground with 0.05 m circular hole diameter. The total release/issue time is 28 min.

### Methodology:

Once baseline study [2] is conducted, similar techniques are used to find temperature effects on propylene leak. Table-1 shows the site, tank, and environmental parameters used for Propylene chemical spill simulations. It is also horizontal cylindrical tank of 50m<sup>3</sup> volume. The design pressure of the storage tank is 2.16 MPa whereas filling factor of 0.9 is considered. The altitude of this industrial area is 7.88 meters located in Deer Park area which is near to Houston, Texas. The average wind speed is considered 3.81 meter/second (8.58 mph) from yearly wind speed data [4]. The wind direction is Southward. Outside ambient temperature is considered as -7 to 47°C (around 20 to 117°F) from yearly temperature data [4]. The average Relative Humidity (RH) considered is 75% from yearly RH data [5]. Similar to Base study, the fractured/punctured hole is located at 1.5 m above the ground with 0.05 m circular hole diameter. Again, the diameter of the horizontal aligned cylindrical tank is 2.6 m and length is 9.42 m. In addition to these, the tank is in unsheltered single storied condition and open country ground roughness.

Parameter	Symbol	Value	Unit
Wind Measuring Height		3	М
Cloud cover (Cloudy level)		40	%
Stability class		D	

Table-1: Atmospheric parameters used for Propylene chemical spill simulations

Following Base study and using Table-1 parameters, the propylene chemical toxic poisoning and vapor cloud explosion accidents were investigated after the propylene storage tank leakage occurred.

### **Toxic Chemical Accident Simulation:**

When a propylene storage tank leaks, a large area of pool of liquid is formed, it turns to vapor rapidly and diffuse in the air. This dispersion will create a large cloud around the leaked area. Depending on the air or wind direction and speed this gas will spread slowly or rapidly. If wind speed is slow a high concentration of gas cloud formed near to the leaked area. If wind speed is high the leaked area gas concentration will not be high enough as it cannot stay on a certain location for a while. As a sample demonstration of simulations, Figure-1 shows concentration (ppm) spreading of propylene towards the direction of wind flow at 29°C. Very high concentration (>17,000 ppm) contour is located near the source and is within 161 m. This concentration is very high enough to create human health hazard. The concentrations between 17,000 to 2,800 ppm contour are located between 161 to 464 m which will create a moderate health hazard. The concentrations between 2,800 to 1,500 ppm contour are located between 464 to 674 m. Lower concentration indicates neighborhood residents will be exposed to propylene slowly and be able to evacuate safely.



Figure-1: Concentration (ppm) contours after propylene leak at 29°C

Propylene release duration (min) at 29°C indicated the releases will be gradually decreasing step by step. It indicates that total 27 minutes will be needed for releasing the propylene from the horizontally aligned cylindrical tank whereas first few minutes a large release will occur compared to slow release for a long duration.

### Simulation of Vapor Cloud Explosion Accident:

Analysis on the fire and explosion accidents consequences in propylene storage tanks shows that Boiling Liquid Expanding Vapor Explosion (BLEVE) which will create by fireball make the largest impact to nearby neighborhoods.

As a sample demonstration of simulations, Figure-2 indicates pressure (psi) dispersion contours after propylene leak at 29°C. It indicates bigger contour formations toward the direction of wind flow. Very high pressure (>8 psi) contour does not exist for this scenario. Next level of

high pressure (between 8 to 3.5 psi) contour is located near the source and is within 108 m. This pressure will be hazardous to humans and properties that can have destructive force. The pressure between 3.5 to 1.0 psi contour is located between 108 to 211 m. Lower pressure indicates neighborhood residents will be exposed to propylene slowly and be able to evacuate safely.



Figure-2: Pressure (psi) contours after propylene leak at 29°C

### **Results and Discussions:**

This study found that the concentration of propylene higher than 17,000 ppm exists between range of 115 to 183 meters for temperature variation of -7°C to 47°C respectively. The intermediate area (325 to 530m) will cause moderate health risk to nearby neighbors. In the yellow areas (472 to 759m), there is no significant health effects other than pungent smell.

Figure-3 shows Distance (m) along varying on concentration (ppm) for different temperatures (°C). As indicated in this figure, higher temperatures lead further away of release of propylene for the same concentration. As temperature remain constant when distance increases, concentration of propylene decreases. The chemical can leak from a hole in a tank and disperse further away with higher ambient temperatures for same the concentration. Any properties and neighborhoods get less concentrations as they are located further from the point of release. On the other hand, any properties and neighborhoods get higher concentrations as they are located near to the point of release.



Figure-3: Distance (m) along varying on Concentration (ppm) for different temperatures (°C)

This study found that the range of fireball influence is up to 163 to 232 meters which is a light injury area for temperature variation of -7°C to 47°C respectively. Areas from 83 to 120m for that temperature variation is a serious injury area (orange area). However, there is no red area which means there will not be any destruction of building collapses.

