Numerical representation of extinguishing gas discharge process

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Abstract. The aim of the work was to provide the analysis of the use of computational fluid dynamics (CFD) for modeling the stage of extinguishing gas discharge to a compartment, which is not taking into account in standard models. The CFD techniques may let to predict gas parameters in dependence of various conditions in a protected area. The investigations were carried out with software ANSYS Fluent 18.2, using Realizable k-ε model and SIMPLE algorithm. The numerical model was validated using experimental data. The subject of the study were standard and newly proposed inert gases. The results showed that adequate selection of input parameter let to simulate the gas discharge stage with high accuracy. The numerical results have a good agreement with the experimental results. The conclusions provide recommendations for the gas discharge prediction based on CFD technique.

1 Introduction

Fire extinguishing using gases is characterized by the least losses related to the extinguishing agent, among all currently known extinguishing agents. For this reason, extinguishing gases are used primarily in places, where stored property is the main value, like server rooms, archives, museums. Extinguishing gases are commonly used in Fixed Gaseous Extinguishing Systems (FGE-systems), operating by total flooding of the protected room [1].

In order to predict the extinguishing gas behavior, designers use models of gas flow through the room described in appropriate standards. The following standard models are currently used:

a) model with a sharp interface between extinguishing gas and air, presented in NFPA 2001 [2];

b) model with wide interface between the gas and air, presented in EN 15004 [3] and ISO 14520-1 [4];

c) model of continuous mixing of extinguishing gas with air, at a constant rate within the volume – valid for areas in which the air is constantly moving [2, 3, 4].

Based on literature study, including analysis of design standards, it was claimed, that known analytical models give only a general view of the extinguishing gas flow process through a protected room. Verification of the applied models indicates discrepancies between the measured and calculated values [5]. The standard models assume significant

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simplifications. One of the most important is omission of the stage of extinguishing gas discharge into the protected space. The extinguishing gas flow process is described from the moment of reaching the design concentration of the extinguishing gas in the room, until the gas leaves the room completely. This stage is related to the maintaining of the retention time of extinguishing gas. The stage of release and distribution of extinguishing gas in the room is not taken into account. The discharge of extinguishing gas is a dynamic process accompanied by supersonic outflow and a process of turbulent mixing of extinguishing gas with air. The standard models do not take into account the temperature drop as a result of the expansion of the extinguishing gas and the phase transition of evaporating liquefied extinguishing gases. After discharge, it is assumed that the temperature inside the protected space is equal to the ambient air temperature [2, 3, 4].

The omission of the extinguishing gas discharge stage limits the accuracy of the description of the gas flow through the room, including the selection of the quantity of extinguishing agent and the influence of automatic relief of over pressures devices on the gas concentration. Limitations of the standard models determine the basis for the validation of extinguishing gas outflow models and attempts to develop them.

Numerical models based on the Computational Fluid Dynamics (CFD) method are increasingly implemented tool in research programs. Using numerical methods, it is possible to gradually limit the scope of simplifications in analytical models and get parameters approximate to the experimental data. One of the most popular computational programs using CFD methods is the ANSYS Fluent Software [6].

The assumption of the research work was to propose a numerical model which take into account the extinguishing gas release phase and examine its impact on the further distribution of gas in the room.

2 Description of gas discharge test

Experimental tests of the release of extinguishing gas into a protected room were carried out in a separate room in the Laboratory of Technical Security Systems in the Main School of Fire Service in Warsaw. The model room was a test chamber with dimensions 5 m x 5 m x 2.8 m. The chamber was equipped in a fixed gaseous extinguishing system for inert gases, a multi-point gas concentration measuring device and a thermocouple grid enabling a multi-point temperature register. To measure gas concentrations, oxygen probes with an electrochemical sensor were used, placed on aluminum measuring poles. First pole was located in the central part of the chamber, while the second pole was placed near the corner of the room. The oxygen concentration and temperature were measured at 5 heights: 28 cm, 84 cm, 140 cm, 196 cm and 253 cm from the floor, what corresponded to 10%, 30%, 50%, 70% and 90% of the height of the protected space.

