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COMPUTATIONAL FLUID DYNAMIC MODEL TO SIMULATE THE DISPERSION OF ATMOSPHERIC NH_3 GENERATED BY A COWSTABLE IN LA LAGUNA, MEXICO

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ABSTRACT

Stalls are one of the main causes of ammonia (NH_3) buildup. These harmful gases have increased their concentration in the air in recent years. However, there are few studies on their dispersion to the atmosphere, since they constitute a passive polluting system in livestock areas. Therefore, the objective of this research was to evaluate the distribution of NH_3 pollutants concerning temperature, humidity, and airflow in a stable, through a computational fluid dynamics model and its analysis using the K2 algorithm. The model consisted of simulated 20 production units with similar environmental conditions and took the initial valuesfrom data obtained from a nearby weather station in a region characterized by semi-arid climatic conditions. The highest concentration of NH_3 was obtained under a wind velocity of 0 ms^{-1} due to the stagnation of the pollutant. The results indicated that levels of only 0.48 ms^{-1} reduce the concentration of NH_3 by 13 %. The results were analyzed using the K2 algorithm to obtain the relationship and inferences between NH_3 emissions, air flow velocity, ambient temperature, and humidity. The analysis of the CFD approach using the K2 algorithm concluded that temperature (85 %) and humidity (98 %) are the main variables that influence the pollution produced by the distribution of NH_3 to the environment derived from livestock activity.

Keywords: Ammonia dispersion, Livestock emissions, Environmental variables, CFD, K2 algorithm, models.

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INTRODUCTION

Weather conditions have a decisive influence on the dispersion of pollutants emitted into the atmosphere and affect chemical reactions (Vira *et al.*, 2022). Wind disperses pollutants and transports them away from its point of emission, while its direction relates to the area of affectation (Wang *et al.*, 2022).

Ammonia (NH_3) at high concentrations, causes throat irritation, lung inflammation, damage to the respiratory tract, and eyes. As the concentration increases, it can produce pulmonary edema. At 50 ppm it causes stress in cattle, inducing low dry matter intake, embryonic deaths due to inhalation poisoning, and low milk or meat production, among others. According to Erisman *et al*. (2008), inefficiencies in the farming system result in large N losses to the environment, including NH_3 emissions to the atmosphere (Houlton *et al*., 2012). Agricultural activities are the world's largest source of NH_3 in the atmosphere (Bouwman *et al*., 1997). The stables are one of the main causes that produce accumulation of ammonia and increase in humidity, these harmful gases increase their concentration in the air if the ventilation is deficient. An ammonia level of > 20 ppm is sufficient to cause damage to the respiratory epithelium, the longer the exposure, the greater the damage caused to the mucociliary system.

Atmospheric NH_3 has undesirable consequences. It contributes to the formation of aerosols with implications for air quality (Aneja *et al*., 2009) and climate change (Adams *et al*., 2001). Its transport and eventual deposit in non-agricultural ecosystems can affect carbon fixation (Pinder *et al*., 2012), eutrophication (Grizzetti, 2011), and biodiversity (Bobbink *et al*., 2010). An annual cost of 18-140 billion USD for NH_3 emissions in the European Union, mainly due to increased mortality associated with aerosols. Without major changes to the current food system, the projected global increase in food demand 70 % by 2050, Conforti (2011) will be accompanied by higher NH_3 emissions (Erisman *et al*., 2008).

Agricultural NH_3 emissions have proven difficult to estimate over space and time, the resolution required for atmospheric models. Detailed models of nitrogen flux in agricultural systems have been developed for livestock operations (Li *et al*., 2012) and mineral fertilizers (Cooter *et al*., 2012). These models require detailed knowledge of local environmental conditions and farming practices that are generally not available. Global NH_3 emission inventories depend on source-specific emission factors, which explain regional practices (Faulkner and Shaw 2008). Recent US National Emissions Inventory (NEI) assessments compiled by the US Environmental Protection Agency (EPA) show good agreement with observations at the national scale (Zhang *et al*., 2022) but large discrepancies at the regional scale (Fisher *et al*., 2011). Uncertainties in NH_3 emissions contribute to large errors in simulated ammonium nitrate, which constitutes a significant fraction of the aerosol (Zhang *et al*., 2020).

