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Modeling of hazards in room with AB-rechargeable batteries

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Abstract. *In current work a numerical modeling of hazards in room with AB-rechargeable batteries is presented. The numerical modeling is done once with the integral method as well as via computer simulation with commercial software package Fluent. A comparison between the obtained numerical results is made and appropriate conclusions for the contaminants in the room are formulated.*

Key words: *numerical simulation, computer simulation, CFD, integral method, pollutants*

1. Introduction

Air contaminants indoors can be classified as primary or secondary ones. The main pollutants are substances directly emitted into the atmosphere from the source. The main primary pollutants that are known to cause damage in concentrations that are high enough are as follows:

- Carbon compounds such as CO, CO_2, CH_4, and Volatile Organic Compounds (VOCs);
- Nitrogenous compounds such as NO, N_2O and NH_3;
- Sulphur compounds such as H_2S and SO_2;
- Halogen compounds such as chlorides, fluorides and bromides;
- Particulate matter (PM) (PV or "aerosols"), or in solid or liquid form, which usually are classified into these groups based on the aerodynamic particle diameter.

Sulphur compounds are responsible for the traditional winter smog of sulphur. These anthropogenic contaminants sometimes can reach lethal concentrations in the atmosphere, as for example during the infamous case in London in December 1952.

Secondary pollutants are not emitted directly from the source; rather they are formed in the atmosphere from primary pollutants (known as "precursors"). The main secondary pollutants that cause damage in high enough concentrations are as follows:

- NO_2 and HNO_3 who are formed by NO;

- Ozone (O_3), formed by photochemical reactions of nitrogen oxides and VOCs;
- Sulphur acid droplets formed by SO_2 and drops of nitric acid formed by NO_2;
- Sulphate and nitrate aerosols (e.g., ammonium sulphate and ammonium nitrate) formed from reactions of drops of sulfuric acid and nitric acid respectively with droplets of NH_3;
- Organic aerosols formed by VOCs.

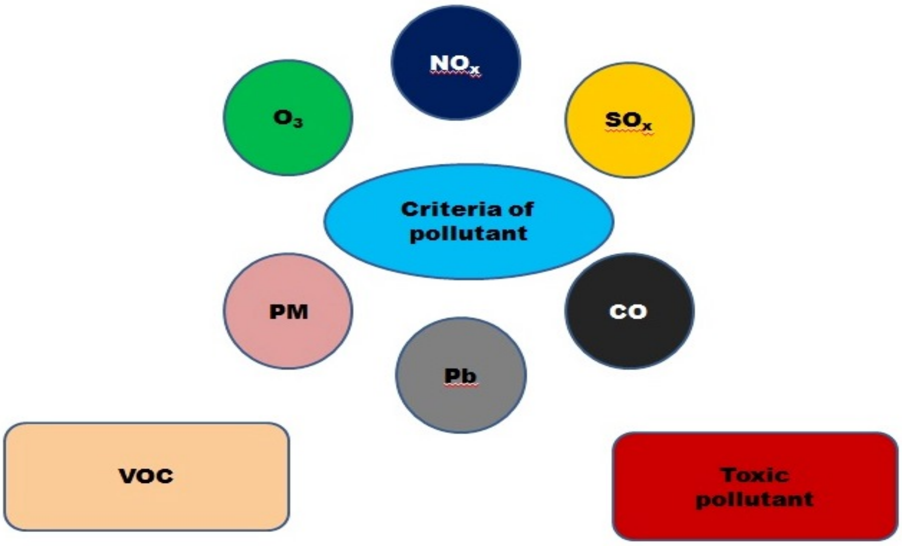

Fig.1 –Pollutants criteria

2. Mathematical model of the flow based on Lagrangian method

Discharge of pollutants (dust, liquid "drops", aerosols, etc.) in the working environment can be approximated to a vertical non-isothermal two-phase flow. Due to the temperature difference between the vertical jet and the ambient temperature an Archimedes force will occur. Of course, it is possible the forced vertical flow of contaminants to flow at a temperature close to that of the medium. However, for general solution non-isothermal nature of the flow will be considered.