The extinguishing agent delivery system consisted of four cylinders with extinguishing gas under the pressure of 20 MPa, capacity 50 dm^3, connected to the pipeline supplying extinguishing gas to the protected space, ending with an outlet nozzle. The set of tanks was equipped with a valve that starts after receiving a signal from the control device via an electromagnetic release.

The measurements were carried out continuously and the results were recorded every 2 seconds and archived in a computer.

The subject of the study were two standard inert gases (IG-100, IG-01) [3, 4] and two newly proposed mixtures of nitrogen and argon with densities similar to air (Table 1). Experimental data obtained during tests were used to validate the proposed numerical model.

Table 1. List of extinguishing gases used in the research program [own work].

No.	Gas composition	d_m [kg/m^3] (t= 20°C, p=1013 hPa, φ = 0%)	$\Delta d^{1)} = \lvert d_m - d_0 \rvert$ [kg/m^3] (t= 20°C, p=1013 hPa, φ = 0%)
1.	IG-100 *N_2 100% v/v*	1.1646	0.0388
2.	IG-01 *Ar 100% v/v*	1.6254	0.4221
3.	Ar 8% v/v - N_2 92% v/v	1.2014	0.0019
4.	Ar 7% v/v - N_2 93% v/v	1.1968	0.0065

$\Delta d^{1)}$ – difference between the density of the extinguishing mixture and the air density, under standard conditions [3] [kg/m^3];
d_m – density of the extinguishing mixture (extinguishing gas in the design concentration and air inside the protected space) [kg/m^3];
d_0 – density of air [kg/m^3].

3 Numerical simulation

3.1 CFD model description

Using the ANSYS Fluent 18.2 software, a numerical representation of the test rig was developed and numerical study of the extinguishing gas flow were carried out. All calculations were performed in the domain with geometry identical to the experimental model, and physical properties of fluids were defined as for extinguishing gases used in experiments (Table 2).

The numerical model took into account the difference in ambient conditions outside and inside the test chamber, which determined the density of air and extinguishing gases used in calculations. The model took into account the stage of release of extinguishing gases into the room and the accompanied phenomena, like intense turbulent movement and temperature drop as a result of the expansion of the extinguishing gas.

3.2 Computational domain and meshing

The geometry of the computational domain was modeled as the area of a rectangular test chamber with dimensions 5 m x 5 m x 2.8 m and a volume of 70 m^3 and the space of the finite area surrounding the chamber with dimensions 5.9 m x 5.9 m x 2.8 m. Chamber leaks were modeled as internal surface elements (first one at the bottom, second one at the top of chamber) with a total area of 200 cm^2. Authors made some simplifications in numerical model. The discharge nozzle, was modeled as a prism on the base of a square. The nozzle outlet area was 4 cm^2 and corresponded to the total area of 24 small outlet openings of the real nozzle (Figure 1). The stream of outgoing gas was directed vertically downwards creating a narrow stream with a circular cross-section. The real nozzle discharges a stream in the shape of an umbrella with a spraying angle from 100° to 180°. Despite the simplification of the nozzle structure, after the discharge of the gas in the entire space of the test chamber, a required distribution of the extinguishing agent was achieved. The extinguishing gas was released to the room for 60 s. In numerical studies a gas outflow was assumed with a constant mass outflow, while in experimental studies the flow rate was variable in time.

In order to represent properly the smallest flow structures, simulations had to be made using a sufficiently dense grid. The numerical domain was discretized using a 3D structured volume grid consisting of six-sided elements. The smallest mesh size was set at 5 mm in the area of the nozzle and the room leakage holes. It was the initial size for further mesh growth function. A grid-sensitivity analysis were performed using six different grid resolutions. These grids had three maximum element sizes (0.05 m, 0.10 m, 0.15 m) and different growth rates (1.15x and 1.20x). On the basis of the analysis of the influence of the grid resolution on the results, the growth rate of 1.20x and the maximum mesh element size of 0.15 m were selected. The generated numerical grid consisted of 128 430 elements. For this grid, the calculated concentration distributions were closest to the experimental data and the required calculation time was the shortest (Figure 1).

