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Eng. ADRIAN BOGDAN ȘIMON-MARINICĂ

DOCTORAL THESIS

MODELAREA ȘI SIMULAREA FORMĂRII COMBUSTIEI AMESTECURILOR EXPLOZIVE

MODELING AND SIMULATION OF THE COMBUSTION FORMATIONS OF EXPLOSIVE MIXTURES

Scientific coordinator,

Prof.univ.dr.habil.ing. MONICA LEBA

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SUMMARY

ACRONYMS AND NOTATIONS

SR EN 60079-11 – Explosive atmospheres. Part 11: Equipment protection through intrinsic security i
SR EN 60079-2 – Explosive atmospheres. Part 2: Equipment protection by pressurized housing p
L.F.L. – Lower flammability limit
U.F.L. – Upper flammability limit
L.E.L. – Low explosion limit
U.E.L. – Upper explosion limit
L.I.E. – Lower explosion limit
L.S.E. – Upper explosion limit
D.M.E. – Dimethyl ether
F.I.D. – Flame ionization detector
P.I.D. – Photoionization detector
U.V. – Ultraviolet radiation
I.R. – Infrared radiation
I.M.S. – Ion mobility spectrometer
I.L. – Working instructions
M.F.C. – Mass flow controllers
3D – Tridimensional
A.C. – Alternative current
V.C.C. – The voltage connected to the circuit
D.I.P. – Dual in-line package
P.C. – Personal computer
FLIR - Teledyne FLIR LLC, ex FLIR Systems Inc.
G.P.L. – Liquefied petroleum gas
C.F.D. – Computational fluid dynamics
C.A.D. – Computer-aided design
I.N.C.D.INSEMEX – National institute for research and development in mine safety and explosive protection
P.V.C. – Polyvinyl chloride
B.O.S. – Background Oriented Schlieren
P.C.C. – Phantom Camera Control
U.D.F. – User – defined functions
C. – Programming language

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INTRODUCTION

Gas mixing systems are equipment used to mix two or more gases in a controlled manner. These systems comes in a wide range of industries, including chemical processing, semiconductor manufacturing and biotechnology.

One of the common applications of gas mixing systems is in semiconductor manufacturing. In this industry, it is important to obtain a precise and consistent gas mixture to ensure the production of plaque (thin plaques, made of semiconductor material such as silicon, and used as a substrate for the manufacture of integrated circuits and other electronic devices) of high quality. The process of producing them requires a controlled mixture of gases such as hydrogen, argon, nitrogen and methane. The gas mixture used to create a plasma that deposits a thin layer of material on the surface of the plaque.

Another application for gas mixing systems is in the chemical processing industry. In this industry, gas-mixing systems create various gases that generates a specific chemical reaction. For example, in ammonia production, nitrogen and hydrogen gases mixed in a reactor to form ammonia. This reaction is extremely exothermic and requires precise control of the gas mixture to avoid accidents.

In the biotech industry, gas-mixing systems used in fermentation processes to control the environment inside the fermenter. These systems combines gases such as oxygen, carbon dioxide and nitrogen to maintain the optimal environment for the microorganisms used in fermentation.

Gas mixing systems are typically composed of several components, including gas flow meters, regulators, valves, and control systems. Gas flow meters measure the flow of each gas, while regulators comes to control the pressure of each gas. Valves control the flow of each gas and the control system coordinates the operation of other components.

There are several types of gas mixing systems available, including batch systems, continuous systems, and semi-continuous systems.

- Batch systems are types of processing systems in which a fixed quantity of materials or substances processed sequentially in a series of defined steps. In a batch system, the operator add all raw materials required for a process at the beginning, the process is completed, and the final product is obtained before another batch is processed. These systems are frequently used in various industries, including chemical, pharmaceutical, food, and materials processing. Operators use batch systems to mix a fixed amount of gases in a single process. These batch systems offer the advantage of a fixed quantity, whereby a fixed quantity of materials are required in a single production process and flexibility by changing process parameters between batches, and quality control by processing each batch separately.
- Continuous systems are types of processing systems where materials enter a process and transform into finished products through a continuous flow, without stops between batches or cycles. In such a system, operators continuously feed raw materials into the processing equipment, and the final product exits continuously as it passes through each processing stage. These continuous systems mix gases continuously.
- Semi-continuous systems combine the two approaches, where a fixed amount of gas is mixed, but the process repeats multiple times. These semi-continuous systems integrate elements from both batch and continuous systems. In such a system, certain stages of the process operate continuously, while others run intermittently or in batches. This type of system provides the flexibility of batch systems and the efficiency of continuous systems, adapting to the specific needs of the process.

Importance and necessity of the Topic. Objectives and Structure of the Thesis

Thesis Objective

The primary objective of the doctoral research focuses on a completely new methodological approach to the analysis of gas mixing systems, with the aim of developing and implementing a gas mixing system in laboratory activities to support the conduct of controlled physical experiments. The intended outcome involves the formation and use of gas mixtures within the explosiveness limits specific to each type of gas introduced into the gas mixer.

Specific Objectives

Identify the specific constructive elements of gas mixing systems.

