

CFD SIMULATION OF CARBON DIOXIDE DISPERSION DYNAMICS IN CLOSED SPACES

Doru CIOCLEA¹, Sorin Mihai RADU^{2}, Alexandru CĂMĂRĂȘESCU³,
Adrian MATEI⁴, Răzvan DRĂGOESCU⁵*

¹National Institute for Research and Development in Mine Safety and Protection to Explosion
INSEMEX Petroșani, Romania, doru.cioclea@insemex.ro

²University of Petroșani, Romania, sorin_mihai_radu@yahoo.com

³National Institute for Research and Development in Mine Safety and Protection to Explosion
INSEMEX Petroșani, Romania, alexandru.camarasescu@insemex.ro

⁴National Institute for Research and Development in Mine Safety and Protection to Explosion
INSEMEX Petroșani, Romania, adrian.matei@insemex.ro

⁵National Institute for Research and Development in Mine Safety and Protection to Explosion
INSEMEX Petroșani, Romania, razvan.dragoescu@insemex.ro

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Abstract: Carbon dioxide is a suffocating gas resulting either from industrial activities from combustion or explosion. There may also be carbon dioxide deposits under pressure, quartered in porous geological formations. This gas can show slow or violent releases with accumulation at ground level. Carbon dioxide is a gas that is both toxic and asphyxiating. This gas can accumulate in closed spaces and when it exceeds the concentration of 12% vol. it becomes lethal. For the protection of working personnel, it is necessary to identify and apply the most effective preventive measures. This requires an understanding of carbon dioxide's behaviour during the build-up phase. The research gives a CFD analysis for determining the dynamics of carbon dioxide dispersion in a confined enclosure.

Keywords: CFD, dispersion, gas dynamics, asphyxiating gas, carbon dioxide, closed spaces

1. Introduction

For the study of complex physical phenomena, including fluid flow, specialized programs known as CFD technique are used as a top technique [1, 2, 3, 4]. In order to simulate gases, the CFD technique and physic-mathematical equations for fluid flow [5, 6, 7, 8, 9, 10, 11]. At the international level, experiments and modelling were performed with the CFD technique to identify the peculiarities that occur in the flow of gases including carbon dioxide [12, 13]. However, the analysis of the dispersion dynamics of this gas, indoors, can bring additional information in order to establish preventive measures [14, 15, 16, 17, 18, 19, 20].

2. Technique used description

The CFD technique for modelling of suffocating and toxic gas used the ANSYS MULTIPHYSICS software package.

The ANSYS package taken into account as follows: Export skills of discretization to the solvents contained in the package, but also to other solvents (such as: Abaqus, Flotran, Nastran, Patran, UGrid, TGrid, etc); Pre and post processors for multiphysics and mechanical solvers; Interface / connection, Pro / ENGINEER, One Space Designer, etc.; Graphical working interface for assembling and interacting mechanical, fluid, electromagnetic systems, geometries and discretization; Parametric generation and modelling application of solids (2D and 3D); Data resources (databases) comprising the technical characteristics of materials mainly used in industry, of toxic and explosive gases and liquids; Ability to automatically discretize (including TGrid) the generated geometries, depending on the type of solver used; Pre- and post-processing for mechanical, structural, thermal and magnetostatic systems; Ability to simulate cyclic loading on the product to anticipate lifespan; Generation and import from Nastran of finite element

* Corresponding author: Radu Sorin Mihai, prof. Ph.D. eng., University of Petroșani, Petroșani, Romania, Contact details: University of Petroșani, 20 University Street, sorin_mihai_radu@yahoo.com

models; Processing the dynamics of rigid and rigid / flexible bodies; Ability to load and manage a batch of solutions. Parallel processing within the package is based on a variational technology applied to static or transient solutions for thermal and structural analysis. The application allows the administration and storage of data from computer simulations.

3. Conditions for modelling

For the modelling regarding the dispersion of carbon dioxide in a closed enclosure, the CFD technique was used on a computerized model, fig. 1, [21, 22].