NH_3 emissions into the atmosphere affect human health, the climate, and ecosystems, due to the formation of secondary aerosols. Despite many studies, there is inadequate knowledge of agricultural sources (Liu *et al*., 2022; Luo, 2022; Viatte *et al*., 2022; Vira *et al*., 2022; Wang *et al*., 2022). The increase in world demand for food causes an increase in the concentration of NH_3 produced by dairy farms. Liu *et al*. (2022) established that the punctual emissions of NH_3 from livestock in 2020 ranged between 16.8 and 126.6 kg N ha^{-1}, with an average emission of 42.0 kg N ha^{-1}, with an increasing trend of 5.8 % annually between 2008 - 2020, mainly in spring and summer. From 2008 to 2018, there have been significant increases in global NH_3 emissions in India at 13 %, tropical

Africa at 33 %, and South America at 18 % with the intensification of agricultural activity (Luo *et al*., 2022).

It is essential to determine the concentration and distribution of gas emissions such as NH3, which is of increasing importance due to its effect on the health and productivity of animals and workers (Chmielowiec-Korzeniowska *et al*., 2018; Qin *et al*., 2020; Tabase *et al*., 2020; Zhang *et al*., 2020; Gautam, 2021; Kim *et al*., 2022; Zhang *et al*., 2022). NH_3 emissions depend on the design and operation of the barn, as well as manure management (Heidarzadeh-Vazifehkhoran *et al*., 2022). Computer models to simulate the generation and dispersion of gases within the stables constitute an effective strategy for contaminant mitigation.

Computational Fluid Dynamics (CFD) is a versatile technique in those multiple areas of knowledge that have contributed to a comprehensive understanding of the complexity of biological systems and had relevance since the end of the 20th century (Rong, 2016; Ben, 2021). CFD became a tool by combining the fundamentals of physics, chemistry, and biology (Ivanov *et al*., 2022). Currently, it is possible to couple CFD to systems based on Artificial Intelligence (Bournet and Rojano, 2022; Xin *et al*., 2022) like the K2 algorithm. The K2 algorithm was developed in the field of artificial intelligence, for approximate reasoning that defines the relationships between multiple variables (De la Torre-Gea, 2014). This work aimed to evaluate the distribution of NH_3 flow generated within a cow stable using a CFD model and its relationship with environmental conditions temperature, humidity, and airflow through probabilistic analysis using the K2 algorithm.

MATERIALS AND METHODS

For this study, it was established the source of contamination as a stable located in the region of La Laguna, Coahuila, Mexico, close to Torreón city, which consists of 20 stables with similar environmental conditions. The results obtained regarding quantity of NH_3 from the approach were considered to establish the source of dispersion pattern of NH_3 to provide an idea of the environmental problem suffered by the region.

By developing a CFD-based methodology, the distribution of atmospheric NH_3 produced by dairy cow barns located in the La Laguna region, which includes the states of Coahuila and Durango, Mexico, was studied; whose geographical coordinates are: 25° 41′ 33″ North latitude, and 103° 23′ West longitude, at an altitude of 1120 m above sea level, during June 15 and 22, 2019, in a region highly characterized by hot weather conditions during the summer that causes environmental pollution.

The stable components were modeled in 3D using the Ansys Geometry version 14.0, commercially available, to obtain the mesh of the modeled objects. The same software tool made it possible to set boundary conditions and initial values of the CFD model (Table 1). Finally, the Ansys Fluent software, simulated ammonia generation. The initial conditions: wind velocity, maximum temperature, and humidity were taken from the corresponding records from June 15 to 22, 2018, 2019, and 2020 from the

Table 1. Boundary conditions and initial values of the CFD model.

