

Modeling Dispersion in the Event of a Leak Ammonia Storage in a Hypothetical Uranium Hexafluoride Production Plant

Camila Stramandinoli Deamatis, Nilce Ortiz

Institute for Nuclear and Energy Research, São Paulo, Brazil Email: camilasdeamatis@usp.br, nortiz@ipen.br

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Abstract

The primary use of ammonia in nuclear plants is in producing uranium hexafluoride (UF₆), a critical compound for uranium enrichment (U-235). Ammonia's widespread use across multiple industries has led to a steady increase in its production over the years. However, due to its toxic properties, conducting comprehensive studies on its dispersion is essential, as leaks can pose significant risks to human health and the environment. Tools like the Areal Locations of Hazardous Atmospheres (ALOHA) system are employed to model the dispersion patterns of hazardous gases, enabling the prediction of toxic substance releases and their spread. This study evaluates ammonia dispersion in scenarios involving tank punctures or valve ruptures, which can lead to accidental leaks, particularly in uranium hexafluoride production facilities. The meteorological factors considered in the dispersion modeling are wind speed, temperature, humidity, and prevailing wind directions. The results demonstrate that low wind speeds and high temperatures significantly impact ammonia dispersion, while fluctuations in humidity have a minimal effect. Furthermore, the observed findings indicate that the prevailing wind direction in the site tends to be most commonly from the East-Southeast (ESE). In this direction, dispersion extends towards vegetated areas and certain uranium hexafluoride production plant sections. However, the results highlight the wind direction variability over time, prompting further investigation into additional simulation scenarios.

Keywords

Ammonia, Uranium Hexafluoride, Nuclear Power Plant, ALOHA, Toxic Gas Dispersion

1. Introduction

Ammonia has diverse applications across a range of chemical industries. It is

widely used in fertilizer production to enhance the growth of crops, grasses, and plants and in the pharmaceutical and textile sectors. Additionally, ammonia acts as an intermediate product in manufacturing plastics and other chemical compounds (Environmental Company of the State of São Paulo, 2021; Rosa et al., 2021). In the fertilizer industry, ammonia is crucial as a primary nitrogen source and vital for plant cultivation (Afif et al., 2016). Its excellent heat transfer properties also make it a popular choice for refrigeration systems (Rosa et al., 2021).

In uranium hexafluoride (UF₆) plants, ammonia is primarily used in the synthesis of ammonium diuranate (ADU-(NH₄)₂U₂O₇). This synthesis occurs through the reaction of uranyl nitrate (UO₂(NO₃)₂) with ammonia, either in its gaseous or aqueous form, leading to the precipitation of ADU. The resulting compound is then calcined to produce UO₃, the initial form of uranium oxide (Paik et al., 2013). The process continues with reducing UO₃ to UO₂, followed by hydro-fluorination to produce UF₄. The final stage involves reacting UF₄ with F₂ to produce uranium hexafluoride (UF₆) (Manna et al., 2017; Morel & Duperret, 2009).

The toxicity of ammonia underscores the significant concern surrounding potential leaks. Any accidental release of ammonia into the environment poses a rapid spread risk, potentially harming nearby individuals and ecosystems (Ng et al., 2023). Accidents in industrial facilities can occur due to pipeline leaks, incidents during transportation, or storage of gases and liquid materials (Casal, 2018). Due to the number of chemical industries and the handling of large quantities of hazardous substances, the frequency of chemical accidents has risen. These accidents often result from human error, inadequate training, manufacturing defects, and poor storage management (Anjana, Amarnath, & Nair, 2018). Hence, predicting the behavior of poisonous releases is paramount (Casal, 2018).

The Areal Location of Hazardous Atmosphere (ALOHA) system is a computational tool for assessing toxic gas dispersion. Its primary objective is to estimate common hazards associated with accidental spills of volatile and flammable chemicals. It facilitates pre-planning and emergency response efforts by generating scenarios based on various factors such as location, chemical properties, atmospheric conditions, and the type of chemical source. Additionally, it shows threat zones and distances from the hazard source (National Oceanic and Atmospheric Administration, 2013; Hoscan & Cetinyokus, 2021).

