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ENSURING THE SAFETY OF CLOSED ENCLOSURES BASED ON COMPUTATIONAL FLUID DYNAMICS ANALYSIS REGARDING THE MODELING OF CARBON MONOXIDE DISPERSION DYNAMICS

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Abstract: *Engaging in industrial activities necessitates the utilization, manipulation, or inadvertent occurrence of hazardous compounds, such as carbon monoxide. The occurrence of this gas in enclosed or partially enclosed areas can have a significant impact on the human body, and at elevated levels, it can result in fatality. Understanding the impact of carbon monoxide on the human body and its dispersion in the atmosphere is crucial for developing effective preventive strategies. This paper presents experiments and CFD (Computational Fluid Dynamics) modeling to establish the dynamics of carbon monoxide dispersion during the accumulation and evacuation stages in a closed enclosure. Toxic and explosive gas - carbon monoxide, discharged within a confined space, there was a display of relatively uniform accumulation phenomenon in the enclosure. The design of the kind of carbon monoxide spreading in the closed area showed a dilution focused on phenomena towards the suction mouths. Carbon monoxide has a high dilution capacity due to the rapid decrease in gas concentrations during the exhaust process.*

Key words: *CFD analysis; exhaust emission; toxic gas; carbon monoxide; dispersion; gas dynamics.*

1. INTRODUCTION

In industrial activities as well as in domestic activities, accidentally or not, there may be phenomena of formation and release of carbon monoxide, a gas extremely dangerous by exposure, for the human body. Carbon monoxide is formed by the incomplete oxidation of organic substances by combustion, fire or explosion.

Carbon oxide is photo-degradable and in this sense, it is estimated that photolysis removes 3.9 million tons of CO from the atmosphere annually [1, 2].

The lack of oxygen in the environment leads to the development of toxic phenomena. There is a 220 times greater attraction between hemoglobin and carbon monoxide than there is between hemoglobin and oxygen [3-5]. Unconsciousness, collapse, and fainting are the symptoms that manifest at concentrations of 50 to 55% HBCO when exposed to 0.1% CO. Syncope, which can lead to death over time, may also occur. Coma and convulsions precede death in approximately 5 hours at a concentration of 66% HBCO (when exposed to 0.2% CO) [6-7]. This level of exposure causes death. When exposed to 1% CO while at 80% HBCO, death happens very quickly. Even a carboxyhemoglobinemia level that is 40% or lower can be lethal for sensitive individuals [24 - 26].

It has been discovered that carbon monoxide poisoning is a factor that contributes to the development of Parkinson's syndrome from a neurological perspective. To avoid the extremely severe effects due to exposure of the human body to atmospheres in which carbon monoxide is accidentally present, the dynamics of its dispersal, especially in confined spaces, must be known in detail. It is also necessary to know the areas inside the enclosure where the concentrations are lower in relation to the source of formation and release of carbon monoxide [10 – 14, 17].

Although the establishment of an efficient ventilation system is known to be the primary protection against the formation of explosive/

toxic atmospheres, the behavior and ventilation capacity of the ventilation system must be known in detail in relation to the atmosphere in which carbon monoxide is present and its geometric shape of the enclosure [11 – 13, 15].

The novelty of the paper consists precisely in the study of these new aspects that are based on the analysis of the dispersion dynamics in the accumulation phase, with the highlighting of the areas with low concentrations.

The analysis of the degree of dispersion is extremely useful for establishing the preventive measures applicable to closed spaces against the phenomena of acute carbon oxide poisoning. The methods used to determine the degree of dispersion are represented both by monitoring the distribution of gas concentrations through laboratory experiments and by CFD analysis of the steps of accumulation and evacuation of carbon monoxide. The results of the analysis of the degree of dispersion revealed that the toxic and explosive gas-carbon monoxide, discharged in the closed enclosure, showed a relatively uniform accumulation process. Carbon monoxide has a high dilution capacity due to the rapid decrease in gas concentrations during the exhaust process.

