Analyzing Ammonia Dispersion Under Varying Atmospheric Conditions Using DRIFT

Atmospheric conditions, such as ambient temperature and relative humidity, can influence dispersion of toxic chemicals. Ammonia is hygroscopic and therefore has complex interactions with water vapor present in the atmosphere. The integral model DRIFT has been utilized to predict ammonia dispersion and downwind concentrations for a range of temperatures and humidities. We have simulated ammonia dispersion for two types of release: (i) long-duration, typical of a leak from a hole in a vessel; (ii) instantaneous release, typical of a catastrophic vessel failure.

The two cases studied in this paper are somewhat idealized representations of what can happen during loss of containment. However, both release scenarios contribute knowledge to how a release of ammonia interacts with the environment, and how this affects downwind dispersion.

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Introduction

A release of a pressure-liquefied industrial chemical, such as ammonia, can result in the formation of a large cloud of vapor. Depending on the release and atmospheric conditions, a cloud of ammonia can travel great distances and pose significant risks to public health and the environment.

The thermodynamic interactions of ammonia with water potentially make ammonia dispersion in a moist atmosphere sensitive to humidity and temperature. Anhydrous ammonia is hygroscopic, it therefore absorbs moisture from the surrounding air and forms a non-ideal solution, releasing heat in the process. This effect is more pronounced than with other substances that either interact weakly or not at all with water. Understanding and predicting the behavior of such releases requires accounting for both thermodynamic interactions and the non-ideal nature of the solution.

Experimentalists investigating the release and subsequent dispersion of a chemical such as ammonia, will often aim to control or at least characterize the storage and source conditions. However, the source conditions of an accidental ammonia release can be difficult to characterize. There are many factors involved, such as location, storage conditions, vessel type, and circumstances relating to the accident. Due to the variable nature of incidents, it is a challenge in modeling to specify conditions which can represent a wide variety of release scenarios. For instance, containment loss might occur suddenly due to a catastrophic failure, or gradually through a prolonged leak from a hole or crack.

In 1992 at a peanut oil mill in Dakar Senegal, a road tanker ruptured, releasing approximately 22 tonnes of liquid ammonia [1]. Overfilling led to overpressures which caused a previously repaired weld to fail, and the tanker burst open. A two-phase flow of ammonia liquid and vapor was produced. The cloud engulfed neighboring offices and restaurants, which were relatively quiet at the time due to the accident occurring during the Ramadan holidays. Even so, there were 129 fatalities and over 1000 injuries. This incident was reviewed and modeled in [2] using the DNV PHAST integral model. Two scenarios were modeled: instantaneous release of 22 tonnes; and a continuous release from a hose failure. Dispersion modeling predicted concentrations of 1500 ppm up to 1.5 km away from the initial tanker position.

In 2019, a farm worker driving a tractor was towing a fertilizer applicator and a trailer carrying two 1000 gallon nurse tanks of ammonia on a public road in Beach Park Illinois. The applicator hose disconnected from the bulkhead adapter, releasing approximately 650 gallons of ammonia. A dense cloud of ammonia vapor was produced, leading to a one mile shelter in place order. A total of 83 people were evaluated at hospital, of which 14 were subsequently hospitalized [3]. Luckily there were no deaths. The time of release (early morning at 04:24), was probably a factor in this, in addition to the size of release (approximately 1.5 tonnes). In an investigation report, the National Transportation Safety Board in the United States concluded that a worn applicator coupling disconnected from the adapter, releasing ammonia through a 1 inch diameter orifice [4]. ASOS weather data for the nearest airport (Waukegan National Airport) indicates a low wind speed of ~0.5 m/s and relative humidity of 85% during the time of release. The orifice was pointing towards the tractor cabin, suggesting a momentum jet could have been impinging onto the tractor.

This brief review of two previous incidents (Dakar 1992 and Illinois 2019) highlights the difficulty in prescribing initial conditions for models. In this study we simulate two different types of release:

- Long-duration release, typical of a hole in a vessel;
- Instantaneous release from a catastrophic failure.

These simulations are not tailored to replicate specific accidents or incidents. Instead, they aim to explore a range of conditions and variables that could potentially occur during an ammonia incident. By doing so, the simulations provide insights into fundamental behaviors of ammonia dispersion in various conditions.

We model the problem using the integral model DRIFT. As one of the few operational models equipped with a sub-model specifically designed to account for ammonia-water interactions, DRIFT is appropriate for this investigation. In addition, it is relatively fast to run, allowing us to comprehensively explore the input space.