ALOHA graphically represents a threat zone, where exposure to toxic vapors, an explosive atmosphere, overpressure from a vapor cloud explosion, or thermal radiation from the fire is possible. The represented threat zones are red, orange, and yellow, where the red zone is the most significant threat zone (National Oceanic and Atmospheric Administration, 2013). The threat zones feature Levels of Concern (LOCs), which are essential tools for assessing the impact of toxic air emissions. LOCs represent specific concentrations of airborne chemicals associated with adverse health effects. ALOHA provides the following guidelines as LOCs: Acute Exposure Guideline Levels (AEGLs), Emergency Response Planning Guidelines (ERPGs), Protective Action Criteria (PACs), and Immediate Danger to Life and Health (IDLH) limits. In this study, the AEGL parameter was selected (National Oceanic and Atmospheric Administration, 2013).

The Acute Exposure Guideline Levels established by a committee composed of members from the United States Environmental Protection Agency (EPA) and industry representatives. AEGL levels classification were according to the severity of the toxic effects resulting from exposure, with level 1 being the least severe and level 3 being the most severe (National Academy of Sciences USA, 2008). Follows a brief from of these three levels:

- AEGL-1: Represented by the color yellow. It may result in notable discomfort, irritation, or non-sensible, asymptomatic effects. These effects are not disabling and are temporary, reversing after exposure stops.
- AEGL-2: Represented by the color orange, it may result in adverse health effects with irreversible, serious, and long-lasting implications.
- AEGL-3: The red indicates a concentration above which the general population, including susceptible individuals, is at risk of experiencing life-threatening or lethal effects.

Google Earth or Google Maps show the treat zones using ALOHA's export feature Keyhole Markup Language (KML) file format (National Oceanic and Atmospheric Administration, 2020).

Meteorological factors, such as wind speed, temperature, and atmospheric pressure, among others, directly impact the dispersion of pollutants and the extent to vulnerable areas (Sanchez et al., 2018; Chakrabarti & Parikh, 2011). Different meteorological variables influence the atmospheric dispersion of pollutants (National Institute of Meteorology, 2024). For example, wind speed considerably influences the dispersion of a chemical product and the extension of impact zones (Sanchez et al., 2018; Inanloo & Tansel, 2015). Although wind speed is a significant factor, other variables, such as temperature and humidity, must also be considered (Sanchez et al., 2018).

The study of ammonia gas dispersion is important due accidents involving this toxic substance can lead environmental and societal impacts (Tan et al., 2017). This substance is corrosive and, when released, poses dangers to humans and wildlife in the area (Ng et al., 2023). The ammonia forms ammonium hydroxide and produces heat when it contacts moist surfaces, such as mucous membranes. Due to its exothermic and corrosive properties, ammonia can cause severe irritation and burns to the eyes, skin, and mucous membranes of the oral cavity and respiratory tract (National Academy of Sciences USA, 2008).

Given the unique characteristics of each industrial process, existing studies typically provide insight only into the specific area where they were conducted (Pouyakian et al., 2023). Therefore, while ammonia dispersion modeling has been explored in various contexts, it is essential to analyze each process's specific scenarios and conditions individually. This study evaluates data to assess the potential consequences of a hypothetical ammonia leak in a uranium hexafluoride

production facility. However, the ammonia dispersion values obtained in this study can be applied to other industries that store ammonia, provided they have similar tank characteristics and weather conditions to those in this research.

2. Materials and Methods

Figure 1 illustrates the methodology employed in this study. Initially, an investigation assessed the characteristics of the studied area, storage conditions, and local meteorological conditions. Together with the initial conditions of ALOHA's program, this information is essential to establish the threat zone.



Figure 1. Methodology summary used to stablish the threat zone.

2.1. Study Area

The hypothetical UF₆ production unit used in this study has a 5000-liter ammonia storage tank. The vertical tank is 2 meters long and 1.78 meters wide.

2.2. Meteorological Conditions

Different meteorological variables influence the atmospheric dispersion of pollutants (Casal, 2018). Information such as wind speed and direction, temperature, and humidity is mandatory for simulations. This study used the meteorological data obtained from the automatic station of the National Institute of Meteorology (INMET). The INMET aims to generate meteorological information through monitoring, analysis, weather, and climate forecasting (National Institute of Meteorology, 2024).

The wind rose graphically represents the frequency of winds according to their direction and speed. So, obtaining information about wind behavior in a specific geographical area is possible. The wind direction represents the wind blows. For example, a north wind direction indicates that it blows from the north towards the south (Casal, 2018).