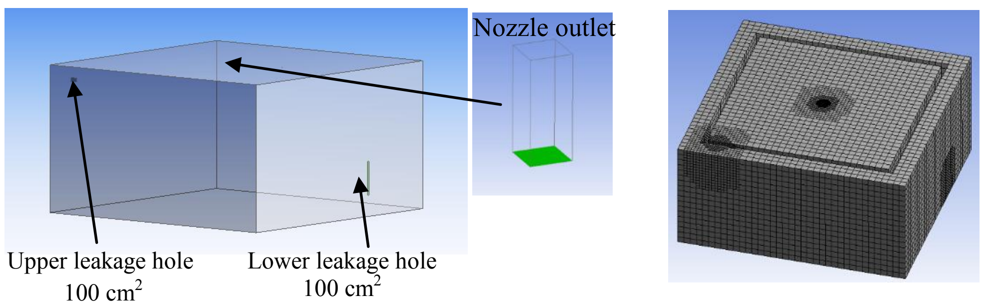

Fig. 1. Numerical model of the test chamber with the arrangement of leakage holes and the simplified numerical model of a nozzle (left) and numerical mesh (right) [own work].

3.3 Boundary conditions and solving setup

On the surface of the walls of the test chamber and the lower (floor) and upper (ceiling) area of the computational domain, wall boundary conditions were established. The walls have assumed the default condition of liquid adherence to the wall (condition without slip). For stationary walls, the speed on the wall was zero. Vertical walls were given a temperature gradient, the upper and lower walls were insulated. A mass flow inlet boundary condition was set on the surface representing the nozzle outlet. The outflow of extinguishing gas into the computational domain lasted 60 seconds. The variability of mass flow rate and pressure at the discharge nozzle during the gas outflow was set using the user-defined functions (UDF). On surfaces limiting the computational domain, a pressure outlet boundary condition was adopted to present a typical outflow into the open space.

The simulations of gas extinguishing gas flow through the room were carried out in the ANSYS Fluent 18.2 program, which is based on the finite volume method. Due to the supersonic flow of the compressible gas, the Density-Based solver was selected. The implicit formulations for the Density-Based solver has been chosen, which is stable and allows faster convergence of the solution [6].

The choice of the turbulence model was based on literature study [7, 8]. Considering the balance between computational time and accuracy, the Realizable k-ε model was used for the simulations. The assumed turbulence intensity was 5%. Mixing and transport of chemical substances were modeled using Species transport model.

Convergence criteria in subsequent time steps were: continuity equation - 10^{-3}, energy equation - 10^{-6}, gas transport equation - 10^{-3}, kinetic energy equation k - 10^{-3}, dissolution rate of kinetic energy dissipation ε - 10^{-3}.

Table 2. Initial and boundary conditions adopted in the numerical model [own work].

No.	Gas concentration	$\Delta d = d_m - d_0$ [kg/m^3] (t= 20°C, p=1013 hPa, φ = 0%)	Mass flow rate [kg/s]	T_{inside} [K]	$T_{outside}$ [K]	gradient T [K]	p [hPa]	Φ [%]
1.	IG-100 *N_2 100% v/v*	-0.0387	0.78	292.15	292.15	0.7	1008	57
2.	IG-01 *Ar 100% v/v*	0.4221	1.12	294.95	295.05	0.5	1015	60
3.	Ar 8% v/v - N_2 92% v/v	-0.0019	0.80	292.55	292.55	0.5	999	65.6
4.	Ar 7% v/v - N_2 93% v/v	-0.0065	0.81	293.15	293.15	0.6	1008	67.7

4 Results and discussion

Numerical tests were initiated at the moment corresponding to the start of the extinguishing agent release to the test chamber.