Solution	Simulation 3D	Doble precision
Model type	Steady-state	
Mesh type	Automatic Patch	Conforming/Sweeping
Minimum element size	0.20 m	
Number of elements	1,652,901	
Viscosity	K - e with buoyancy	
Energy equation	Active	
	Domain entry	
Velocity inlet	0.15 m s^{-1}	
Turbulent kinetic energy	1.00 J	
Air temperature	315.00K	
Species	Active	
NH_3 concentration	100 %	
RH	100 %	
Domain exit	Outlet pressure	1.00 Pa
Kinetic energy	1.00 J	
Solar radiation	900.00 W m^{-2}	
Diffuse solar radiation	400.00 W m^{-2}	
Solar calculator	Active	
Material Physical properties	Air	Soil
Density (kg m^{-3})	1.22	1,400.00
Specific heat of the air (J $kg^{-1}K^{-1}$)	1,006.43	1,738.00
Thermal conductivity (W m^{-1} k^{-1})	24.20 e^{-3}	1.50
Coefficient of thermal expansion (K^{-1})	3.39 e^{-3}	
Airborne gases	NH_3	Water steam
Thermal conductivity (W m^{-1} k^{-1})	0.04	0.04
Viscosity ($kgm^{-1}s^{-1}$)	1.72 e^{-05}	1.72 e^{-05}
Mass diffusivity (kg $m^{-1}s^{-1}$)	2.88 e^{-5}	2.88 e^{-5}
Thermal diffusion coefficient (kg $m^{-1}s^{-1}$)	-8e-06 t + 6 e-05	-2.50 e^{-3} + 0.13

nearest meteorological station called "El Cuije" in Mexico located at 1,033 m from the stable, whose geographical coordinates are: 25° 41′ 24″ North, 103° 20 22′ West.

1. The proposed methodology to develop the CFD model was in three stages:
2. Continuous flow discretization: Field variables consisted of a number finite of values at points called nodes.
3. Discretization of the equations of motion based on the values of the nodes.
4. System solution of algebraic equations and obtaining the values of the variables in all the nodes.

Each production unit in the stable was 60 m long and 40 m wide, and the height was 10.8 m at the eaves and 12 m at the top (Figure 1). The longitudinal axis of the