Figure 2 represents the annual average for the year 2023. It illustrates that the prevailing wind direction throughout that year was between east (E) and southeast (SE).



Figure 2. The wind rose chart for the site.

The meteorological data used in this study were obtained from the INMET automatic station, with records available from the start of its operations in August 2006 until December 2023. Variables such as wind speed, temperature, and relative humidity were analyzed specifically during nighttime periods, as the simulations were conducted during this time frame. Figures 3-5 show the distribution of wind speed, temperature, and humidity, respectively, represented by histograms. This study considered that INMET performs regular calibrations on its stations, ensuring data reliability. However, some values were not recorded in the database. The table detailing the number of recorded and missing data is available in Appendix A of this paper.

Figure 3 shows a histogram with the percentage of occurrences of different wind speed ranges during nighttime from 2006 to 2023 and the number of times each range occurs is represented above each bar in the histogram. Pearson's skewness coefficient of 1.18 confirms the positive skewness, indicating that the data have a longer tail to the right. In another words, the highest bars in the histogram correspond to wind speeds between 0 and 5 meters per second, this indicates that wind tends to be calmer during nighttime. Although most wind speed measurements are low, there are some extreme values above 10 meters per second, though these occur at relatively small percentages.

Figure 4 presents the distribution of temperature during nighttime. The nighttime temperature distribution was found to be nearly symmetrical, with a Pearson's skewness coefficient of 0.20, indicating a predominance of slightly higher temperatures during the nighttime, but the skewness is minimal, suggesting a relatively

balanced distribution between lower and higher temperatures. The most frequent nighttime temperatures are concentrated around 20° C, representing about 16% of observations. Although there is this concentration of temperatures, the histogram shows that extreme temperatures, such as those above 30° C or below 10° C, also occur, albeit with a frequency less than $2\%^{1}$.



Figure 3. Histogram of wind speeds during the nighttime period from 2006 to 2023.





¹Artificial intelligence technology by OpenAI, was used to assist in reviewing the text in this paragraph.

The histogram in **Figure 5** shows the humidity distribution and a Pearson's skewness coefficient of -1.05, representing a left-skewed distribution. This means that most humidity values are concentrated between 80% and 100% during the nighttime.



Figure 5. Histogram of humidity during the nighttime period from 2006 to 2023.

The histograms illustrating the distributions of minimum and maximum wind speeds, maximum and minimum temperatures, and maximum and minimum humidity in **Figures 3-5** provide a comprehensive view of the climatic variations in the dataset from 2006 to 2023. While there are fluctuations throughout the year, a consistent trend can be identified over the different years analyzed.

2.3. Scenarios Studied

Table 1 describes the data used as initial conditions at ALOHA for all simulations, including the chemical product, location, tank dimensions, hole diameter, and wind directions. This information is essential for modeling the leak scenario and analyzing the possible consequences.

Data summary					
Chemical Name	Ammonia (NH ₃)				
CAS Number	7664-41-7				
Wind direction	ESE, NWN e SW				

Table 1. Data summary for ALOHA modeling.

Continued	
Tank volume	5000 liters
Tank length	02 meters
Tank Diameter	1.78 meters
Time	Night
Opening diameter	0.5 centimeters

This research analyzes ammonia dispersion, varying the observation points and variations in wind speed, temperature, and humidity. Five scenarios were conducted, each focusing on analyzing a different meteorological condition parameter. Within these parameters, several simulations were carried out. The scenarios are described in **Figure 6**. The methodology employed in this study is similar to that of Sanchez et al. (2018) and Anjana et al. (2018), utilizing diverse scenarios to predict ammonia dispersion. This approach enables a more comprehensive analysis of meteorological conditions and their effects on dispersion.



Figure 6. Scenarios studied under different meteorological conditions.

3. Results and Discussions

The extreme values used in the simulations were determined by analyzing the data provided by INMET from August 2006 to December 2023 (National Institute of Meteorology, 2024).

3.1. Scenario 1: Wind Speed Variations

• Maximum wind speed:

The highest wind speed recorded since August 2006 was November 03, 2023, at 25.4 meters per second. The temperature used in the simulation was 20.3 °C, the average recorded on this date. In the conditions adopted for this simulation, the reach of the toxic ammonia cloud for AEGL 3, AEGL 2, and AEGL 1 were 10, 18, and 42 meters, respectively.