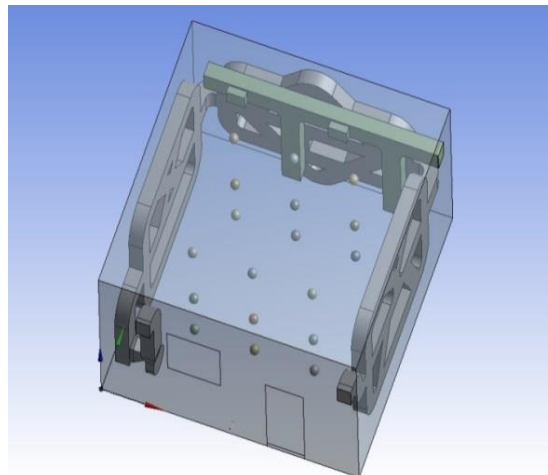


Fig. 1. Site modelling

At the level of the modelled enclosure, three sets of points were formed, as shown in Table 1, at altitudes of 0.5, 1.5, and 3m from the floor (fig. 2). Set points are used to regulate the evolution of gas concentrations during simulation.

Table 1. Coordinates of control points

	P1A	P1B	P1C	P1D	P1E	P1F
X ₁	1.5	2.8	4.1	1.5	2.8	4.1
Y ₁	1.5	1.5	1.5	4.0	4.0	4.0
Z ₁	0.5	0.5	0.5	0.5	0.5	0.5
	P2A	P2B	P2C	P2D	P2E	P2F
X ₂	1.5	2.8	4.1	1.5	2.8	4.1
Y ₂	1.5	1.5	1.5	4.0	4.0	4.0
Z ₂	1.5	1.5	1.5	1.5	1.5	1.5
	P3A	P3B	P3C	P3D	P3E	P3F
X ₃	1.5	2.8	4.1	1.5	2.8	4.1
Y ₃	1.5	1.5	1.5	4.0	4.0	4.0
Z ₃	3.0	3.0	3.0	3.0	3.0	3.0

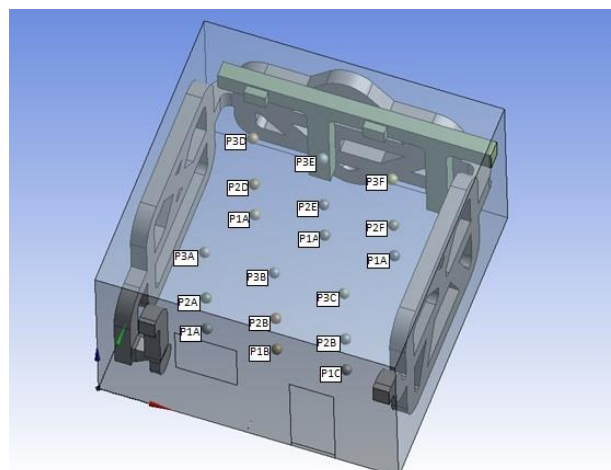


Fig. 2. Location of control points

4. CFD modelling

The conditions imposed for modelling were:

Carbon dioxide has maximum concentration;

The carbon dioxide introduction device was placed 0.15 meters from the floor;

Carbon dioxide is introduced using an 8 mm diameter hose;

The gas flow rate introduced is 4.5 l/min;

Modelling time was 10 minutes;

The maximum value of carbon dioxide was established at 1% Vol.

Following the simulation of carbon dioxide, the results are presented at the levels 1, 2 and 3.

The evolution of carbon dioxide concentration at level 1 is shown in Figure. 3.