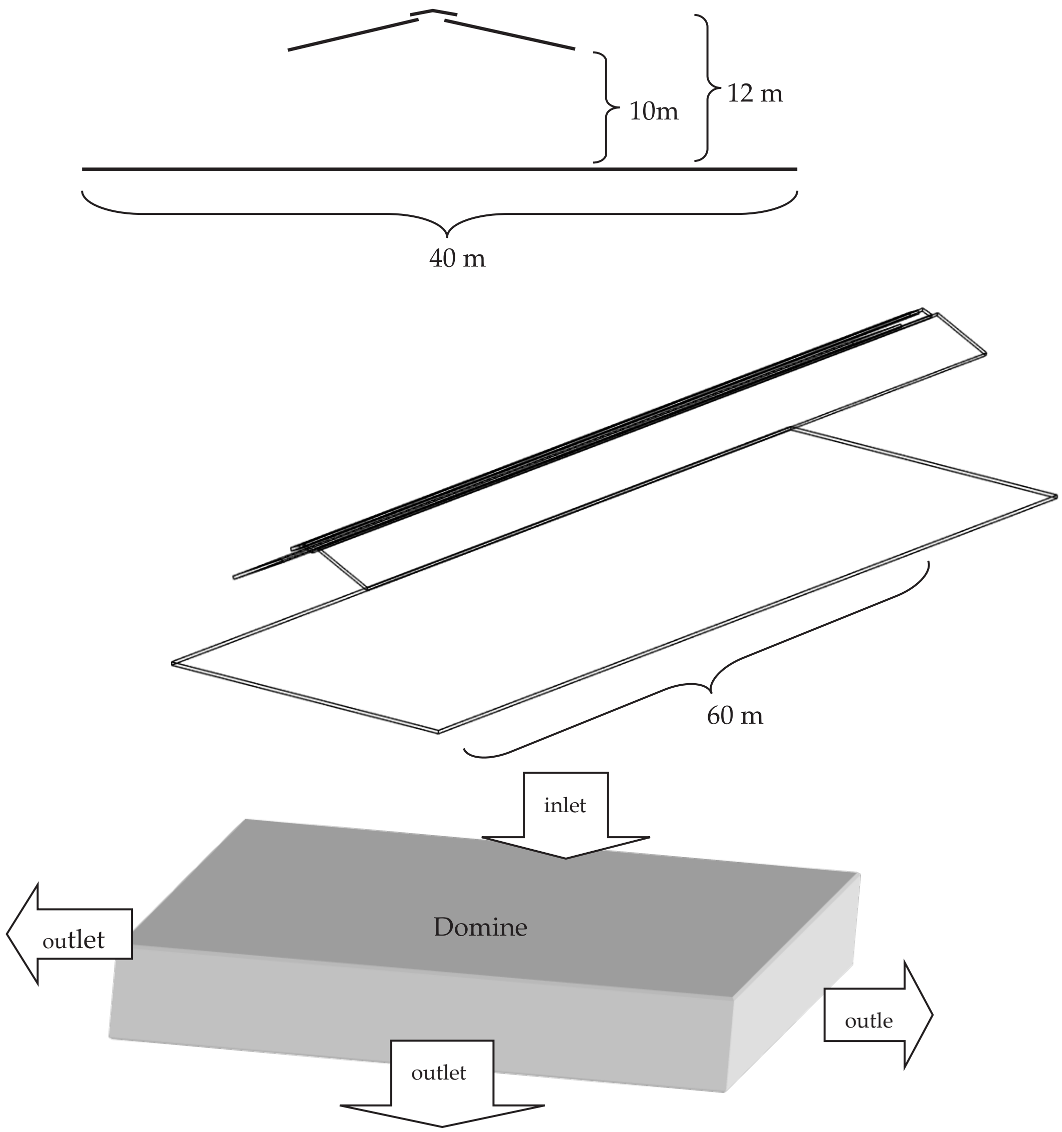

Figure 1. Unit production dimensions and domine.

domain is in the east-west direction, and three sides are completely open, in boundary conditions of 100 m long by 100 m wide and 40 m high.

From the CFD model, a sample of 11,952 records was taken in a vertical plane, at a distance of 40 m from the domain entrance (1/2 the length of the barn), with data on temperature, NH_3 concentration, relative humidity, and height. With them, a database was created and discretized in 5 intervals for each variable, between 300 K and 315 K, 0 to 100% NH_3 and Relative Humidity, and 0 to 40 m of height.

CFD model was validated by analyzing two data sets of temperature; the first from 24 daily measurements from the "El Cuije" weather station: in July 2021 and the second from data calculated from the CFD model for the same dates (Figure 2). The standard error was computed, finding only 1.49 % of variation between the data set and CFD data, with a standard deviation equal to 1.93 K, which means that the approximation by the CFD model is acceptable (Rico-García *et al*., 2011).

The variables were defined in a discrete domain, and the functional relationships described the causal inferences expressed in terms of conditional probabilities (Equation 1) using the most common method of Machine learning called the K2 algorithm (De la Torre-Gea *et al*., 2014).

$$f(i,\pi \mathrm{i}) = \prod_{j=1}^{qi} \frac{(\boldsymbol{ri} - \mathbf{1})!}{(\boldsymbol{Nij} + \boldsymbol{ri} - \mathbf{1})!} \prod_{k=1}^{ri} \alpha ijk \tag{1}$$

Where:

π_i: a data set of NH_3 of node x_i

$q_i = |\varphi_i|$

φ_i: list of all possible instantiations of the variables of x_i in database D. That is, if p_1, .. , p_s

are the parents of xi, then φi is the Cartesian product $\{v^{p1}_{1}, \ldots, v^{p1}_{rp1}\}$x . . . x$\{v^{ps}_{1}, \ldots, v^{ps}_{rps}\}$ of all the possible values of attributes p_1 through p_s.