2. MATERIALS AND METHODS

Because it has such a direct impact on the human body, the problem posed by the existence of poisons in industrial facilities is indicated. one that is of the utmost importance [10]. Workers have the potential to be exposed to the action of hazardous substances for either brief or extended periods of time, which may result in acute intoxication or work-related illnesses. The phenomenon of gas dispersion has occurred as the subject of a significant amount of research on a global scale [12, 14, 17 - 21, 23, 24]. On the other hand, in particular, the dynamics of the dispersion of harmful gases indoors have received less research. If there is an unintentional emission of carbon oxide within a confined industrial setting location, the outcomes of the comprehensive analysis study can be utilized to pinpoint regions of sanctuary or evacuation pathways in case of an emergency that this occurs [2, 5, 6 - 8]. To simulate the dispersal of gas dynamics, specialized programs known as the CFD technique are used as a state-of-the-art technique [6, 7, 11 - 13, 15, 16]. CFD instruments use the Navier Stokes system of physical equations [9, 10, 21 - 26]. To optimize efficiency, the process of solving algebraic equations is performed utilizing the calculation technique. CFD instruments are more accurate and closer to the real situation of the modeled phenomenon even if sometimes the data obtained differs from the data obtained experimentally.

2.1 Technical infrastructure

At INCD INSEMEX Petrosani, there is an industrial ventilation laboratory, the experiments concerning the setting up of the processes of formation and dispersion of dangerous atmospheres were done what was [4]. The experimental system that was utilized includes apparatus for data collecting in addition to a monitoring system that includes six pulleys to which six monitors for more than one gas the ALTAIR type is attached. These detectors can detect quantities of oxygen, carbon monoxide, carbon dioxide, and methyl chloride. The speed at which gas spreads and the dynamics behind the production of poisonous atmospheres can both be determined with the help of pulleys, which can build a changing spatial arrangement. Studying how well closed structures can let air flow through them that run the danger of producing potentially dangerous, poisonous, or suffocating atmospheres requires the employment of a complicated ventilation system with a changing structure. This is done to ensure how safe and healthy it is to work where the experiment took place.

The ventilation system comprises a 3kW engine for spinning blades fan unit a group of rectangle pipes measuring 300/400 mm, which regulate the mood inside of the building. Together, these components manage the air quality inside the building.

The air suction system comprises a network of rectangular pipes, including short and long branches, specifically intended to ventilate enclosures containing gases of varying specific weights, ranging from low to medium to high. The purpose of these short and long branches is to draw air into the enclosure.

2.2 Laboratory experiments

The CFD method was used to look at the motion of toxic gas dispersion using the set of tools called ANSYS MULTIPHISICS. This package includes a set of specialized solvers designed specifically for the analysis and resolution of the systems being considered: The mechanical, thermal, and stability aspects are utilized to address structural and thermal issues, regardless of whether they are linear or not. A distinct task that is comparable to Design Space, featuring basic thermal and structural computation capabilities. The software FLOTRAN is capable of handling multiphysics simulations. An appropriate solvent for fluid dynamics is CFX or a solvent with similar properties. This tool is designed to connect and integrate answers in physics and multiple physics. Expert in solving fluid-structure reactions that go both ways, utilizing multiphysics and CFX type solvers. A computational tool for solving fluid dynamics problems, such as the Fluent software or a similar program. This tool is designed to simulate the production and reduction of NOx in combustion systems. This tool is designed to solve problems related to drying and melting processes. MHD module.

This module is designed to handle multiphase flows, specifically those including particle distribution. I am an expert in solving fluid dynamics problems specifically related to polymers and glass materials. This solver is designed to handle the complex dynamics of solids, fluids, and gases, as well as their interactions, in both two-dimensional and three-dimensional settings.

Furthermore, the CFD technique employs the Navier-Stokes equations that are tailored for the laminar flow of actual fluids to model the dynamics of gas buildup and dilution.