The main objective of this study is to examine the impact of atmospheric conditions, such as humidity and temperature, on the dispersion of ammonia.

Methodology

Long-duration release

Due to the difficulty in characterizing the initial conditions for a release such as the Beach Park incident, we chose to model a large-scale pressure-liquified experimental release of ammonia. The Desert Tortoise field trials conducted in 1983 are chosen as a suitable test case. Conditions for the selected Desert Tortoise trials are mostly taken from the SMEDIS database [5]. Temperature and pressure were recorded at the orifice. The release rate of 80 kg/s was estimated from the initial mass of ammonia in the vessel and the time taken to empty (126 s). For this release we increase the release duration to 10000 s, to produce a long-duration type release.

For the purpose of this study, 100% liquid has been assumed at the exit nozzle which is consistent with the normal assumption for a padded release, but does not account for flashing that may have been induced by pressure losses, e.g. due to the presence of a knee-bend immediately upstream of the exit orifice in Desert Tortoise.

Instantaneous release conditions

A source-term calculation of the expansion from storage to atmospheric conditions is not carried out in this study. This allows us to focus on the downwind dispersion behavior. We model the release from the point at which the ammonia has reached atmospheric pressure (101325 Pa) and its temperature is at its boiling point (-33.34 °C).

The total mass of ammonia is 20 tonnes, similar to the Dakar incident which was 22 tonnes. To simulate different fills of a vessel, we take the liquid fraction to vary from 0 to 0.3. This might be typical of a road or storage tanker, where there is a vapor space above the fill line. Ammonia vapor at 20 °C and atmospheric pressure has a relative density compared to air of approximately 0.6 [6]. Therefore when the liquid fraction is zero, the cloud is expected to be initially buoyant, and remain buoyant as it disperses into the atmosphere. The cloud is initially stationary and released from ground level. The aspect ratio of the initial cloud is assumed to have an aspect ratio of 1, i.e. height equal to width.

Problem overview

Table 1 summarizes the source conditions for the two release configurations.

Parameter	**Long-duration**	**Instantaneous**
Source type	Momentum jet	Catastrophic
Orifice diameter (m)	0.081	-
Temperature (K)	294.65	239.81
Release pressure (Pa)	1.01E+06	101325
Liquid fraction	1	0.0, 0.1,…, 0.3
Release rate (kg/s)	80	-
Release duration (s)	10000	-
Inventory (tonne)	-	20
Release location (m)	(0, 0, 1)	(0, 0, 0)

Table 1 Geometry and source conditions for the two types of release. Parameters marked with an asterisk are sensitivity inputs to the model.

We wish to study the dispersion of ammonia from two different release types. Therefore, initial conditions which are inputs to the dispersion model will vary between the two different release scenarios. However, where possible, conditions have been matched between the two scenarios. This allows for a comparison between the two cases. A summary of the atmospheric conditions is provided in *Table 2*.

Parameter	**Value**
Temperature* (°C)	0, 3, …, 30
Pressure (Pa)	101325 (atm)
Relative humidity* (%)	0, 10, …, 80
Reference height (m)	2
Roughness length (m)	0.003
Pasquill stability class	D
Friction velocity (m/s)	0.442
Wind speed (m/s)	2

Table 2 Atmospheric conditions. Parameters marked with an asterisk are sensitivity inputs to the model.

The atmospheric stability was assumed to be neutral (Pasquill D), with a wind speed of 2 m/s. We assume zero rainout because this leads to the formation of a pool and subsequent vaporization. This is considered to be a separate problem which will not be considered in this study, but could be included in future investigations. In addition, there is no heat transfer to or from the ground.

Numerical model

Both release scenarios are modeled using DRIFT version 3.7.19. DRIFT (Dispersion of Releases Involving Flammables or Toxics) is a gas dispersion model, originally developed by the UK

Atomic Energy Authority (UKAEA), and subsequently maintained by ESR Technology, with the support of the UK Health and Safety Executive (HSE). DRIFT is used within HSE to model atmospheric dispersion of toxic and flammable substances for the purpose of providing public safety advice on hazardous substance consent applications and land-use planning. Model evaluation of DRIFT has been undertaken for a variety of release scenarios [7, 8]. A mathematical description of DRIFT can be found in the report by Tickle and Carlisle [9].

In total, given all possible combinations of the sensitivity inputs, there are 198 runs for the long-duration release, and 792 runs for the instantaneous release.