The non-isothermal nature of vertically transmitted flow requires knowledge of buoyancy (Archimedes) force which is calculated by the expression:

$$dF_A = -\left[\int(\rho-\rho_{ok})\,g\,df\right]dx \qquad (1)$$

The system of equations of motion of the two phases is as follows:

$$\frac{\partial}{\partial x}\left[y^j U_g \rho_g\right] + \frac{\partial}{\partial y}\left[y^j V_g \rho_g\right] = 0 \qquad (2)$$

$$\frac{\partial}{\partial x}\left[y^j U_p \rho_p\right] + \frac{\partial}{\partial y}\left[y^j V_p \rho_p\right] = 0 \qquad (3)$$

$$\left[y^j U_p\right]\frac{\partial \chi}{\partial x}+\left[y^j V_p\right]\frac{\partial \chi}{\partial y}=-\frac{\partial}{\partial y}\left[y^j \chi V^{'}\right]-\overline{\chi V_p^{'}} \qquad (4)$$

$$\left[y^j \rho_g U_g\right]\frac{\partial U_g}{\partial x}+\left[y^j \rho_g V_g\right]\frac{\partial U_g}{\partial y}=-\frac{\partial}{\partial y}\left[y^j \rho_g \overline{U_g^{'} V_g^{'}}\right]-F_x y^j-\left(\rho_2-\rho_g\right)\pi g y^{2j} \qquad (5)$$

$$\left[y^j \rho_p U_p\right]\frac{\partial U_p}{\partial x}+\left[y^j\left(\rho_p V_p+\overline{\rho_p^{'} V_p^{'}}\right)\right]\frac{\partial U_p}{\partial y}=-\frac{\partial}{\partial y}\left[y^j \rho_p \overline{U_p^{'} V_p^{'}}\right]+F_x y^j \qquad (6)$$

$$\left[y^j \rho_g U_g\right]\frac{\partial h_g}{\partial x}+\left[y^j \rho_g V_g\right]\frac{\partial h_g}{\partial y}=-\frac{\partial}{\partial y}\left[y^j \rho_g \overline{h_g^{'} V_g^{'}}\right]-$$
$$-\left[y^j \rho_g \overline{h_g^{'} V_g^{'}}\right]\frac{\partial U_g}{\partial y}-Q y^j+F_x y^j\left(U_g-U_p\right)+F_y y^j\left(V_g-V_p\right)-\sum_{i=1}^{3}\overline{F_i^{'} V_{pi}^{'}} \qquad (7)$$

$$\left[y^j \rho_p U_p\right]\frac{\partial h_p}{\partial x}+\left[y^j\left(\rho_p V_p+\overline{\rho_p^{'} V_p^{'}}\right)\right]\frac{\partial h_p}{\partial y}=-\frac{\partial}{\partial y}\left[y^j \rho_p \overline{h_p V_p^{'}}\right]+Q y^j \quad (8)$$

$$p=\chi R T_g \qquad (9)$$

In two-phase vertical non-isothermal jets forces of interfacial interactions are decisive in their solution with implementation of the two-fluid circuit - without considering them it is not possible to create mathematical models of two-phase turbulent flow. Determining the impact of the forces of interfacial interaction on the development of the two-phase flow is a necessary element in the creation of numerical models.

The motion of a single particle impurity described by the method of Lagrange leads to an equation of the following type:

$$\sum_{i=1}^{N}\overrightarrow{f_i}=\overrightarrow{f_A}+\overrightarrow{f_S}+\overrightarrow{f_T}+\overrightarrow{f_G}+\overrightarrow{f_{TM}}$$

Then the implemented revisions and laying described in [7] lead to the following equation of the seventh order of the speed of the gas phase:

$$A\overline{U_{gm}^{*}}^{7}+B\overline{U_{gm}^{*}}^{6}+C\overline{U_{gm}^{*}}^{5}+D\overline{U_{gm}^{*}}^{4}+E\overline{U_{gm}^{*}}^{3}+F\overline{U_{gm}^{*}}^{2}+G\overline{U_{gm}^{*}}+H=0 \qquad (10)$$

The equation is solved by the method of Newton-Rapshan successively and defines the basic parameters of the flow.

$$\overline{U_{pm}}=L_{11}+L_{12}\overline{\rho_{gm}}\,\overline{U_{gm}^{*}}^{2}+L_{13}\overline{\rho_{gm}}\,\overline{U_{gm}^{*}}+L_{14}\overline{\rho_{gm}}+L_{15} \qquad (11)$$

$$\overline{T_{pm}}=e^{\frac{\left(\bar{x}-\bar{x}_0\right)}{L_{106}}}\left(\overline{T_{p01}}+L_{97}\right) \quad (12)$$

$$\overline{T_{gm}}=L_{94}+L_{95}\overline{T_{pm}} \qquad (13)$$

$$\overline{R_u} = L_4 + L_3 F_x \left(\frac{\overline{U_{pm}} - \overline{U_{gm}}}{\overline{U_{pm}^2}} \right) \quad (14)$$

$$\overline{R_p} = \frac{R_u}{Sc_t} \quad (15)$$

$$\overline{R_T} = \frac{R_u}{\Pr_t} \quad (16)$$

In this section is given the mathematical model of the flow and its solution using intregral method.