$r_i = |V_i|$

V_i: list of all possible values of the attribute x_i

α_{ijk} : number of cases in D in which the attribute x_i is instantiated with its k^{th} value, and the variables of x_i in π_i with the j^{th} instantiation in φ_i.

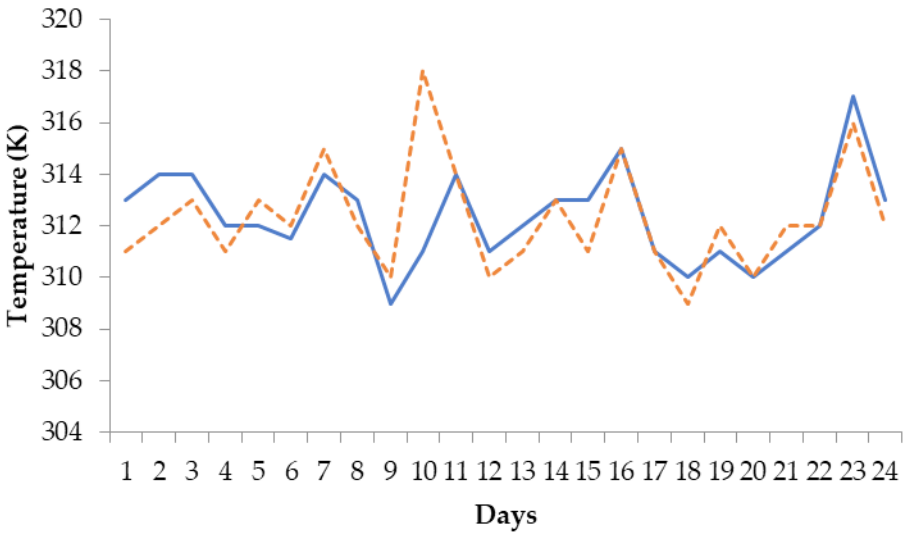

Figure 2. CFD model validation: weather station data solid line, CFD data dotted line.

$N_{ij} = \sum_{k=1}^{ri} \alpha_{ijk}$. That is, the number of instances in the database in which the variables of x_i in π_i is instantiated with the j^{th} instantiation in φ_i.

RESULTS AND DISCUSSION

The results obtained from the CFD simulation show a behavior where the mass of NH_3 (%) depends on the airflow patterns related to the ventilation systems. The highest concentration of NH_3 occurs in the center of the barn at 0.1 m height, where the mass of NH_3 (%) depends on the airflow patterns related to the ventilation systems, these results agree with Rong and Aarnink (2019), Gautam (2021), and He *et al*. (2022) indicate.

According to studies previously cited by Doumbia *et al*. (2021), the highest concentration of NH_3 was found in high-temperature conditions (315 K) and is the main influencing parameter. The maximum temperature of 308 K improves environmental conditions and significantly reduces the dispersion of NH3, as indicated by Doumbia *et al*. (2021), Chen *et al*. (2021), and Ahmadi *et al*. (2022).

On the other hand, the highest concentration of NH_3 was obtained under conditions of air velocity of 0 ms^{-1} due to the stagnation of the pollutant. Therefore, levels of only 0.48 ms^{-1} reduce the concentration of NH_3 by 13 %, improving environmental conditions, as previously cited works point out (Doumbia *et al*., 2021; Chen *et al*., 2021; Ahmadi *et al*., 2021; al., 2022).

NH_3 emissions are generated from the 0.1 m boundary layer without airflow. Figures 3 and 4 show the decrease of the contaminant as its dispersion towards the highest layers and wind velocity increases.