Concentrations are measured along the centerline ($y = 0$) for a range of downwind distances ($x = 0$ to 10 km). To assess cloud lift-off for the instantaneous case, concentrations at each downwind coordinate x are recorded at 3 separate heights: $z = 1$, 10, 100 m.

The distance to AEGL-3 (10 mins exposure, 2700 ppm) are reported in the analysis as a measure of the clouds' extent. According to the National Research Council [10]: "AEGL-3 is the airborne concentration (expressed as ppm or mg/m^3) of a substance above which it is predicted that the general population, including susceptible individuals, could experience life-threatening adverse health effects or death".

Results: effect of liquid fraction on the instantaneous release

We first focus our attention on the instantaneous release. To determine if the cloud becomes buoyant and lifts-off from the ground, concentrations are reported at 1, 10, and 100 m. At each downstream location x, the height at which the maximum concentration is reached is recorded. We then assess the cloud behavior according to the following three characteristics:

1. The cloud is initially buoyant and remains buoyant. The height at which the maximum concentration is found is always greater than 1 m.
2. The cloud is initially buoyant, but further downwind the maximum concentration is recorded at the lowest height of 1 m.
3. The cloud travels along the ground, such that the maximum concentration is always recorded at 1 m.

By applying these criteria for each case and assigning a value on the behavior, we can then correlate this to the values given to the input parameters.

A Pearson correlation test is performed for each variable and reported in *Table 3*. The Pearson correlation coefficient (r) measures the strength and direction of a linear relationship between two variables, ranging from -1 (perfect negative correlation) to +1 (perfect positive correlation), with 0 indicating no linear relationship. The P-value assesses the statistical significance of this correlation; a low P-value (typically below 0.05) implies a statistically significant relationship. Conversely, a high P-value indicates a lack of statistical evidence for a significant correlation.

The strongest correlation between lift-off behavior and input parameter is observed with the liquid fraction. This suggests that liquid fraction is a dominant input, which greatly influences the cloud buoyancy and therefore whether or not it lifts off from the ground.

Input variable	**Correlation Coeff (r)**	**P-Value**	**Correlation**
Liquid fraction	-0.90	0.00	Strong negative correlation.
Relative humidity	0.11	0.00	Weak positive correlation.
Temperature	-0.05	0.13	No statistical significance.

Table 3 Pearson correlation coefficient and P-value for testing correlation between input variables and cloud lift-off.

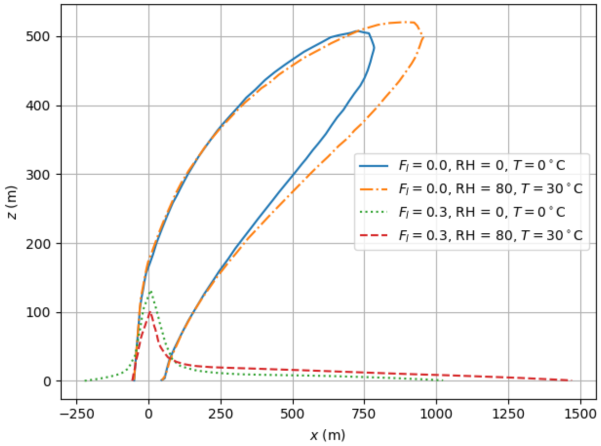

Figure 1 Contours of AEGL-3 (2700 ppm) for various liquid fractions $\boldsymbol{F_l}$*, temperatures, and relative humidities.*

Contours of AEGL-3 (2700 ppm) from a side-view of the cloud are presented in *Figure* ***1***. In these figures the wind is travelling left to right. These represent the maximum extent at which 2700 ppm is recorded, and are therefore not a snapshot of the cloud at a particular time. *Figure 1* illustrates the findings of *Table 1*- here the main difference between the contours of AEGL-3 (2700 ppm) stems from the value of the liquid fraction. For a gaseous release where $F_l = 0$, the cloud is initially buoyant and remains buoyant. Increasing the liquid fraction to 0.3 results in dense-gas dispersion behavior.

Going forward, we only consider the instantaneous release with a liquid fraction of 0.3. This is in order to compare concentration values with the long-duration release at a height of $z = 1$ (m).

Results: effect of weather conditions on dispersion

Figure 2 is a plot of concentration as a function of downwind distance at a height of $z = 1$ m. The instantaneous release produces concentrations near the source that are nearly two orders of magnitude lower than the long-duration leak. This is due to the immediate mixing of ambient air into the ammonia cloud for the instantaneous case.