Varying Distance (m) along on pressure (psi) for different temperatures ( $^{\circ}$ C) for 3.5 to 8 psi pressure follows the linear equation: Distance (m) along on varying Pressure (psi) = 0.6869 x Temperatures ( $^{\circ}$ C) + 88.663. Whereas, varying Distance (m) along on pressure (psi) for different temperatures ( $^{\circ}$ C) for 1 to 3.5 psi pressure follows the linear equation: Distance (m) along on varying Pressure (psi) = 1.2798 x Temperatures ( $^{\circ}$ C) + 174.3. As indicated in these equations, higher temperatures lead further away of release of propylene. As temperature remain constant when distance increases, pressure decreases with propylene release. The propylene can leak from a hole in a tank and disperse further away with higher ambient temperatures. Any properties and neighborhoods get less pressure as they are located further from the point of release. On the other hand, any properties and neighborhoods get higher pressure as they are located near to the point of release.

Varying Release Rate (kg/min) with respect to different Temperature ( $^{\circ}$ C) follows the linear behavior following the equation: Release Rate (kg/min) = 27.313 x Temperature ( $^{\circ}$ C) + 1661.7. As indicated in this equation, higher temperatures lead to higher amount of release of propylene. The propylene can leak from a hole in a tank and disperse faster with higher ambient temperatures, therefore neighborhood residents will get the release of propylene faster.

This Aloha software is used in Engr-4350 (Industrial Loss Prevention) class where Junior and Senior students take the class. As they will be graduating soon and will be future worksite leader and trainer, they need to know cheaper ways to analyze chemical spills and mitigation, therefore this software will help reducing the cost of giving training in worksites. Students downloaded this software in their laptops and lab classrooms which helped them to learn and practice the software on their own pace. After learning this software students did a few projects related to their worksite chemical problems and reported their supervisors liked their proactive these leading roles in terms of safety aspects of companies which caused them to motivate to learn in depth of this software.

The amount of instruction and scaffolding given to students during the implementation include: at least one example was demonstrated from Aloha in the classroom by the instructor, students were given a week to practice the same problem and to get familiar with the sofware, a randomly selected student from the class demonstrated another exmple in another week, radom selection of students' for different students was conducted for different examples and it went on for six different examples from the manuals. At the end of pacticing and demsonstraing all the examples a case study was given to apply the knowledge of the demonstrated examples.

My approach for collecting student feedback related to Aloha was Blackboard and Canvas software which are Learning Management System (LMS) for course evaluation and students's learning. Typically, instructors get students' response/feedbak after the end of the semester. In addition to that students' verbal comments were considered as student feedback related to this software. All of these indicated that they like this software and a useful, cheap, and easily avaiable software to use during chemical spills in their worksites.

Appendix shows problem statements and other examples of materials provided to the students.

### **Conclusion:**

This analysis can help to identify how far in terms of distance will be considered to evacuate citizens safely and who need to do quick evacuation. It will be also helpful to guide safety supervisors to focus and set emergency levels in different hazardous areas in addition to placing safety warnings and signs in the storage tank areas to avoid any occurrence of fire and static current or sparks.

This software is used in the classrooms for this kind of study over the years to teach chemical spill. Students' comments and responses indicate that they like this software as it is easy to use and has very user-friendly Graphical User Interface (GUI). Classroom and training class discussions using this software will save money to do chemical spill mitigation and control in house with expensive devices. Furthermore, to the best of the author knowledge, this is the first reported work where chemical spill hazards related to air temperature using this software is used which is an inexpensive way to prepare and control chemical spills.

### Acknowledgments:

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### **Appendix (Problem statements and examples of materials**

### provided to the students)

### Example-1: A Tank Source (Puddle and Pool Fire) -Modeling a Toxic Vapor Cloud

In a small industrial park outside Baton Rouge, Louisiana, a 500-gallon, 4-foot-diameter, vertical tank contains liquid benzene. On June 20, 2016, at 10:30 p.m. local time, a security guard discovers that liquid is leaking out of the tank through a 6-inch circular hole located 10 inches above the bottom of the tank. He also sees that the liquid is flowing onto a paved area in the industrial park. The guard thinks that the tank has just been filled that evening.

The temperature on scene is 80°F, with the wind from the southwest at 7 miles per hour (as measured at a height of 10 meters by a fixed meteorological tower at the site). The sky is more than half covered by clouds and the humidity is about 75%. A thunderstorm is approaching from the southwest. There is no low-level inversion. There are very few buildings in the industrial park and a large grassy field is located to the northeast of the industrial park.

The Local Emergency Planning Committee has requested that on-scene responders use ERPG-2 concentrations to define the toxic endpoints in their analysis of benzene hazards.