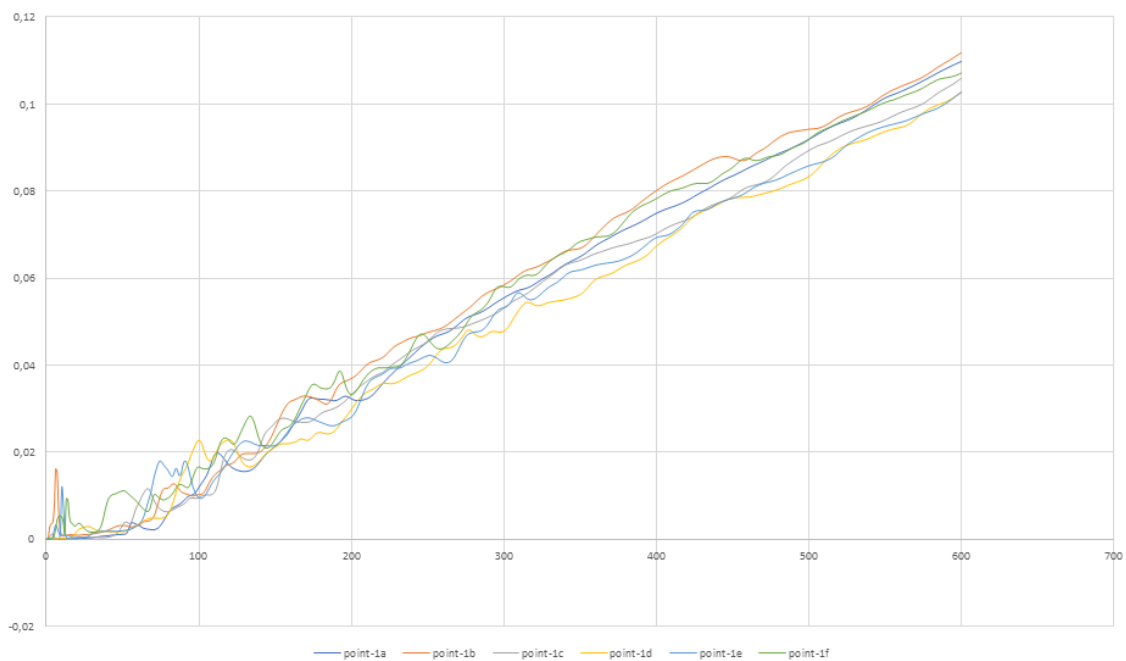


Fig. 3. Dynamics of carbon dioxide dispersion at level 1

The evolution of carbon dioxide concentration at level 2 is shown in Figure 4.

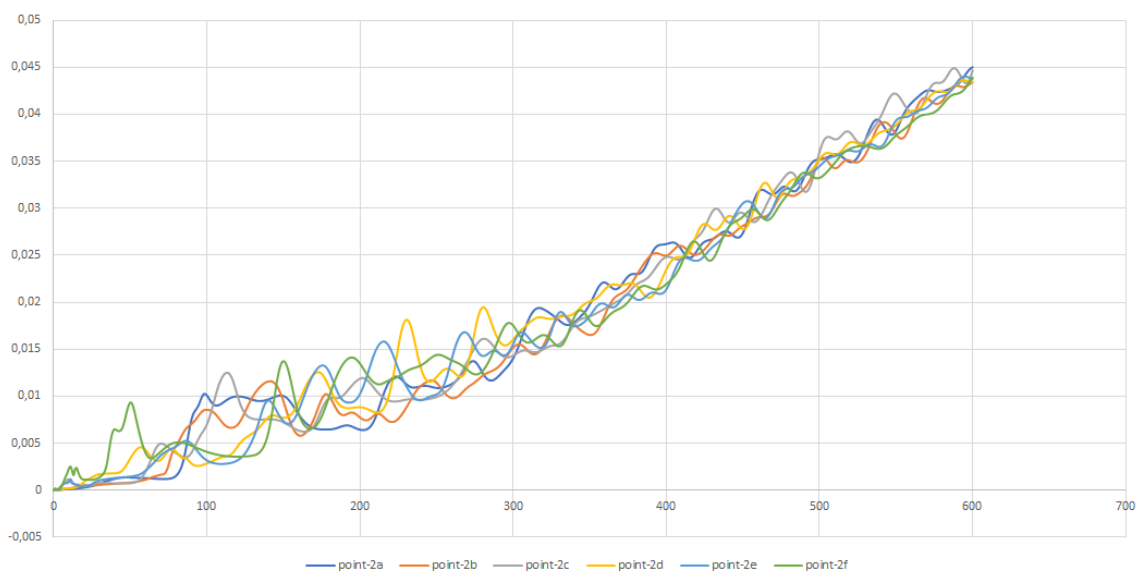


Fig. 4. Dynamics of carbon dioxide dispersion at level 2

The evolution of carbon dioxide concentration at level 3 is shown in Figure 5.