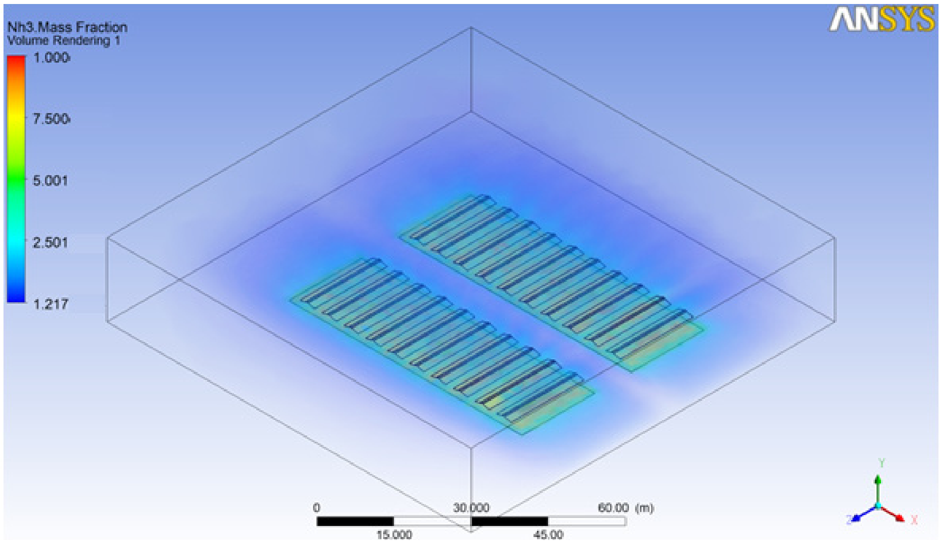

Figure 3. CFD model showing the dispersion of NH_3 concentration.