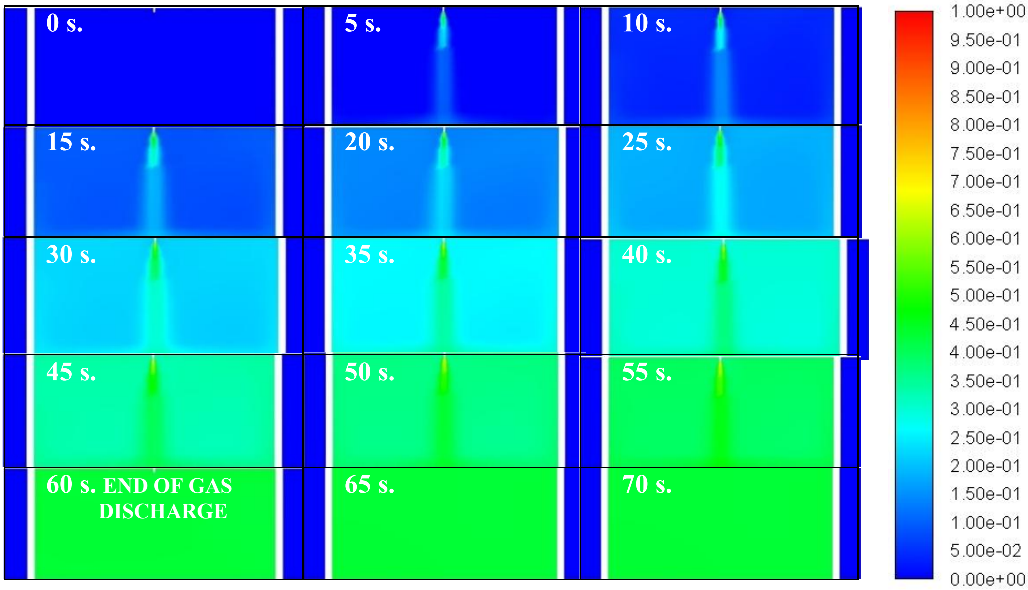

Fig. 2. Distribution of extinguishing gas concentrations in the test chamber at the discharge stage, gas mixture Ar 8% v/v - N_2 92% v/v [own work].

During the outflow, the speed of gas molecules increased violently. After exceeding a certain speed limit, the flow became turbulent and the stream was broken down into a series of vortices. After end of the outflow in the entire volume of the test chamber uniform distribution of the extinguishing agent was obtained (Figure 2).

The numerical tests confirmed the view about the complexity of the process of extinguishing gas discharge into the room. The discharged stream of gas caused the effect of "sucking" the mass of air and directed it vertically downwards. The maximum gas velocity near the nozzle outlet was about 377 m/s. This fact allows to classify the discussed outflow as a supersonic. The vertical stream of gas was moving at a speed of 90 m/s, and in the rest of the chamber the mass of gases moved at a speed of up to 10 m/s. After the finish of discharge, the turbulences were still visible in the room, changing their range and direction.

The numerical values of gas concentrations well reflected the actual change in concentrations in the room after discharge. In some cases the numerical model allowed to obtain values very close to the experimental data (Table 3).

Table. 3. Summary of the concentrations obtained after the extinguishing gas discharge.

No.	Gas composition	Gas design concentration [%]	Gas concentration reached after discharge (experimental study) [%]	Gas concentration reached after discharge (numerical study) [%]
1.	IG-100 *N_2 100% v/v*	43.8	46	45
2.	IG-01 *Ar 100% v/v*	43.8	46.5	47.6
3.	Ar 8% v/v - N_2 92% v/v	44.9	45	45.5
4.	Ar 7% v/v - N_2 93% v/v	44	46	43.8

The modeled maximum values of gas concentrations deviated from the actual values by an average of 2%. The standard model underestimated the predicted value of maximum concentration achieved after discharge of extinguishing gas into the room by about 5%.

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The discharge of the extinguishing agent leads to the adiabatic expansion of extinguishing gas, stored under high pressure in the cylinder. The results of measurements indicated that the periodic temperature drop in the chamber was about 4 K (Fig. 4). The temperature decreased up to 290 K. After the discharge, locally lower temperature slowly increased and equalized with the ambient temperature as a result of heat exchange between gases and test chamber elements. The resulting temperature inside the chamber was 291.98 K (Figure 3).