3. RESULTS

3.1 Results of the laboratory experiments

An experiment was conducted in the laboratory to study the dynamics of creating a toxic atmosphere using carbon monoxide and CO. This study aimed to ascertain the ventilation capacity of enclosed spaces where there is a potential for the development of atmospheres that could be explosive, poisonous, or asphyxiating. This device features six different flow variations and five different suction lips at the level of the experimental cage. The following configuration can be found for the suction openings: There are three suction ports that provide horizontal suction, and there are two suction openings that provide vertical suction. This fan has a centrifugal drive and is a type V20-450D-3kW. This special fan can achieve a flow rate of 2800 m3/h. At a suction mouth level, the flow that was achieved on average was 3.11 m3 per minute. The average flow that could be achieved at the level of the experimental enclosure was 15.55 meters cubic feet per minute. The following were the conditions for the first round of testing parameters: 23.8 degrees Celsius, 9.460 pascals, 53.7%, and 34.8 liters per minute (similar with the considerations of [14 - 22]).

The gas flow velocity at the discharge mouth was 53.7 m/s. The removal of carbon oxide inside the enclosure was done using a support located 0.25 m from the floor on the east wall in the middle of its base side. The hose was fixed in a horizontal position.

The MSA-ALTAIR detection devices were positioned at a moderate level on the six pulleys, with the suction and detection sections set at a height of 1.8 meters above the ground.

Following the phase that consisted of releasing carbon dioxide into the enclosure and turning off the equipment that was responsible for its discharge, the enclosure's air system was turned on. The structure of the enclosure's ventilation system was accomplished with the assistance of flow fluctuations.

The SCADA-type command and control system was responsible for operating both the flow variators and the ventilation system.

The experiment was conducted for a total duration of 243 minutes. The duration allocated for ventilation was 30 minutes. Figure 1 illustrates the graphical representation of the dispersion dynamics in a closed enclosure.

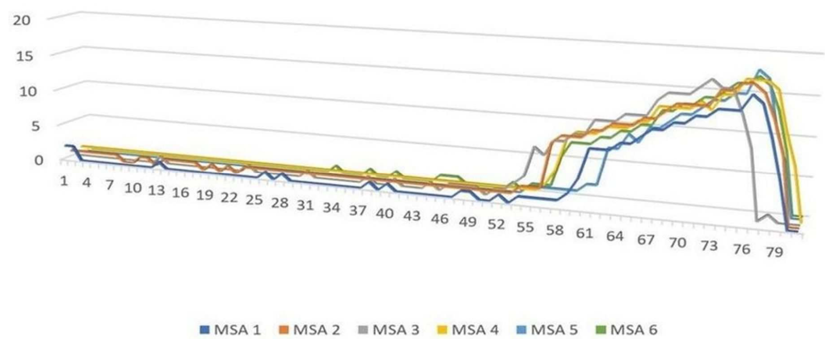

Fig. 1. Carbon oxide dispersion dynamics in a closed enclosure.

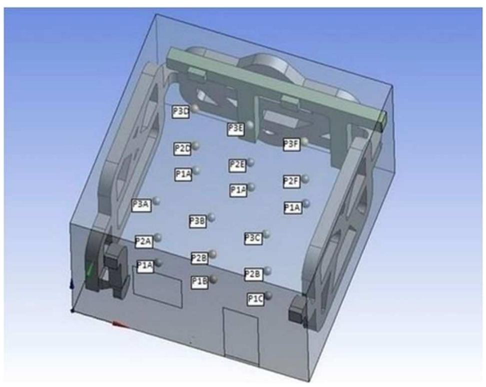

Fig. 2. Location of control points.