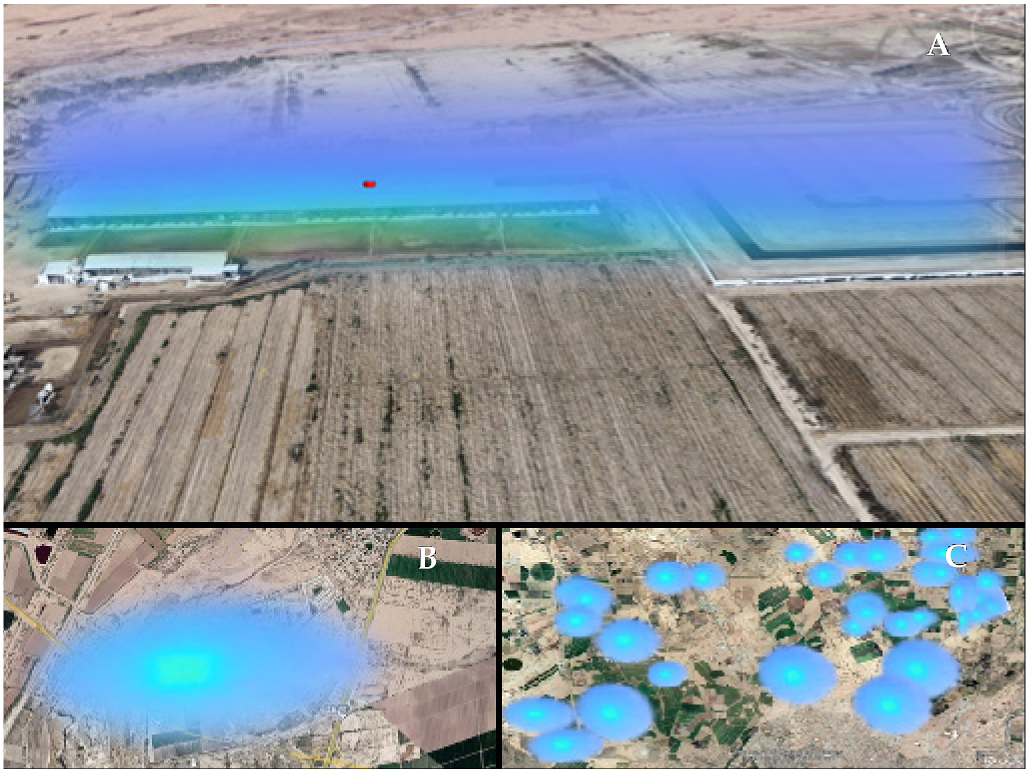

Figure 4. Transposition of the CFD simulation of the dispersion of NH_3. A: next to a residential community; B: in the location of the stable of La Laguna, Mexico; C: Dispersion of NH_3 from 30 stables conurbation to Torreón city, from 340 registered in La Laguna, Coahuila, Mexico.

Long-term measurements of ammonia concentrations were carried out at three different sites typical of urban, rural, and industrial areas in the La Laguna region of Mexico. NH_3 at the rural site shows a single peak of 14.9 ppm at midday, due to temperature-favored volatilization of agricultural emissions. Showing higher NH_3 levels in summer, ambient temperature was the common determining parameter of atmospheric NH_3 levels, as indicated in Figures 3 A to C.

The NH_3 emissions they generate from the limit layer of 0.1 m without airflow. Figure 5A shows the decrease in the pollutant as its dispersion increases towards the highest layers and wind velocity.

Wind velocity is an important factor in the distribution of NH_3 concentration. Figure 5B shows the effect of the eaves of the barn on the airflow, which causes vertical stagnation zones between 0 to 5 m high and 10 to 12 m below the eave.

Temperature and wind velocity are associated with increasing NH_3 concentrations, in agreement with Viatte *et al*. (2022). However, the highest concentrations of NH3 are associated with Humidity in the central part of the stable, as shown in Table 2. When only a concentration of 0.5 % NH_3 at 298 K temperature and 0 ms^{-1} air velocity, 90 % of these conditions were found at 0 m height with 0.5 % humidity, *i.e*. on the wet surface.

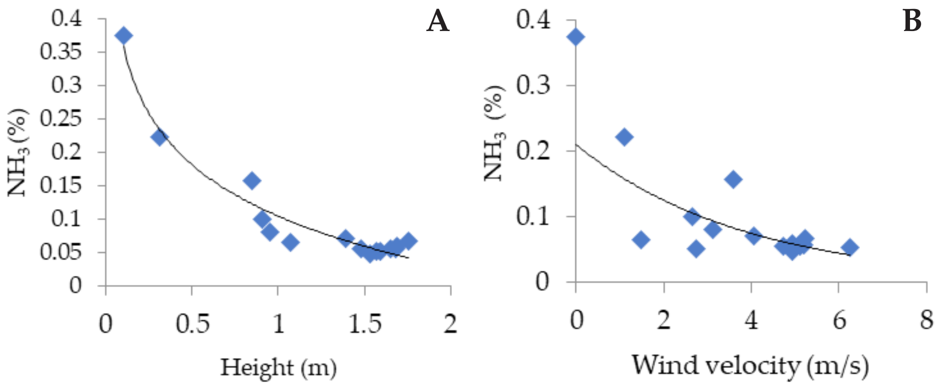

Figure 5. A: NH_3 and height relationship; B: NH_3 and wind velocity relationship.

Table 2. Probabilistic analysis of the CFD domine using the K2 algorithm.

	X (m)	Y (m)	Z (m)	H_2O (%)	NH_3 (%)	T (K)	Wind velocity (ms^{-1})
	55.00	0.10	55.00	0.37	0.37	310.70	0.00
A posteriori probability	0.79	0.26	0.77	0.98	1.00	0.85	0.32

The CFD model's approximation analyzed using the K2 algorithm showed that the NH_3 concentration is related to humidity, temperature, and wind velocity, whose gradients depend on height, as shown in Figure 6 like the studies carried out using CAM-chem and Fourier transform infrared spectrometry by Vira and Wang *et al*. (2022), the volatilization of NH3 is when the highest temperature and humidity occurs on the surface of the stable.