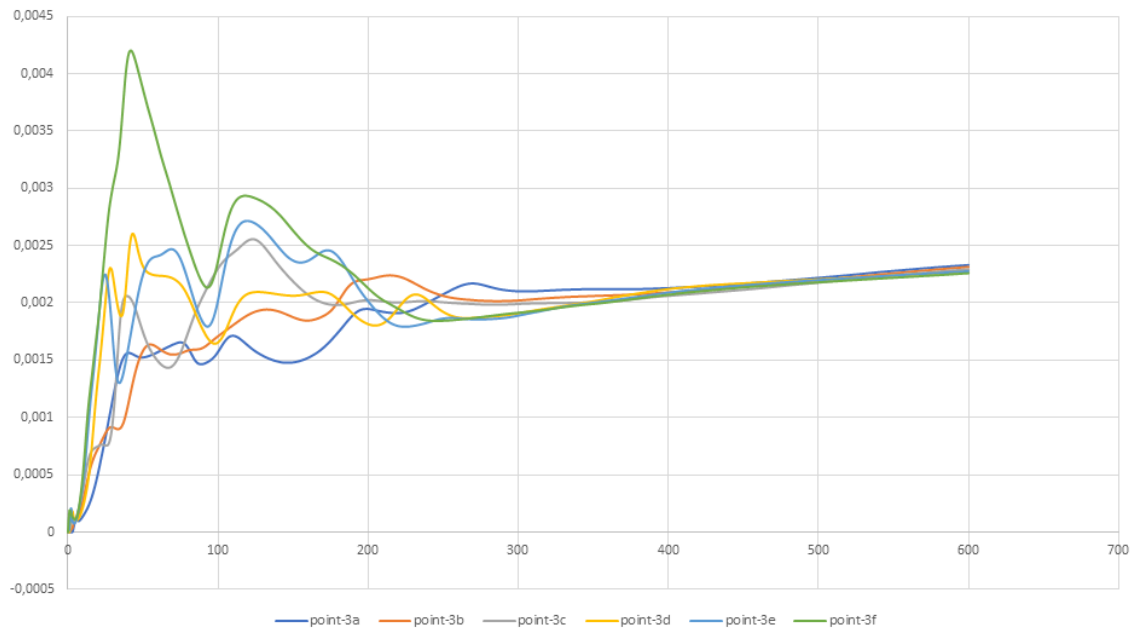


Fig. 5. Dynamics of carbon dioxide dispersion at level 3

The results are shown graphically in Figures 6-9.

In Figure 6 at 1 min., in Figure 7, at 2 min. the carbon dioxide disperses parallel to the floor facing of opposite wall.

Additionally, the jet of carbon dioxide rises on the opposite wall up to half its height and diffuses slowly.



Fig. 6. Carbon dioxide dispersion at 1 minutes



Fig. 7. Carbon dioxide dispersion at 2 minutes

In Figure 8 and 9, at 9 min. respectively 10 min., carbon dioxide disperses parallel to the floor going up the opposite wall towards the ceiling. In addition, the carbon dioxide jet rises firmly on the opposite wall up to half its height. From the floor, carbon dioxide diffuses progressively vertically, evenly, in a firmly established stage, up to about half the height of the enclosure.