3.2 CFD modeling

To determine the mechanics of how toxic gases spread were performed using the CFD technique, modeling the carbon monoxide dispersion in a closed enclosure [4]. To simulate the dynamics of accumulation and dilution of gases, the CFD mechanism uses the Navier - Stokes equations. To simulate in a way this is as close to the experimental settings as possible survey was performed the computerized model Figure 2. At the level of the simulated enclosure, 3 sets of points are located at elevations 0.5 m (p1A/B/C/D/E/F), 1.5 m (p2A/B/C/D/E/F), and 3 m (p3A/B/C/D/E/F), respectively from the hearth Figure 4. Point sets are utilized to track the progression of gas concentrations during the modeling duration.

3.2.1 Accumulation

The following parameters have been determined for modeling: (1) The concentration of carbon monoxide introduced is 230 parts per million (ppm). (2) The gas is introduced near the eastern wall, specifically at 0.15 meters from the hearth. (3) The rate at which the gas is discharged inside the enclosure is 4.5 liters per minute. (4) The dispersion of carbon monoxide happens under constant pressure. The experimental site experiences typical atmospheric conditions, including pressure, temperature, and humidity. Additionally, the simulation time is set to 10 minutes. (6) The gas concentrations were reported as molar fractions.

The carbon monoxide dispersion inside the closed enclosure was modeled (levels 1, 2, and 3).

The graphical representation findings for an accumulation duration of 10 min. may be observed in Figures 5. At the 1-minute mark, starting from the beginning of the modeling process. The carbon oxide jet exhibits a planar configuration that is parallel to the floor and possesses a small curvature in the direction of its flow. After 2 minutes the commencement of the modeling process, the carbon oxide jet is flat and parallel to the floor. Additionally, the carbon oxide jet ascends on the adjacent wall, exceeding half the height.

After 3 minutes after initiating the modeling process, the carbon oxide jet assumes a planar configuration that is parallel to the floor. The fluid jet is set firmly at the floor to the opposite wall, rising in the form of a plane jet parallel to the vertical wall. Additionally, the jet of carbon oxide disperses at the ceiling at a length of less than half its length.

At the 4-minute mark, during the initial stages of modeling, the carbon oxide jet exhibits a planar configuration that is parallel to both the floor and the opposing wall. The fluid jet is firmly established at the floor and the opposite wall, it lies on the ceiling as an inhomogeneous jet along its entire length and disperses inhomogeneously on the access wall. The dispersion at the enclosure level is in the incipient development phase.

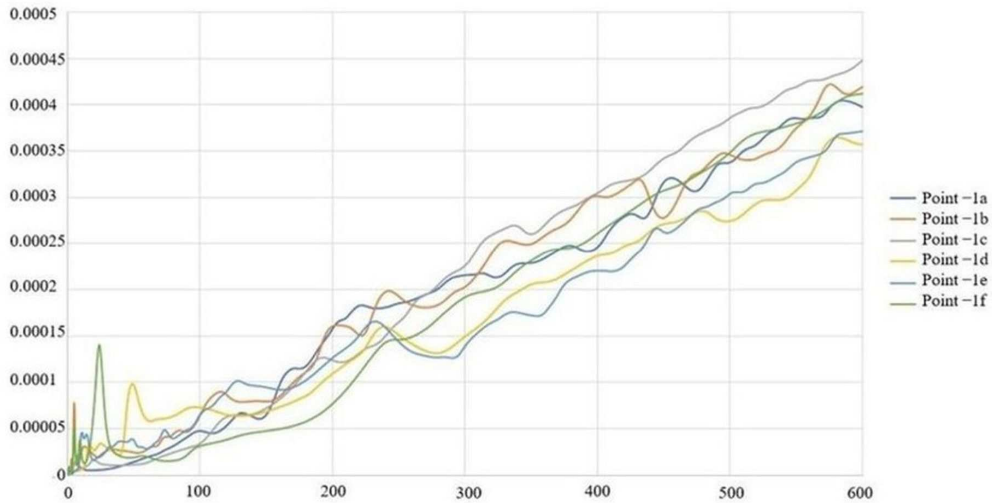

Fig. 3. Level 1-Dynamics of carbon oxide dispersion.