• Minimum wind speed:

The lowest wind speed recorded since 2006 was zero meters per second. However, the minimum speed allowed by ALOHA is one meter per second. Therefore, the adopted value was for the simulation. In this case, the temperature used in this simulation was 20.3 °C and the humidity 50%, matching the previous simulation's conditions and allowing a comparison of the toxic gas dispersion, where the only variable was the wind speed. In this simulation, with the minimum wind speed, the reach of the harmful ammonia cloud for AEGL 3, AEGL 2, and AEGL 1 were 74, 204, and 511 meters, respectively.

• Wind Speed Variations:

The study includes some additional scenarios to analyze the impact of wind speed on ammonia dispersion. Table 2 summarizes the meteorological data used in the ALOHA modeling for this scenario. These simulations of wind speed variations demonstrate that as wind speed decreases, the distance the gas reaches increases, as shown in the results in Figure 7.

Table 2. Meteorological conditions for ALOHA modeling—Wind speed variation.

Meteorological Conditions												
Wind speed (m/s)	1	2	3	4	5	7	10	13	15	18	22	25.4
Temperature (°C)	20.3	20.3	20.3	20.3	20.3	20.3	20.3	20.3	20.3	20.3	20.3	20.3
Humidity (%)	50	50	50	50	50	50	50	50	50	50	50	50



Figure 7. Threat zone behavior according to wind variation.

Among the simulations considering different wind speeds, the greatest ammonia dispersion occurred at a wind speed of 1 meter per second. The increase in ammonia dispersion compared to the dispersion observed at a maximum speed of 25.4 meters per second is 640% for AEGL-3, 1033.33% for AEGL-2, and 1116.67% for AEGL-1.

Wind is a relevant parameter for gas dispersion (Anjana, Amarnath, & Nair, 2018; Tan et al., 2017; Casal, 2018). The simulations indicate that a decrease in wind speed increases ammonia dispersion, with larger areas affected by the gas plume. According to Casal (2018), concentrations in a plume are inversely

proportional to wind speed, as wind exerts a dragging effect on the gas cloud. Thus, the results of these simulations on wind speed variations align with Casal's (2018) assertion that wind speed directly affects the dispersion of gas clouds, with stronger winds dispersing the gas more quickly and reducing the threat range.

Although wind speed is a significant factor, other meteorological variables must also be considered (Sanchez et al., 2018). Accordingly, additional simulations were conducted in this study and are presented below.

3.2. Scenario 2: Temperature Variations

• Maximum temperature

The highest temperature recorded since 2006 was 38.8°C on October 07, 2020. The average wind speed recorded that day was 3.4 meters per second. In the conditions adopted for the simulation, the range of the toxic ammonia cloud, according to concentrations for AEGL 3, reaches 40 meters; for AEGL 2, it is 108 meters; and for AEGL 1, it is 263 meters.

• Minimum temperature

The lowest temperature recorded since 2006 in winter was 1.9°C on October 05, 2021. The wind speed used was 3.4 meters per second, the same speed used in the maximum temperature simulation, so it was possible to compare the distance reached by the gas. The dispersion range of the toxic ammonia cloud for the conducted simulation was as follows: for AEGL 3, it extended to 21 meters; for AEGL 2, it reached 56 meters; and for AEGL 1, it extended to 134 meters.

• Temperature Variations:

The study includes seven additional points to assess the effect of temperature variations on ammonia dispersion. The summary of data on meteorological conditions used in ALOHA modeling for this scenario is presented in **Table 3**. The results are in **Figure 8**. The results show that an increase in temperature favors ammonia dispersion. The findings indicate that increasing temperature favors the dispersion of ammonia. The increase in ammonia dispersion compared to the minimum and maximum temperatures was 90.48% for AEGL-3, 92.86% for AEGL-2, and 96.27% for AEGL-1.

Meteorological Conditions										
Temperature (°C)	1	1.9	5	10	15	20	25	30	35	38.8
Wind speed (m/s)	3.4	3.4	3.4	3.4	3.4	3.4	3.4	3.4	3.4	3.4
Humidity (%)	50	50	50	50	50	50	50	50	50	50

Table 3. Meteorological conditions for ALOHA modeling—Temperature variation.