Dimension a gas mixing system.

Perform mathematical analysis for controlling the dosage of each type of gas used in the mixer.

Identifying the specific features of the control objectives necessary in the construction of the gas mixer.

Development and experimentation with the gas mixer by supplying known gases and brought to desired concentrations.

Thesis structure

The doctoral thesis begins with an introductory section that outlines the importance, purpose, and objectives of the research. The main body includes five chapters that detail the scientific approach, along with an appendix, making up 150 pages. The work features 103 figures, 26 tables, and a list of bibliographic references cited throughout. The thesis systematically presents the author's research, covering results from the documentation phase, mathematical calculations for optimizing gas mixture dosing, experimentation procedures, data interpretation from measurements, and design aspects. The author constructs the thesis as a cohesive unit based on case studies and concludes with results from using the gas mixer developed by the author in controlled laboratory experiments.

In **Chapter I**, titled **"Current state of research on explosive mixtures"** presents the principles of gas mixture formation and the fundamental laws of gases. The chapter covers the equipment for flow and volume measurements and describes static systems for producing explosive mixtures. It also examines systems for producing gas mixtures at atmospheric pressure. Additionally, the chapter presents volume measurements by highlighting intermediate and secondary standards. This chapter aims to derive, organize, and correlate the important fundamental relationships that exist in both pure gases and mixed gases.

Chapter II, titled **"Theoretical aspects of the characteristics and parameters of explosiveness of air–flammable gas mixtures"** focuses on a study of estimating explosion pressures resulting from the combustion of explosive mixtures. The chapter establishes the mathematical framework needed to determine the airflow required underground, particularly at the work front. Burning rate and explosion intensity depend on several factors, including the composition and concentration of reactants, ignition source, the size and shape of the mixture, and the presence of obstacles or features that induce turbulence in the mixture. Additionally, the presence of oxygen is crucial for combustion to occur, as reactions require oxygen to generate heat, pressure, and gases.

It is important to highlight that running a specialized program resulted in an explosion pressure of 78 mbar for turbulent-free burning. According to details on damage from overpressure explosions, this explosion pressure causes deformation and movement of corrugated metal panels and projects wooden panels of houses outward. In the analyzed case, the maximum explosion pressure produced low-intensity dynamic effects, such as damage to some drywall partitions.

The **Chapter III**, titled **"Laboratory techniques for creating explosive/gaseous mixtures"** begins with an introduction summarizing the law of partial pressures. The main section of the chapter focuses on methods for creating explosive mixtures using laboratory equipment from INCD INSEMEX Petroșani. This includes a gas mixing setup with an initiator, a dosing system with a digital dispenser for preparing mixtures, and a laboratory system for analyzing oxygen in combustible gases.

In **Chapter IV**, titled **"Design and experimentation of an automatic gas mixing system"** the chapter briefly presents the design of a programmable gas mixer. This mixer is necessary for preparing mixtures of flammable gases (explosive or toxic) to obtain mixtures at concentrations within the explosiveness range, between the lower explosive limit and the upper explosive limit for combustible gases, or within pre-established limits for alarm purposes, corresponding to percentages of the lower explosive limit or the lethal dose limit. The system operates with an accuracy of 0.1% volumetric fractions, using the principle of mixing two volumetric flows controlled by a programmable microcontroller. Gases are stored and transported at atmospheric pressure through cylindrical injectors with a capacity of 10 liters, an internal diameter of 10 centimeters, driven by stepper motors, so the gas circuit does not include valves.

At the end of the chapter, the experiment involved testing the automatic system with electric control for preparing flammable gas/air mixtures, using both methane and hydrogen. The tests achieved concentrations ranging from the lower explosive limit to the upper explosive limit, starting from 5% volumetric methane up to 15% volumetric methane.

Chapter V, titled **"Computerized simulations of explosions of explosive mixtures in glass tubes"** focuses on gas explosion events, both in private and domestic settings. The chapter includes a technical analysis of the factors that led to these events. Identifying the causes of the event involves determining the likely source of initiation for the explosive mixture, discovering the source of the combustible gas, and analyzing how the mixture formed. Due to the geometric complexity of the space where the explosion occurred, the incident, reflected, or composite shock waves generated by the explosion can create an event footprint that questions the location of the initiation source. Based on the possible sources found on site, researchers must conduct analyses using finite element and volume methods. The factors considered in the computerized simulations include the geometry of the space, the nature of the combustible gas leak, its dispersion, and the resulting thermal and mechanical effects. The Computerized Simulations Laboratory at INCD INSEMEX Petroșani conducted the analyses and simulations in this chapter.

In **Chapter VI**, titled **"Conclusions, personal contributions, and future research directions"** The discussion highlights the most important results from analyzing theoretical concepts, models, approaches, case studies, and experimental research. The author emphasizes contributions to the doctoral research on two interrelated and interdependent levels: the theoretical level and the practical level, with a focus on how these results apply in practice. The final part of the chapter outlines several future research directions that could enhance understanding and knowledge in the development, programming, and experimentation with gas mixing systems. This chapter synthesizes the conclusions and explicitly states the contributions to the field of research addressed.