After 5 minutes of modeling, the carbon oxide jet takes on a flat shape that is parallel to the floor and the opposite wall (Figure 4). The fluid jet is firmly established at the floor and the opposite wall, it lies on the ceiling as an inhomogeneous jet along its entire length with lamination in its middle after which the jet disperses inhomogeneously on the access wall to the floor. 6 minutes after initiating the modeling process, the carbon oxide jet assumes a planar configuration that is parallel to both the floor and the opposing wall. The fluid jet is firmly established at the floor and the opposite wall, it lies on the ceiling like an inhomogeneous jet along its entire length. presenting a strong lamination in the middle of it. The jet of carbon oxide disperses inhomogeneously on the access wall presenting a splay at the floor level. The dispersion at the enclosure is in the middle development phase.

Figure 5 shows that at the 10-minute mark of the modeling process, the carbon oxide jet is positioned horizontally and parallel to both the floor and the opposing wall. The fluid jet is firmly established at the floor and the opposite wall, it lies on the ceiling like an inhomogeneous jet along its entire length, presenting a strong lamination in the middle of it. The carbon oxide jet disperses inhomogeneously on the access wall, rotating at the floor level over the main jet.

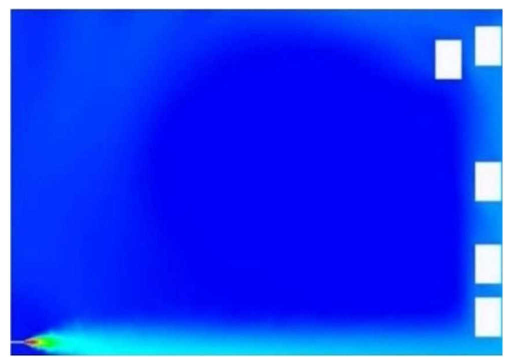

Fig.4. Evolution of carbon monoxide dispersion at 5 min, from the start.

3.2.2 Evacuation

The following aspects have been established for modeling: (1) The phenomenon of dilution of carbon monoxide is carried out under the influence of the ventilation system; (2) At the level of a suction mouth, the flow was measured and found to be an average of 3.11 m3/min; (3) The established average flow rate was 15.55 m3/min at the same level as the experimental enclosure; (4) The atmospheric pressure, temperature, and humidity are frequently observed at this location experimental site; (5) The simulation time is set to 10 minutes. The graphical representation findings illustrate the dilution and evacuation time of 4 minutes. The range of numbers is from 13 to 27.

Table 1.

Gas values at control level 1 have changed throughout time due to evolution.

Time Step [s]	point-1a	point-1b	point-1c	point-1d	point-1e	point-1f
0	0.000818784	0.000895205	0.000897455	0.000744098	0.000732304	0.000732304
1	0.000819622	0.000900675	0.000700902	0.000749271	0.000747043	0.000747043
2	0.000814734	0.000897624	0.000838018	0.000750744	0.000779731	0.000779731
……	…………	…………	…………	…………	…………	…………
600	1.21E-05	1.26E-05	1.25E-05	1.24E-05	1.19E-05	1.19E-05

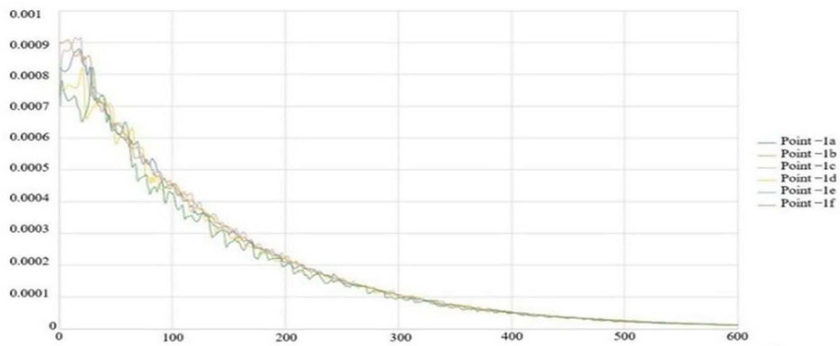

Fig. 5. Dynamics of carbon monoxide dispersion at level 1.