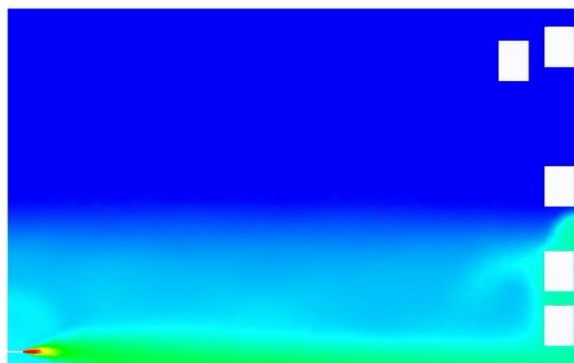


Fig. 8. Carbon dioxide dispersion at 9 minutes

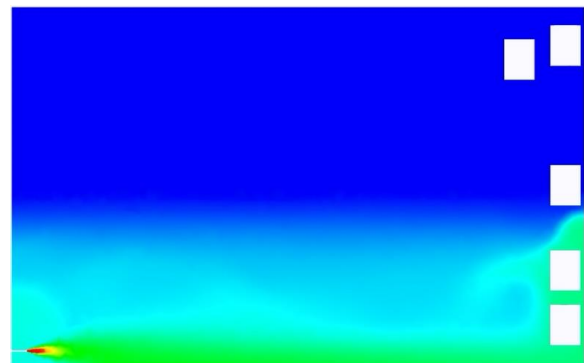


Fig. 9. Carbon dioxide dispersion at 10 minutes

5. Discussions

From modelling indoor asphyxia gas dispersion we can formulate the following observations:

The carbon dioxide dispersion was monitored on 3 levels: Lower Level 1, Middle Level 2, Upper Level 3;

The gas dispersion at first level has a variable evolution in the initially turbulent phase. The flow becomes laminar as the flow process stabilizes;

The gas dispersion at second level has a variable evolution in the medium turbulent phase. The flow initially becomes turbulent as the flow process stabilizes;

The gas dispersion at third level has a variable evolution in the highly turbulent phase, but it becomes laminar as the flow process stabilizes;

The Gd parameter that characterizes the degree of dispersion showed a variable evolution as follows:

Gd at first level vary from 4.217 to 4.526% Vol./h;

Gd at second level vary from 1.717 to 1.855% Vol./h;

Gd at third level vary from 0.088 to 0.092% Vol./h;

CFD simulation of carbon dioxide revealed a dispersion phenomenon oriented along the flow direction. Carbon dioxide disperses in the form of a flat jet attached to the floor, up to the level of the opposite wall. Vertically, the gas is diluted unevenly.

The carbon dioxide concentration gradually decreases and becomes relatively uniform and reduced in the accumulation area at floor level. If the carbon dioxide were to disperse continuously, the atmosphere inside the enclosure would be displaced from the floor to the ceiling.

6. Conclusions

For the study of the dispersion dynamics of asphyxiating gases, the modelling of the dispersion of carbon dioxide was carried out using the CFD method;

At first level, second level and third level, the flow has a variable evolution in the early, medium and strongly turbulent phase. The flow becomes laminar as the flow process stabilizes;

The Gd parameter that characterizes the degree of dispersion showed a variable evolution and presented value between 0.088 and 4.526 % Vol./h;

The simulation of carbon dioxide presented a dispersion oriented in the direction of flow, presenting the shape of a jet stuck to the floor up to the level of the opposite wall. The gas disperses unevenly vertically from the floor level.

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References

- [1] **Guillemaud V.**, 2007
Modélisation et simulation numérique des écoulements diphasiques par une approche bifluide à deux pressions, Université de Provence - Aix-Marseille I, Français, Thèse pour obtenir le grade de Docteur.
- [2] **Liu B., Liu X., Lu C., Godbole A.R., Michal G.**, 2016
Computational Fluid Dynamics Simulation of Carbon Dioxide Dispersion in a Complex Environment, Journal of Loss Prevention in the Process Industries, 40 419-432. Research Online is the Open Access Institutional Repository for the University of Wollongong.
- [3] **Lovreglio R., Ronchi E., Maragkos G., Beji T., Merci B.**, 2016
A Dynamic Approach for the Impact of a Toxic Gas Dispersion Hazard Considering Human Behaviour and Dispersion Modelling, Journal of Hazardous Materials, DOI: 10.1016/j.jhazmat.2016.06.015
- [4] **Pagnon S.**, 2012
Stratégies de modélisation des conséquences d'une dispersion atmosphérique de gaz toxique ou inflammable en situation d'urgence au regard de l'incertitude sur les données d'entrée, l'École Nationale Supérieure des Mines de Saint-Étienne, Thèse pour obtenir le grade de Docteur
- [5] **Bardina J., Thirumalainambi R.**, 2004
Web-Based Toxic Gas Dispersion Model for Shuttle Launch Operations, Proceedings of SPIE - The International Society for Optical Engineering, DOI: 10.1117/12.544853.