3. Numerical analysis of vertical non-isothermal jet flow modeled in a confined space.

In this section numerical analysis of vertical non-isothermal stream is presented and the modeling phase of the flow in a confined space in particular. Here the initial conditions, the velocity, the temperature and the boundary thicknesses within the boundary layer are listed.

The numerical study is conducted under the following initial conditions: $U_{g0} = U_{p0} = 3m/s$; $T_{g0} = T_{p0} = 303K$; $D_p = 10\mu m$; $y_0 = 0{,}5m$

On Fig. 2 the distribution of the velocity of the gas phase and the phase of impurities are shown. The graph demonstrates that the velocity along the height of the room almost does not change and the jet reaches the batteries which are situated on the floor as fast as desired.

Fig. 3 shows the temperature distribution of the gas phase and the phase of the impurities along the height of the room. It can be seen that the change in temperature is not significant.

Fig. 4 illustrates the distribution of the three boundary thicknesses of the boundary layer- respectively for impurities Rp, temperature Rt and velocity Ru. The graph concludes that the temperature thickness is greatest, followed by the velocity and impurities' one is the smallest $R_t > R_u > R_p$. Due to $R_t > R_u$ presence of diffusion of heat from the stream to the external environment is observed. Considering that Rp is the smallest value, diffusion of impurities out of the jet is not expected. This is a very significant technology result in the evacuation of impurities from the working environment.