The temperature variation simulations in this study and those by Bondžić et al. (2021) suggest that higher temperatures increase the area at risk from ammonia dispersion. Although the plume's reach was less significant than wind speed variations, the results still show that temperature plays a role in gas dispersion. Casal (2018) highlights that wind speed and direction are the dominant factors in gas



cloud dispersion, while temperature has a comparatively smaller effect.

Figure 8. Threat zone behavior considering to temperature variation.

3.3. Scenario 3: Humidity Variations

This research also considered the humidity variation, which ranged from a minimum value of 0% to a maximum of 100%. In this case, the scenario was a temperature of 20°C and a wind speed of 3.4 meters per second. Table 4 summarizes the data on meteorological conditions used in ALOHA modeling for this scenario.

The results presented in Figure 9 showed that altering humidity values does not result in any variation in the distance reached by the gas, indicating that variations in humidity do not affect ammonia dispersion.

able 4. Meteorological conditions for ALOHA modeling—humidity variation.												
Meteorological Conditions												
Humidi	ty (%)	0	10	20	30	40	50	60	70	80	90	100
Temperat	ure (°C)	20	20	20	20	20	20	20	20	20	20	20
Wind spee	ed (m/s)	3.4	3.4	3.4	3.4	.4 3.4 3.4 3.4 3.4 3.4 3.4		3.4	3.4			
200 180 160 140 (E) 120 100 80 60 40 20 0						•		•	•		AE AE	GL 3 GL 2 GL 1

Humidity (%)



In this study, humidity was considered, but it did not affect ammonia dispersion. Similarly, the research conducted by Silva Júnior, de Oliveira, and Fiates (2022) indicates that humidity is an irrelevant factor in ammonia dispersion.

3.4. Scenario 4: Critical Variations

In the simulations with varying wind speeds, the speed increased when the toxic cloud decreased. On the other hand, increasing temperature favors dispersion in models when temperature changes. However, with humidity, no change in the dispersion range was observed. This scenario involved studying the worst case observed for ammonia dispersion in Scenarios 1 and 2. Scenario 1, where the wind variation on ammonia dispersion was studied and observed with a wind speed of 1 meter per second, resulted in the greatest dispersion. Scenario 2, which examined temperature variation, found that a temperature of 38.8°C led to the greatest ammonia dispersion. Therefore, the study used these values for the simulation in this scenario. Since humidity proved irrelevant, the value of 50% remained constant. The simulation results consider the parameters presented in **Figure 10**.

Figure 10 shows the threat zone for this simulation. The dispersion range of the toxic ammonia cloud for AEGL 3 extended to 101 meters; for AEGL 2, it reached 280 meters; and for AEGL 1, it extended to 710 meters.

Figure 11 presents a Graphic representation of the threat zone. Considering the most relevant wind direction, ESE, the average gas dispersion affects uninhabited regions. However, the red danger zone affects part of the uranium hexafluoride unit, becoming a concern for workers. Another area of concern susceptible to impact is the vegetation surrounding the installation, which may harbor wildlife at risk of exposure. Safeguarding both the workers and the local environment is paramount.



Figure 10. Threat zone obtained using the ALOHA for Scenario 4.

Risk modeling based on realistic worst-case scenarios is necessary to minimize potential risk and can provide a more accurate description of the consequences in extreme situations (Juwari et al., 2024). Therefore, this scenario involved studying previous scenarios' worst-case observations for ammonia dispersion.

3.5. Scenario 5: Wind Direction Variations

As previously discussed, the wind exhibits different directions over time. Given this variability, in addition to the simulation in the East-Southeast (ESE) direction, simulations were also conducted in the West-Northwest (WNW) and Southwest (SW) directions to investigate the areas affected by ammonia dispersion. Studying these scenarios aims to assess the impacts under different wind conditions. The WNW and SW directions were selected for these simulations because, according to the wind rose shown in **Figure 2**, they were the other predominant directions.

The dispersion range of the toxic ammonia cloud in this simulation was: for AEGL 3, it extended to 101 meters; for AEGL 2, it reached 280 meters; and for AEGL 1, it extended to 710 meters. **Figure 11** shows the graphical representation for the East-Southeast, West-Northwest, and Southwest directions.