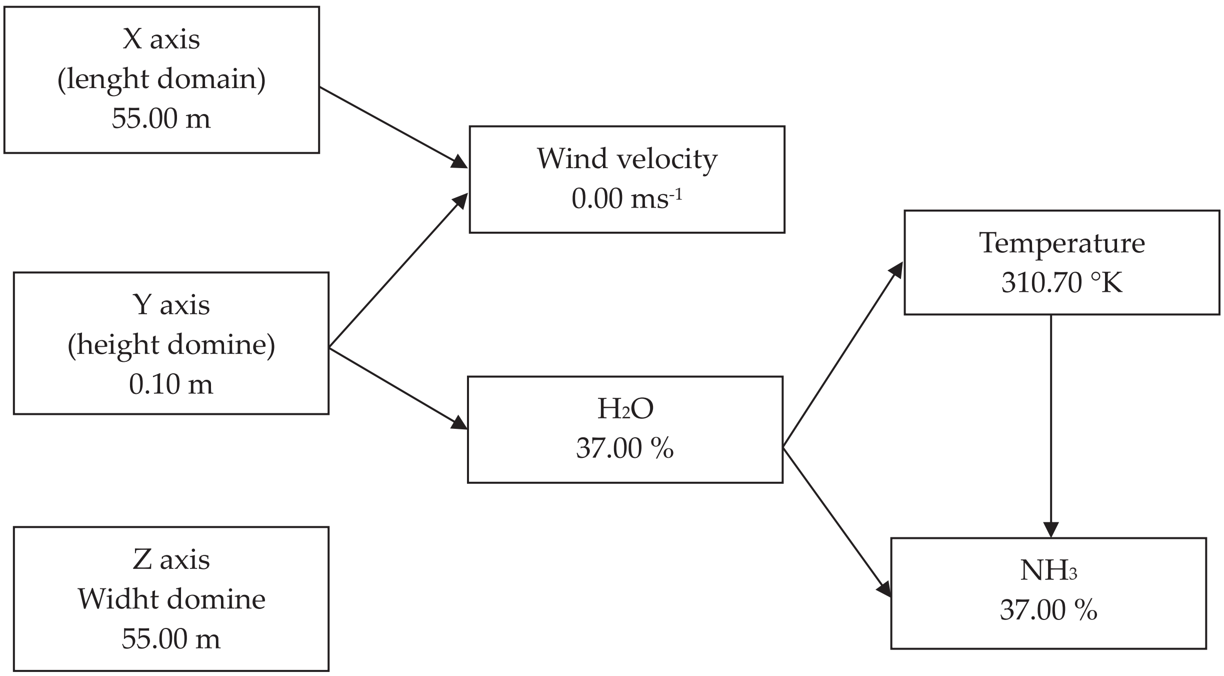

Figure 6. Relationships between the domain dimensions and the variables studied concerning the concentration of atmospheric NH_3 using the K2 algorithm.

CONCLUSIONS

To conclude, the results of this study underscore the significant influence of airflow patterns, temperature, and humidity on the distribution and concentration of NH_3 within cow stable. The CFD simulations demonstrate that NH_3 concentrations are highest near the barn center at lower heights (0.1 m), particularly under low wind velocity and high humidity conditions. This aligns with findings from prior studies, emphasizing that reduced airflow leads to NH_3 stagnation, while even slight increases in wind velocity facilitate dispersion, improving air quality. Temperature was also a critical factor, as increased temperatures enhanced NH_3 volatilization, with peak concentrations observed under high-temperature conditions, similar to observations by Doumbia *et al*. (2021) and Chen *et al*. (2021).

The probabilistic analysis using the K2 algorithm further confirms that NH_3 dispersion is governed by a combination of environmental parameters, with temperature, wind velocity, and humidity gradients varying with height. These results have practical implications for managing NH_3 emissions in agricultural facilities, indicating that optimized ventilation and temperature control could effectively reduce NH_3 concentration and improve environmental conditions.

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