In Figure 6, it is observed that at time 0 when the introduction of carbon monoxide has been stopped, the fluid with high concentration is still present on the floor and the opposite wall, inhomogeneous on the ceiling along its entire length with a strong lamination in its middle, the carbon monoxide disperses inhomogeneously on the access wall rotating at the level of the floor.

Phase 0 shows the maximum gas dispersion at the enclosure and captures the moment between stopping the introduction of the carbon monoxide jet and starting the ventilation installation.

It is observed that 10 s. from the start of modeling the jet of carbon monoxide introduced into the floor disappears. Under the influence of the ventilation installation, the gas cloud is firmly located on the opposite wall and lies both on the floor and at the ceiling in inhomogeneous laminar form towards the suction mouths. The gas concentration reduction at the enclosure level is in the incipient evolution phase.

In Figure 7, notes that within 20 seconds of the start of the modeling of the dilution and discharge of CO gas accumulated in a closed enclosure, the gas cloud with higher concentration located in the access wall is dislocated and diluted inhomogeneously and moves to the floor and ceiling in the form of spurs towards the suction mouths. In the central area, the gas cloud is visibly diluted and moves turbulently towards the suction mouths.

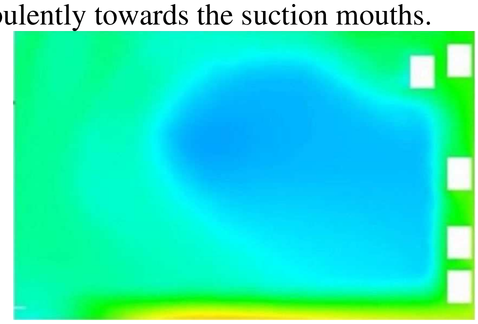

Fig. 6. The evolution of the carbon monoxide dispersion at time 0, the introduction of CO stopped.

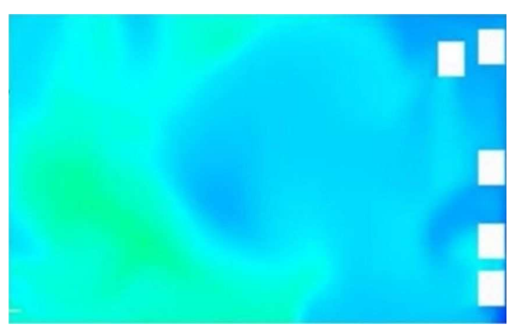

Fig. 7. CO dispersion - 20s, after stopping.

It is observed that in the 30 s, from the start of modeling, the gas cloud with higher concentration located in the central area is dislocated and diluted inhomogeneously and moves turbulently towards the suction mouths. In the area of the entrance wall, at the floor and ceiling. areas with accentuated dilution appear. The gas dilution at the enclosure is in the reduced dilution phase.

It is observed that in the 40 s, from the inception of the modeling process, the gas cloud with homogeneous concentration has a relatively uniform distribution at the enclosure and moves turbulently towards the suction mouths. In the area of the inlet wall, respectively in the area of the suction mouths. areas with accentuated dilution appear. The gas dilution at the enclosure is in the lower average development phase.

In Figure 8 it is observed that at 50 s, respectively at 1 min, from the start of modeling, the gas cloud with relatively homogeneous concentration has uneven distribution at the enclosure and moves turbulently towards the suction mouths. In the area of the inlet wall, respectively in the suction mouths, areas with accentuated dilution appear. The gas dilution at the enclosure is in the medium development phase.