As wind direction changes over time, estimating the vulnerable population in different directions around the hazardous materials storage facility is essential for effective preparedness and timely evacuation in the event of an accident (Anjana, Amarnath, & Nair, 2018). Therefore, other directions were simulated. Based on the simulations conducted for this scenario, it is observed that in the event of an accident with wind blowing in the West-Northwest (WNW) and Southwest (SW) directions, ammonia dispersion does not extend beyond the nuclear plant's premises. The affected area remains confined to the nuclear plant, without impacting inhabited regions. This means that under these specific wind conditions, there is no risk of ammonia contamination for nearby communities. However, considering the most relevant wind direction, ESE, the gas dispersion also affects uninhabited regions. Another area susceptible to impact is the vegetation zone. Additionally, in all directions, the AEGL-3 zone affects part of the uranium hexafluoride unit, making it a concerning area for the facility's workers.

Given its toxicity, ammonia leakage poses a significant concern, as any accidental release of ammonia into the environment risks spreading quickly and causing harm to nearby individuals and damage to the ecosystem (Ng et al., 2023). The harm caused by NH₃ to humans, animals, and the environment should not be underestimated (Wang et al., 2022). Because exposure to ammonia can lead to various pulmonary symptoms in workers' respiratory systems (Soltanzadeh et al., 2024). According to Casal (2018), predicting the behavior of a toxic release enables an assessment of the accident's effects. This provides essential information for developing safety measures and emergency response plans. Implementing practical strategies and technical solutions can effectively decrease vulnerability to such incidents (Soltanzadeh et al., 2024).

In the study, the affected area does not impact inhabited regions; however, it does affect the plant area, which can pose risks to workers in that area. To minimize the risk in the event of an accidental leak, the study by Anjana et al. (2018)



Figure 11. Graphical representation of the threat zone – Directions ESE, WNW and SW.

proposes measures for ammonia storage facilities to mitigate potential risks, such as: the construction of high walls around the ammonia storage facility can prevent ammonia dispersion by inhibiting the wind effect, and water spray nozzles controlled by ammonia detectors can be installed since ammonia is soluble in water, thereby reducing risks and preventing air pollution. With the installation of water spray nozzles suggested by Anjana et al. (2018), a warning system could be integrated to alert workers and emergency response teams. Alongside this, the development of an Emergency Action Plan (EAP) becomes necessary, as simulation training for evacuating the affected area can ensure that everyone knows how to respond adequately to emergencies².

4. Conclusion

This study demonstrates that the meteorological conditions with the greatest impact on ammonia dispersion are low wind speeds and high temperatures, while variations in humidity showed minimal influence on gas dispersion. Additionally, it was found that the prevailing wind direction in the analyzed region is East-Southeast (ESE). However, since wind direction varies over time, other predominant directions were also considered. The simulations revealed that, regardless of wind direction, ammonia dispersion affects the facility, and the ESE direction impacts surrounding vegetation. This raises concerns for the safety of workers, and local wildlife.

As a result, implementing preventive measures is essential. Regular inspections of tanks, valves, and pipelines should be conducted to ensure the integrity of ammonia storage infrastructure. Although the likelihood of an accident is low, this ²Artificial intelligence technology by OpenAI, was used to assist in reviewing the text in this paragraph.

study underscores the importance of having a comprehensive Emergency Action Plan in place. This plan should include personnel training for proper evacuation procedures in the event of a leak. By increasing awareness and preparedness among facility workers, potential damage can be minimized, and an effective emergency response can be ensured.

Since factors such as weather conditions and storage variables—like tank size, stored volume, and location directly influence the dispersion of toxic gases such as ammonia, each industry must conduct studies tailored to its specific context. Therefore, future research can focus on assessing operational risks involving conditions that were not addressed in this study.

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Conflicts of Interest

The authors declare no conflicts of interest regarding the publication of this paper.

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Appendix

Table A1 presents the valid and unrecorded records by year (2006-2023) during the night for the meteorological data used in this study. For unknown reasons, some data were not recorded.

Year	Valid Records	Invalid Records
2006	1725	270
2007	4137	207
2008	4482	104
2009	4331	0
2010	4314	30
2011	4226	116
2012	4258	97
2013	4261	83
2014	4278	65
2015	4259	85
2016	4323	32
2017	4344	0
2018	4271	72
2019	3480	863
2020	4030	324
2021	1434	2910
2022	3185	1158
2023	4344	0

Table A1. Number of valid and invalid records by year from 2006 to 2023.