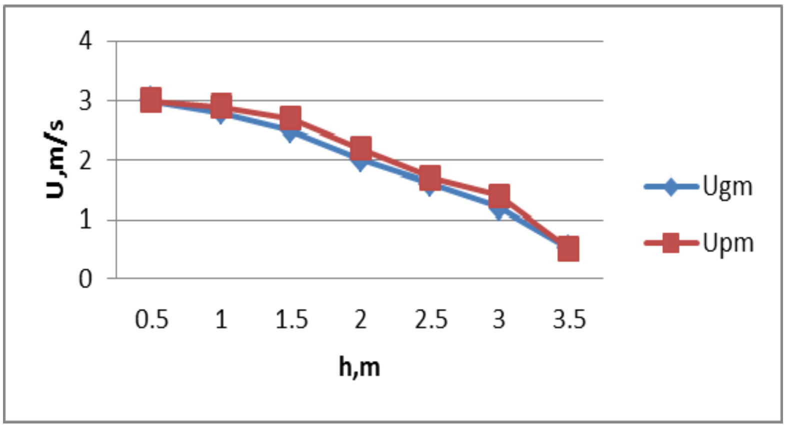

Fig. 2– Distribution of velocity of gas phase and phase of impurity

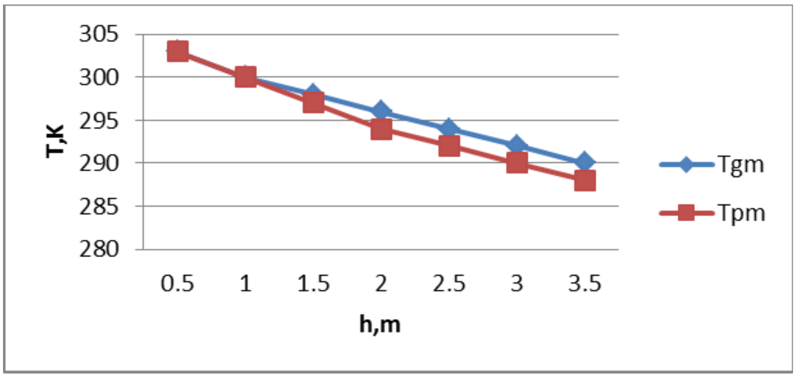

Fig.3– Distribution of temperature for gas phase and phase of impurity

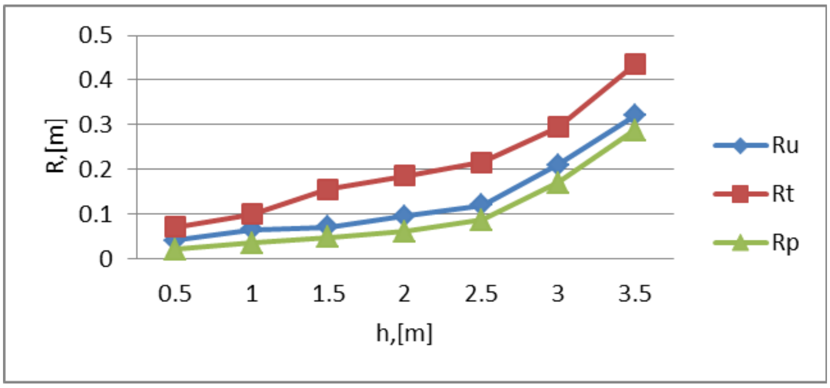

Fig.4. – Distribution of boundary layer thicknesses Ru, Rt and Rp

In section three is given the numerical results for velocity and temperature for both phase. Also is shown the distribution for three boundary layer thicknesses Ru, Rt and Rp.

4. Computer simulation of a room with AB- rechargeable batteries

The same scenario of a ventilated room with AB-rechargeable batteries is modeled and simulated by commercial software package Fluent.

The geometry of the room with AB-rechargeable batteries is shown on Fig. 5.

The aim of the computer simulation is to show the distribution of the temperature and velocity field in order to make a comparison between the data obtained by Fluent and results for the velocity and temperature obtained by the Integral method.

For the numerical simulation a relatively simple geometry of the room considered is built, using Fluent's pre-processing panel Gambit. It consists of a rectangular room with AB-rechargeable batteries ordered in rows and situated on the floor. The numerical grid is generated with Gambit's meshing tools and consists of four control volumes. At this stage the boundary conditions are defined as well.

For the 3D computer simulation a pressure based solver is used. The turbulent model chosen for the simulation is based on the Reynolds averaged Navier-Stokes equations. Standard k-ε turbulent model is selected. Appropriate boundary conditions are defined.

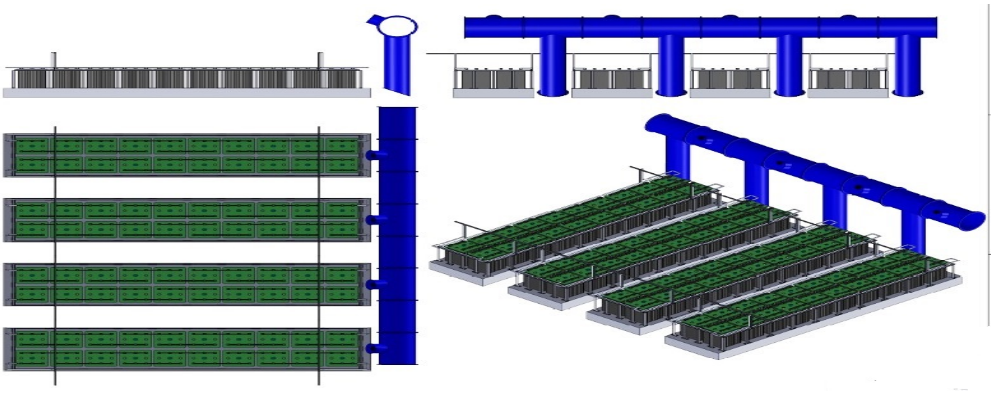

Fig.5 Geometry of the ventilated room with AB-rechargeable batteries

The visualization of the results of the numerical solution is made in the software FLUENT. In it is defined the parameters of the boundary conditions and turbulent models are selected. On the following figures are presented visualizations of the velocity and the temperature fields respectively.