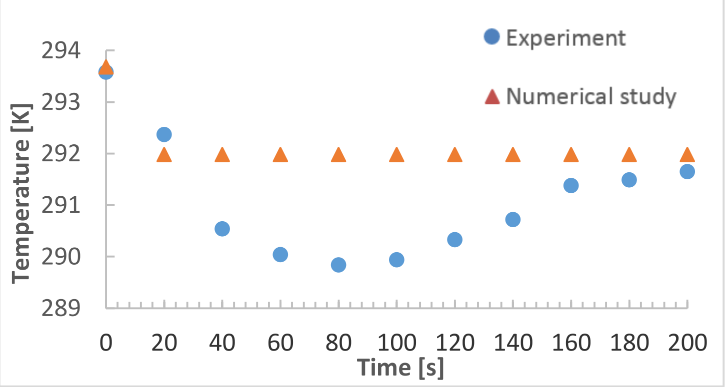

Fig. 3. Comparison of calculation results with measurements - temperature variation at 0.9 H in the central part of the chamber, gas mixture Ar 7% v/v - N_2 93% v/v [own work].

Numerical solution interpreted the general course of temperature changes in the room in a simplified way. Small discrepancies appeared between 20. s and 160. s of flow. The result temperature in the chamber was about 292 K. The gas outflow decreased the room temperature by 2 K. The temperature difference about 2 K affects the variability of the width of the density range about 0.008 kg/m^3. This density variation can cause significant changes in retention times values, especially for gases with density close to air.

4.1 Comparison between simulation and observation

As a result of numerical simulations, the course of flow processes of extinguishing mixtures through the test chamber was examined in order to compare the obtained results with the results of experimental tests and calculations using the standard model.

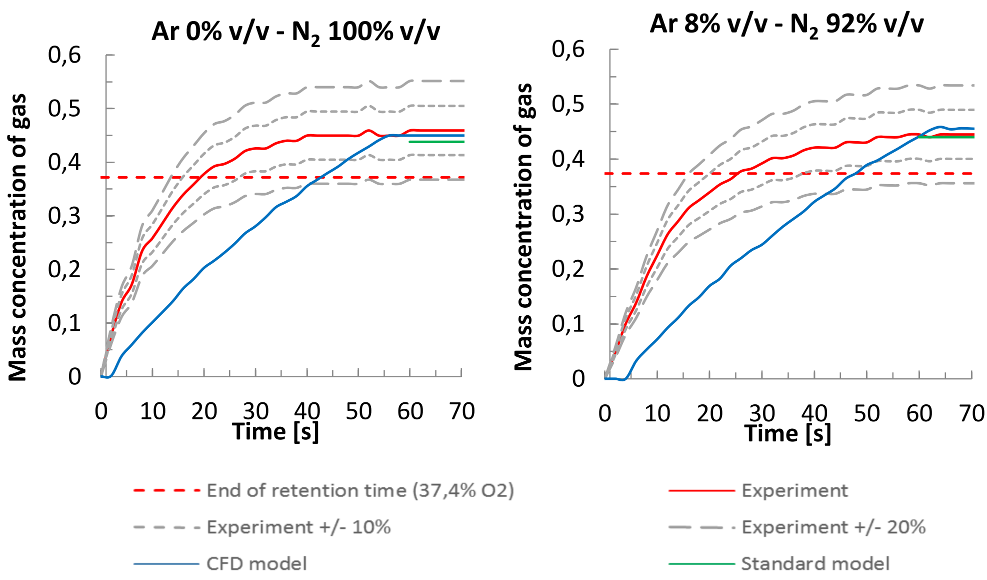

Fig. 4. Distribution of extinguishing gas concentration at 90% of chamber height, gas mixture Ar 0% v/v - N_2 100% v/v, Ar 8% v/v - N_2 92% v/v [own work].

Analyzing the graphs it can be stated, that numerical model predicted gas discharge stage with good accuracy. The process of discharge and the obtained values of gas concentration were close to real values. In some cases the results were better than values obtained using standard model, which not take into account the discharge stage at all.

5 Conclusions and future work

The numerical CFD method is a useful engineering tool that can support the study of fixed gaseous extinguishing system.

The analysis of velocity fields, gas concentrations and temperature authorizes the statement that the numerical method provided good convergence with experimental results.

The stage of extinguishing gas discharge is very important. It affects not only the formation of vortex structures responsible for mixing of extinguishing gas with air during direct outflow. It also affects the further disposition of gas in the room.

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