For the instantaneous case, lower ambient temperatures lead to higher concentrations in the region $x < 10$ m. However, the opposite is true for $x > 10$ m, where higher ambient temperatures produce higher concentrations. A reasonable agreement is found between the current data (instantaneous, 30 °C, 80% RH) and the results of [2], who modeled a similar release.

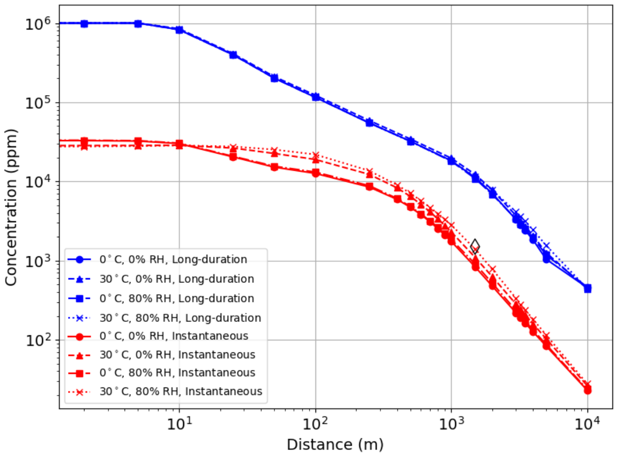

Figure 2 Concentration profiles at a height of 1 m. A select number of cases have been chosen to illustrate the difference between the two types of release. A black diamond marker represents the distance to 1500 ppm reported in [2]

Figure 3 and *Figure 4* present the distance to AEGL-3. The color bar limits are automatically pinned to the minimum and maximum of the data. As was identified in *Figure 2*, the long-duration release results in greater distances to AEGL-3, because a larger cloud is produced. Increasing the temperature from 0 to 30 °C and the relative humidity from 0 to 80% leads to an increase in the distance to AEGL-3 of: (i) 15% for the long-duration release, (ii) 35% for the instantaneous release. Although the concentrations predicted from an instantaneous release are lower, the ambient temperature and relative humidity have a greater effect on this type of release, in relative terms.

However, the contours also reveal how the parameters temperature and relative humidity affect the cloud extent. In the long-duration case, the distance to AEGL-3 increases as both temperature and relative humidity increases. The distribution is smooth, unlike the contour produced for the instantaneous case where there is a sharp transition in the temperature range 10 to 15 °C.

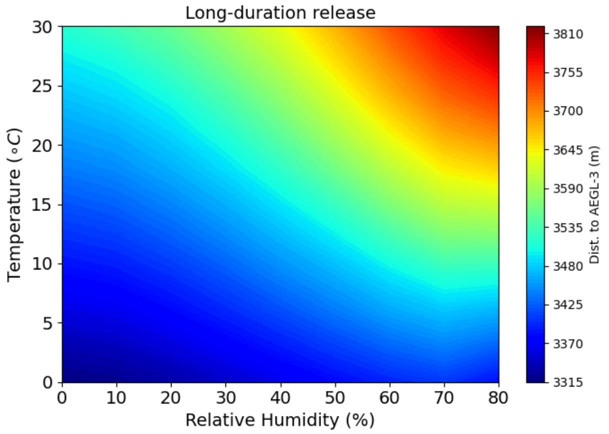

Figure 3 Contours of distance to AEGL-3 for a long-duration release.

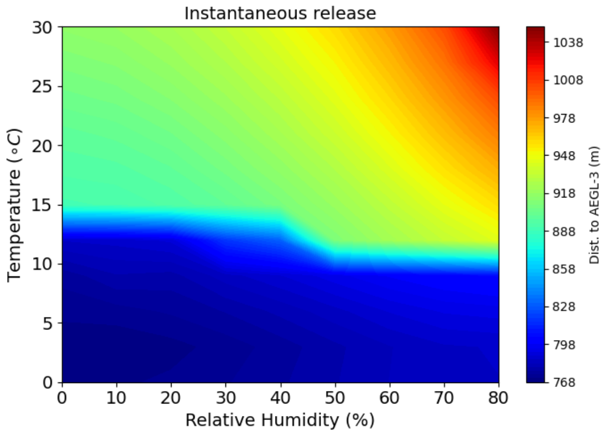

Figure 4 Contours of distance to AEGL-3 for an instantaneous release.