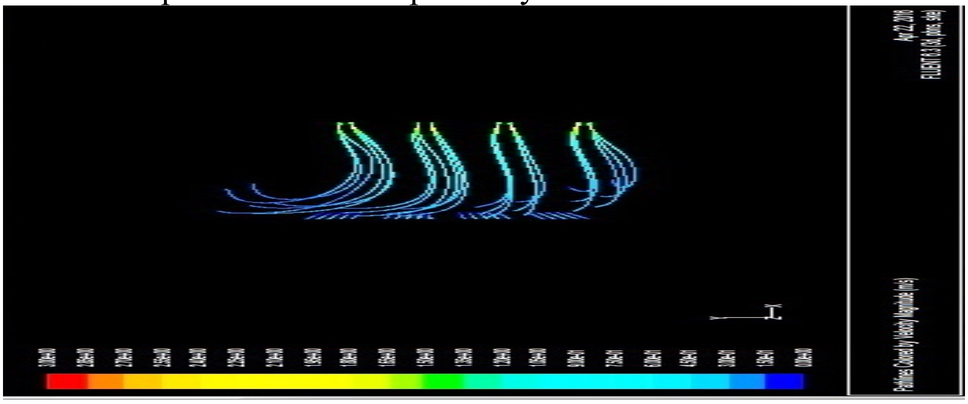

Fig.6 – Visualization of velocity of fluid flows

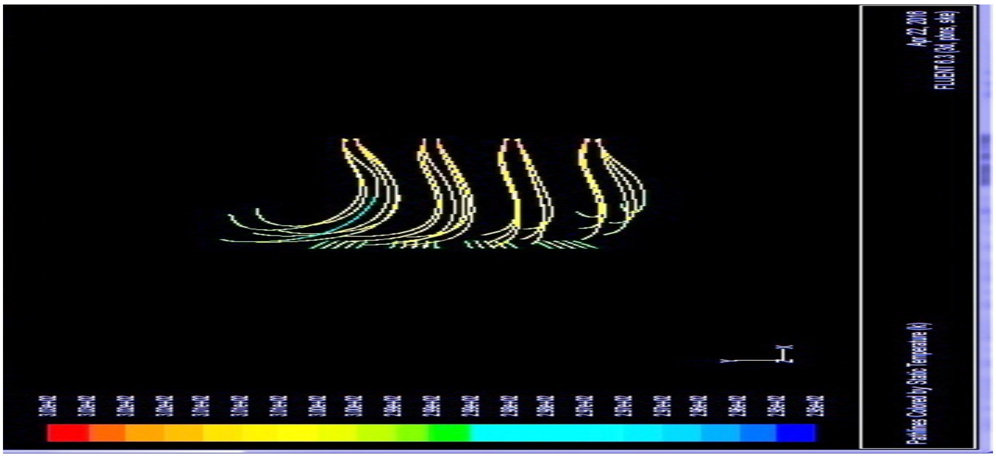

Fig.7 - Visualization of temperature of fluid flows

Fig.8 – Visualization of velocity vectors in the room

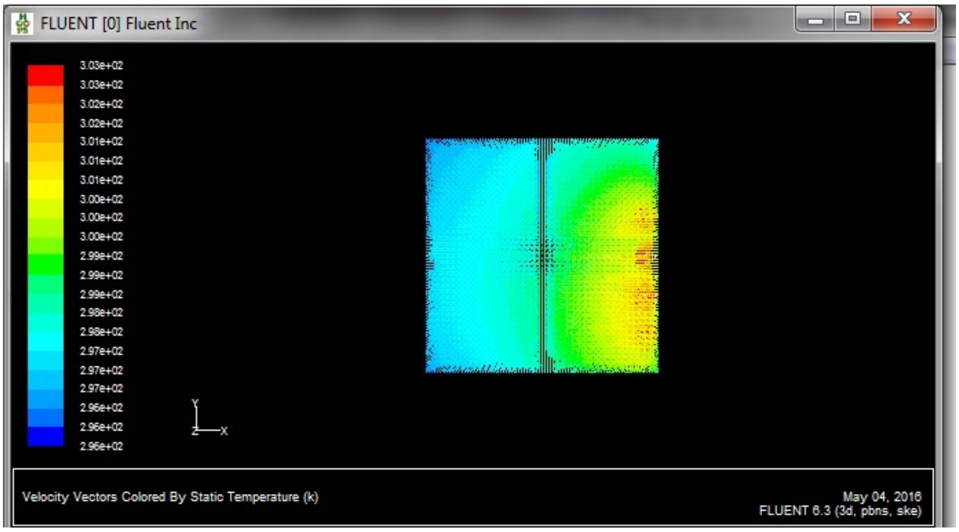

Fig.9 - Visualization of temperature vectors in the room

On fig. 6-7 are given the visualization of the velocity and temperature of the flow. On fig. 8-9 are given the visualization of velocity and temperature vectors in the room. The boundary conditions are the same use in Section 3.

5. Conclusion:

This paper discusses the numerical modeling of hazards in room with AB-rechargeable batteries. First is presented the mathematical model of the vertical non-isothermal two-phase flow and the complexity of the obtaining of solution for this two-phase turbulent flow. Second the numerical analysis of vertical non-isothermal stream modeling the flow in a confined space is given. Based on the previously presented analytical solution are shown. This paper finishes with a comparison analysis between the numerical solution (based on analytical model) and numerical simulation with Fluent software.

Based on the numerical simulations and the obtained numerical results it is shown that values of the speed and the temperature in both cases are close. This gives us reason to conclude that the resulting distribution model is correct and can be used to calculate the parameters of hazards in a room that can be of great benefit in practice.

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