- [6] **Florescu I.**, 2007
Fluid Mechanics. ALMA MATER Publishing House, Bacău
- [7] **Lauret P.**, 2014
Modélisation de la dispersion atmosphérique sur un site industriel par combinaison d'automates cellulaires et de réseaux de neurones, l'École Nationale Supérieure des Mines de Saint-Étienne, Thèse pour obtenir le grade de Docteur
- [8] **Moussa N.A., Devarakonda V.V.**, 2014
Prediction of Toxic Emissions from Chemical Fire and Explosion, Fire Safety Science - Proceedings of the 11th International Symposium, pp. 1457-1468
- [9] **Pădurean I.**, 2012
Fluid Mechanics and Hydraulic Drives, Eurostampa Publishing House, Timisoara, ISBN 978-606-569-504-7
- [10] **Popescu D., Dinu R.C.**, 2012
Fluid Mechanics and Hydraulic Machines. University of Craiova Publishing House, ISBN: 606-14-0432-2
- [11] **Robertson T., Dunbar J.**, 2005
Guidance for Evaluating Landfill Gas Emissions from Closed or Abandoned Facilities, U.S. Environmental Protection Agency Office of Research and Development, Washington, EPA-600/R-05/123a
- [12] **Chiodini G., Costa A., Rouwet D., Tassi F.**, 2016
Modelling CO₂ Air Dispersion from Gas Driven Lake Eruptions, Geophysical Research Abstracts, Vol. 18, EGU2016-17572, EGU General Assembly 2016.
- [13] **Goodfellow H., Tahti E.**, 2001
Industrial Ventilation Design Guidebook, Academic Press, San Diego, California, USA
- [14] **Dejean G., Iatcheva E. e.a.**, 2011
Pollution de l'air intérieur de l'habitat, L.E.N. MÉDICAL, ISBN : 978-2-914232-67-8, Imprimé en France
- [15] **Kletz T.**, 2001
Learning from Accidents - Third edition - First published as Learning from Accidents in Industry 1988, Reprinted 1990, Second edition 1994, Third edition 2001, British Library Cataloguing in Publication Data, Library of Congress Cataloguing in Publication Data, ISBN 0 7506 4883 X
- [16] **Mannan S.**, 2005
Lees' Loss Prevention in the Process Industries, Imprint Butterworth - Heinemann, ISBN 978-0-7506-7555-0
- [17] **Suess M.J., Craxford S.R.**, 1978
Manuel de gestion de la qualité de l'air des villes, Organisation Mondiale de la Sante, Bureau Régional de l'Europe, Copenhagen, ISBN 92 9020 201 7
- [18] **Voicu V.**, 2002
Fight Against Emissions in Industry, Technical Publishing House, Bucharest
- [19] **x x x**, 2013
Air Contaminants, ASHRAE Handbook Fundamentals
- [20] **x x x**, 2007
Guidance on Evaluation of Development Proposals on Sites where Methane and Carbon Dioxide Are Present, The National House-Building Council - NHBC, RSK Group PLC, Report edition No. 04
- [21] **Cioclea D.**, 2020
Development of Techniques and Methods to Prevent the Formation of Explosive and / or Toxic Atmospheres Specific to Industrial Areas, INSEMEX Petroșani Study - NUCLEU Project
- [22] **Cioclea D.**, 2023
The Superior Valorisation for Energy Purposes of Coal Deposits under the Conditions Imposed by Environmental Strategies, INSEMEX Petroșani Study - NUCLEU Project



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