In this example scenario, you'll determine: Distance to the ERPG-2 level if the puddle evaporates and forms a toxic vapor cloud.

### Instructions:

\*Follow 'ALOHA Sample Examples' file from page-3 to page-14.

\*You need to upload your simulation file in Blackboard as attachment

\*Your file name need to be this format: "ENGR-4330 Simulation-1 Exp-1 Last name First Name"

### Example-2: A Tank Source (Puddle and Pool Fire) -Modeling a Pool Fire

In a small industrial park outside Baton Rouge, Louisiana, a 500-gallon, 4-foot-diameter, vertical tank contains liquid benzene. On June 20, 2016, at 10:30 p.m. local time, a security guard discovers that liquid is leaking out of the tank through a 6-inch circular hole located 10 inches above the bottom of the tank. He also sees that the liquid is flowing onto a paved area in the industrial park. The guard thinks that the tank has just been filled that evening.

The temperature on scene is 80°F, with the wind from the southwest at 7 miles per hour (as measured at a height of 10 meters by a fixed meteorological tower at the site). The sky is more than half covered by clouds and the humidity is about 75%. A thunderstorm is approaching from the southwest. There is no low-level inversion. There are very few buildings in the industrial park and a large grassy field is located to the northeast of the industrial park.

The Local Emergency Planning Committee has requested that on-scene responders use ERPG-2 concentrations to define the toxic endpoints in their analysis of benzene hazards.

In this example scenario, you'll determine:

- Distance to the ERPG-2 level if the puddle evaporates and forms a toxic vapor cloud. (Note: Get data from Example-1).
- Thermal radiation threat if a lightning strike (or other ignition source) ignites the puddle and forms a pool fire.

For this example, you want to assess the threat assuming that the pool fire occurs soon after the puddle forms. Therefore, you don't need to enter new information for time, atmospheric conditions, or puddle size.

### Instruction:

\*Follow 'ALOHA Sample Examples' file from page-15 to page-19

\*You need to upload your simulation file in Blackboard as attachment

\*Your file name need to be this format: "ENGR-4330 Simulation-2 Exp-2 Last name First Name"

#### Example-3: A Tank Source (Multiple Scenarios) -Modeling a BLEVE

On June 25, 2016, at 12:30 p.m., a train derails in a highly industrialized section of Columbia, South Carolina. Among the derailed cars is a tank car of propane in a U.S. Department of Transportation (DOT) class 112J400W car with a listed capacity of 33,800 gallons. The tank is approximately 70 feet long and the tank appears to be intact. The propane has been liquefied under pressure.

At the time of the accident, the air temperature is 70°F, with the wind from 360° at 10 miles per hour (measured at a height of 10 meters by the National Weather Service). The sky is completely overcast and the relative humidity is 67%. There is no low-level inversion.

The tank needs to be removed from the tracks and the cargo off-loaded. The tank has already been subjected to significant stress during the wreck and it is conceivable that it could fail during this effort. Possible failure scenarios include: A sudden catastrophic failure leading to a Boiling Liquid Expanding Vapor Explosion (BLEVE);

In order to plan a safe response and ensure public safety, the potential severity of these threats must be evaluated. You'll use ALOHA to predict the threat zone the potential scenario.

#### Instructions:

\*Follow 'ALOHA Sample Examples' file from page-20 to page-27.

\*You need to upload your simulation file in Blackboard as attachment

\*Your file name need to be this format: "ENGR-4330 Simulation-3 Exp-3 Last name First Name"

### Example-4: A Tank Source (Multiple Scenarios) - Modeling a Flash Fire or Vapor Cloud Explosion

On June 25, 2016, at 12:30 p.m., a train derails in a highly industrialized section of Columbia, South Carolina. Among the derailed cars is a tank car of propane in a U.S. Department of Transportation (DOT) class 112J400W car with a listed capacity of 33,800 gallons. The tank is approximately 70 feet long and the tank appears to be intact. The propane has been liquefied under pressure.

At the time of the accident, the air temperature is 70°F, with the wind from 360° at 10 miles per hour (measured at a height of 10 meters by the National Weather Service). The sky is completely overcast and the relative humidity is 67%. There is no low-level inversion.

The tank needs to be removed from the tracks and the cargo off-loaded. The tank has already been subjected to significant stress during the wreck and it is conceivable that it could fail during this effort. Possible failure scenarios include:

- A sudden catastrophic failure leading to a Boiling Liquid Expanding Vapor Explosion (BLEVE). (Note: Get data from Example-3).
- A leak leading to a flash fire or a vapor cloud explosion;

In order to plan a safe response and ensure public safety, the potential severity of these threats must be evaluated. You'll use ALOHA to predict the threat zones for each of these potential scenarios. For the last scenario, you'll model the release assuming a seam fails on the tank, creating a rectangular hole 40 inches long and 0.1 inch wide.