In Figure 9, at 3 min, from the start of modeling, the gas cloud evolves from a relatively inhomogeneous concentration, uneven distribution at the enclosure, and turbulent displacement towards the suction mouths. In the area of the inlet wall, respectively around the suction mouths, areas with accentuated dilution appear. The gas is being diluted now enclosure level is progressive in the phases of upper average development, pronounced, and almost complete.

Fig. 8. CO dispersion - 1 min, after stopping.

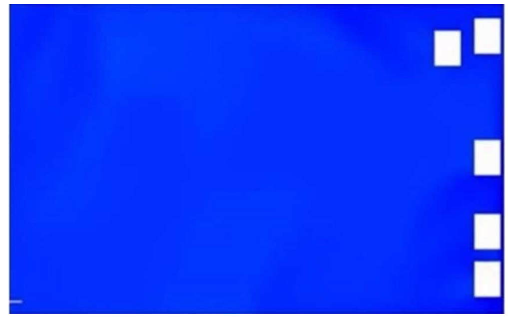

Fig. 9. CO dispersion – 3 min, after stopping.

4. DISCUSSION

4.1. Discussions of the laboratory experiments results

The experiment on the dispersion of hazardous gasses in a confined carbon monoxide containment yields the following deductions:

The process of dispersing indoor presence of carbon oxide has had 3 distinct stages, namely: the incubation period in which the gas is dispersed and diluted and which has detectable concentrations from 0 to 2 ppm at the level of measuring devices MSA ALTAIR; the accumulation period in which the gas is dispersed and reaches progressively increasing gas values at the level of the MSA ALTAIR measuring devices; the duration of time during which the gas is removed from the space by means of a ventilation system that has a changeable structure.

4.2. Discussion of the CFD modeling results

From the modeling of the dispersion of toxic gases indoors using carbon oxide CO, the further deliberations can be inferred: The indoor dispersion of carbon oxide gas was regulated through a system of 18 control points, evenly distributed across three different levels.

4.2.1. Accumulation

The dispersion process at level 1 has a varied progression. Hence, a range of distinct gas concentrations was discovered for the initially turbulent flow at all control sites. The medium level 2 dispersion procedure is marked by a fluctuating progression. Therefore, a range of gas concentrations specific to the turbulent flow was discovered at all control sites. The process of dispersal at the higher level 3 exhibits a fluctuating progression.

4.2.2. Evacuation

The dilution and evacuation process at levels 1 lower, 2 medium and 3 uppers, exhibit a fluctuating progression. At the lower level 1, there were fluctuations in the precise gas concentrations within the turbulent flow, on the first third followed by a laminar flow on the next two-thirds of the process. at all control points. except for carbon oxide concentrations at point 1f. At average level 2, fluctuations in the concentrations of gases in turbulent conditions medium flow was found, in the first half followed by a laminar flow in the second half of the process. at all control points. At level 3 higher, a fluctuation in the concentrations of certain gases was observed in the turbulent upper flow during the first half of the operation followed by a laminar flow in the second half of the process, at all control points. The enclosed gas dispersion and specific parameter Gd, exhibited distinct variations based on the location of the control points in the plan. Modeling the dilution and evacuation of carbon oxide from the enclosed enclosure exhibited a phenomenon of dilution with a specific orientation towards the suction mouths. The flow of carbon oxide is in the form of a turbulent and inhomogeneous cloud. The gas flow moves under the depression of the ventilation system from the area of the inlet wall unevenly to the suction and discharge area. The concentration of carbon oxide in the initial phase is maximum in the area of the inlet wall, gradually decreases by dilution as it is re- moved, and becomes relatively uneven and low in the outlet area at the mouth. Carbon oxide has a high dilution capacity due to the rapid de- crease in gas concentrations during the exhaust process.