To further explore this, we extract the data at ambient temperatures of 15 °C, and plot the relative concentration as a function of distance and relative humidity in *Figure 5* and *Figure 6*. Concentrations are normalized by the 0% humidity case, which is why the relative concentration is equal to 1 at 0% RH.

In the long-duration case, increasing humidity has little effect for $x < 1$ km. However, a dip in the profiles of relative concentration at $x = 1$ km indicates that an increase in humidity leads to a slight reduction in concentration. Further downwind, the relative concentration increases to a maximum of approximately 1.2. Therefore, increasing the humidity from 0 to 80% results in a 20% increase in the concentration in the region $1 < x < 10$ km.

For the instantaneous release, an increase in the relative humidity has a more pronounced effect. In fact, there is a maximum increase in concentration of roughly 40%. There are two peaks observed in the profiles of relative concentration in *Figure 6* at approximately 100 m and 1500 m.

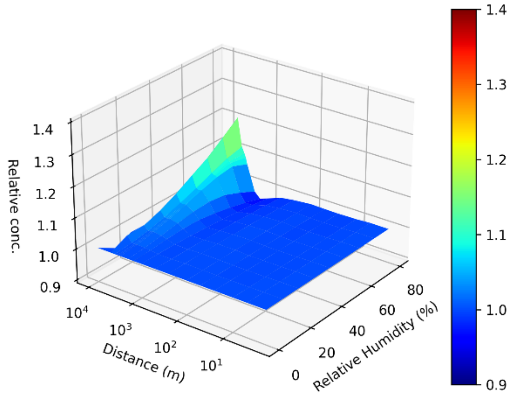

Figure 5 Relative concentration profiles as a function of distance and relative humidity for the long-duration release. Data are normalized by the concentration at 0% relative humidity.

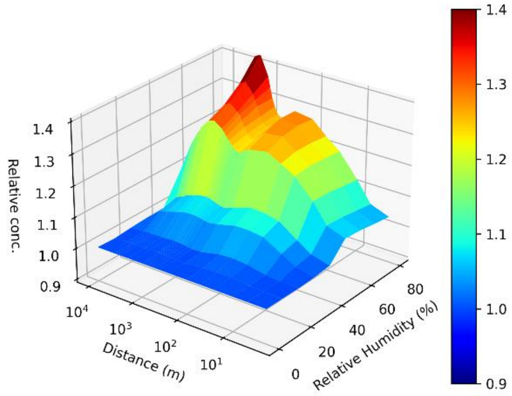

Figure 6 Relative concentration profiles as a function of distance and relative humidity for the instantaneous release. Data are normalized

by the concentration at 0% relative humidity.

Conclusions

Atmospheric conditions, such as ambient temperature and relative humidity can affect dispersions of toxic chemicals, including ammonia which is hygroscopic and therefore has complex interactions with water vapor present in the atmosphere.

We have simulated ammonia dispersion for two types of release: (i) long-duration, typical of a leak from a hole in a vessel; (ii) instantaneous release, typical of a catastrophic release. These two cases are somewhat idealized representations of what can happen during loss of containment.

The integral model DRIFT has been utilized to predict ammonia dispersion and downwind concentrations for a range of temperatures and humidities. For the instantaneous release, the liquid fraction in the initial cloud was varied, and this was shown to have a strong impact on the cloud's behavior. A liquid fraction of 0.3 was found to result in a dense blanket cloud of ammonia for all inputs tested. Conversely, a liquid fraction of 0 produces a buoyant cloud, due to the lower density of ammonia compared to air.

The relationship between dispersion behavior and ambient conditions (temperature and humidity) was complex. The distance to AEGL-3 (2700 ppm) has been used as a marker to assess the cloud size. Generally speaking, for both long-duration and instantaneous releases, increasing the temperature and humidity resulted in a greater distance to AEGL-3. However, when considering a fixed temperature, the effect of varying humidity was dependent on distance from the source. Concentrations in the far field ($x > 1$ km) for the high humidity case at 15 °C were approximately 20% higher for the long-duration release, and 40% higher for the instantaneous release.

This study has shown that humidity and temperature have a modest effect on ammonia dispersion behavior. The effect is more pronounced for the case of an instantaneous release compared to a long-duration release. In addition, the effect is dependent on downwind distance.

Further work could explore the sensitivity of liquid fraction on the buoyancy and lift-off behavior of the cloud in the range 0 to 0.3.

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