Now that ALOHA has displayed the thermal radiation hazard from a BLEVE, you want to assess the threat if the tank leaks and a flammable vapor cloud forms instead. If this situation occurs, either a flash fire or a vapor cloud explosion could occur, depending on the scenario specifics. For both of these scenarios, you will need to begin by estimating the flammable area of the vapor cloud. You do not need to enter new information for time, atmospheric conditions, or tank size.

### Instructions:

\*Follow 'ALOHA Sample Examples' file from page-28 to page-36

\*You need to upload your simulation file in Blackboard as attachment

\*Your file name need to be this format: "ENGR-4330 Simulation-4 Exp-4 Last name First Name"

#### Example-5: A Tank Source (Multiple Scenarios) -Modeling a Jet Fire

On June 25, 2016, at 12:30 p.m., a train derails in a highly industrialized section of Columbia, South Carolina. Among the derailed cars is a tank car of propane in a U.S. Department of Transportation (DOT) class 112J400W car with a listed capacity of 33,800 gallons. The tank is approximately 70 feet long and the tank appears to be intact. The propane has been liquefied under pressure.

At the time of the accident, the air temperature is 70°F, with the wind from 360° at 10 miles per hour (measured at a height of 10 meters by the National Weather Service). The sky is completely overcast and the relative humidity is 67%. There is no low-level inversion.

The tank needs to be removed from the tracks and the cargo off-loaded. The tank has already been subjected to significant stress during the wreck and it is conceivable that it could fail during this effort. Possible failure scenarios include:

- A sudden catastrophic failure leading to a Boiling Liquid Expanding Vapor Explosion (BLEVE). (Note: Get data from Example-3).
- 2) A leak leading to a flash fire or a vapor cloud explosion. (Note: Get data from Example-4).
- A breach leading to a jet fire from the tank.

In order to plan a safe response and ensure public safety, the potential severity of these threats must be evaluated. You'll use ALOHA to predict the threat zones for each of these potential scenarios. For the last two scenarios, you'll model the release assuming a seam fails on the tank, creating a rectangular hole 40 inches long and 0.1 inch wide.

Now that you've considered the flammable area and the overpressure hazard from a vapor cloud explosion, you want to assess the thermal radiation threat if the tank leaks and the escaping propane is quickly ignited, so that a jet fire occurs instead. Therefore, you don't need to enter new information for time, atmospheric conditions, or tank size.

### Instructions:

\*Follow 'ALOHA Sample Examples' file from page-37 to page-39

\*You need to upload your simulation file in Blackboard as attachment

\*Your file name need to be this format: "ENGR-4330 Simulation-5 Exp-5 Last name First Name"

### Example-6: A Direct Source and a MARPLOT Map

At 3 p.m. on June 4, 2016, a train traveling on the Southern Railway near Manassas, Virginia, collides with a stalled truck at Lee Highway (U.S. Route 29). Three 150-pound chlorine cylinders that were in the truck bed are damaged during the collision and simultaneously release their contents. At the time of the release, winds are out of the east at about 6 miles per hour, measured at a height of 3 meters. One-third of the sky is covered by clouds, the humidity is about 80% and the air temperature is 72°F. There is no low-level inversion.

The land between the accident site and the intersection of John Marshall Highway (State Route 55) with Lee Highway is flat with no obstructions. Two workmen repairing potholes on Lee Highway just west of this intersection are overcome by fumes and treated at a local hospital for chlorine gas inhalation. To what approximate concentration of chlorine might the workmen have been exposed?

You'll evaluate this scenario first by using ALOHA to obtain a source strength estimate and a threat zone estimate, and then by displaying the threat zones on a MARPLOT map in order to obtain a concentration estimate for the location where the workmen were injured.

### Instructions:

\*Follow 'ALOHA Sample Examples' file from page-40 to page-53

\*You need to upload your simulation file in Blackboard as attachment

\*Your file name need to be this format: "ENGR-4330 Simulation-6 Exp-6 Last name First Name"

# Simulation-7, due by 12/6, by 9pm At

📎 Edit

Find a historical chemical spill incident (

<u>https://en.wikipedia.org/wiki/List of industrial disasters</u> ) and evaluate the hazard emission scenario by using ALOHA to obtain a source strength, as well as different threat zones estimates, and then display the threat zones on a MARPLOT map in order to obtain a concentration estimate for the location where the neighborhoods and workmen were in potential hazard zone.

Instructions:

\*You need to write a nice report related to that incident: cause, how it could be avoided, lesson learn etc.

\*You need to attach your simulation files in that file

\*You need to upload your file in Blackboard as attachment

\*Your file name need to be this format: "ENGR-3375 Simulation-7 Independent Study Last name First Name"

\*You can submit the Simulation file early, if you want

Points 50

Submitting a text entry box or a file upload