5. CONCLUSIONS

The subsequent deductions were derived from analysis of the carbon monoxide dispersion and dilution dynamics both experimentally and by CFD modeling. The process of dispersing carbon oxide in the closed enclosure presented 3 distinct stages, namely: the incubation period (155.75 and 176.25 minutes), the accumulation period (51 and 69 minutes), and the ventilation period (12 and 19.25 minutes). The toxic gas - co discharged the enclosed space exhibited a relatively uniform accumulation phenomenon at the enclosure. Proven by the fact that gas concentrations were identified regarding the detection devices between 16-18 ppm. Compared to the value of the global average concentration concerning the aggregate capacity of the enclosure of 15.86 ppm.

The kinetics of explosive dispersion, poisonous, and asphyxiating gases were studied by modeling the dispersion of carbon oxide within a confined space using the computational fluid dynamics (CFD) technique. The process of dispersing carbon oxide at the lower level 1, level 2 and level 3 exhibits a fluctuating progression. Therefore, a range of gas concentrations was discovered for the initially turbulent, medium, and extremely turbulent flow at all control points.

The spatial distribution of carbon oxide dispersion and progressive dilution within the closed enclosure, as represented using the gradient (Gd), exhibited distinct variations based on the location of the control points. The rate at which carbon oxide disperses and becomes diluted within a confined enclosure is determined by the gradient. Gd the progressive reduction of the gas's concentration gradient as it becomes increasingly diluted. The concentration of Gd at lower level 1 ranged from 2.144 to 2.689 ppm/h. At the average level 2, it ranged from 1.806 to 2.710 ppm/h. At the upper level 3, it ranged from 2.108 to 3.270 ppm/h.

The simulation of carbon oxide dispersion within the enclosed space revealed a phenomenon where the dispersion was aligned with the direction of the gas jet being released. The carbon oxide flows as a flat jet that is adhered to the floor and extends up to the height of the opposite wall. The procedure of diluting and removing co at a lower level 1, level 2 and level 3 is characterized by a turbulent, turbulent medium and turbulent upper flow, on the first third followed by a laminar flow on the next two-thirds of the process at all control points. The rate at which carbon oxide spreads and becomes less concentrated within the closed space, denoted as Gd, exhibited a fluctuating pattern that depended on the location of the control points in the plan. At the lower level, the values ranged from 4.430 to 5.328 ppm/h. At the average level, the values ranged from 3.643 to 5.073 ppm/h. The simulation of carbon oxide dispersion in the enclosed space revealed a phenomenon of dilution that was directed towards the suction openings.

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Dinamica fluidelor computațională și experimentări privind dinamica dispersiei monoxidului de carbon în spații închise

Desfășurarea activităților umane de natură industrială implică utilizarea, manipularea sau prezența accidentală a unor substanțe toxice, cum ar fi oxidul de carbon. Prezența acestui gaz în spații închise sau semiînchise poate afecta grav organismul uman, iar atunci când concentrațiile sunt ridicate poate duce la deces. Cunoașterea modului în care oxidul de carbon afectează corpul uman și a modului în care se dispersează în aer este foarte importantă pentru stabilirea unor măsuri de prevenire. De asemenea, pentru a stabili căile de evacuare și zonele de refugiu, este necesar să se cunoască dinamica de dispersie a oxidului de carbon atât pe orizontală, cât și pe verticală. Această lucrare prezintă experimente și modelarea CFD (Computational Fluid Dynamics) pentru a stabili dinamica dispersiei monoxidului de carbon în timpul etapelor de acumulare și evacuare într-o incintă închisă. Gazul toxic și exploziv - oxidul de carbon, evacuat într-o incintă închisă, a prezentat un fenomen de acumulare relativ uniform în incintă. Modelarea dispersiei monoxidului de carbon în incinta închisă a evidențiat un fenomen de diluție orientat spre gurile de aspirație. Monoxidul de carbon are o capacitate de diluție ridicată datorită scăderii rapide a concentrațiilor de gaz în timpul procesului de evacuare.

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