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NUMERICAL SIMULATION OF HEAVY AND LIGHT POLLUTANTS MOTION AS A TOOL OF EXPERIMENTAL DATA VERIFICATION

Computational Fluid Dynamics (CFD) codes including software ANSYS Fluent represent worldwide accomplished group of tools for fluid mechanics phenomena numerical simulations. These codes are based on numerical solution of partial differential equations that are not to be solved analytically. The only way of numerical data verification is to execute comparison with experimental data respecting the same boundary conditions. This article deals with experimental data verification by using CFD code ANSYS Fluent 12.1.4 as a tool for numerical simulations. Comparison of pollutant's plume and its scattering considering different density of each pollutant is the main point of the problem. Results are presented by means of commented graphs and pictures.

Key words: Aerodynamic Tunnel, Computational Fluid Dynamics (CFD), Physical Experiment, Numerical Model, Pollutant

1. Introduction

Toxic gas leak industrial accidents in the past proved how dangerous these accidents could be for living environment and inhabitance. That is why it is advisable to prevent these accidents before they happen. When designing and optimizing preventive measures, it has been very helpful to utilize some tools of mathematical (numerical) modelling. Numerical modelling enables the investigator to predict a possible way of running the accident and its impact on the surrounding area. Research on physical and chemical properties of the gaseous chemical substance, whose presence is assumed at the accident, is also one of the main points of preventive measures creation process.

For this purpose, low scale physical models including simple or complex terrain and source of pollutant inserted could be used for investigation of gas pollutant motion and scattering phenomena depending on defined physical properties. For example, it is possible to observe and then even formulate general principles of different pollutant motion and scattering in real atmospheric boundary layer that way.

Physical experiment results could finally be used for verification of numerical models, CFD codes for example. In case of equivalence between experimental data and numerical data which is up to investigator's mind and demands, numerical model is considered to be verified successfully and can be used for the next progress and investigation of the issue only by way of numerical simulation. Of course, the simulations could cover a low scale experiment as well as the real scale experiment. Final results obtained by this kind of analysis could be very helpful in the process of designing industrial building's safety and security systems, searching for the ideal location of gas detectors or choosing and securing the most sufficient ways for evacuation. One of many possible comparative issues is the main point of the following lines.

2. Physical Experiment in Aerodynamic Tunnel

In 2008 physical experiment of light and heavy pollutant's motion and scattering in a low speed aerodynamic tunnel was executed. Flow field was vertically stratified as simulating the real air velocity profile out in the atmospheric boundary layer. Low speed aerodynamic tunnel belongs to the Aerodynamic laboratory of Academy of Science of the Czech Republic (nearby Prague, the capital city of the Czech Republic). Main objectives of the experiment were:

1. *Proving* the functionality of a gauging system when detecting chosen gas pollutants;
2. *Detection* of pollutant plume position and range measuring concentration in points;
3. *Optimization* of pollutant concentration measuring method in points of a space.

The experiment was executed in the gauge section of the low speed aerodynamic tunnel (see *Fig. 1*). Gauge section has the following dimensions: 2 [m] (length), 1.5 [m] (width) and 1.5 [m] (height). The space of gauge section represents simple flat terrain with a chimney placed right in the middle of the floor, i.e. in the distance of 1 [m] from the gauge section threshold and 0.75 [m] from both sidewalls (*Fig. 3*). Chimney (small nozzle) serves as a source of the air-pollutant mixture. The nozzle has cylindrical shape with following dimensions: 20 [mm] (height), 6 [mm] (outside diameter) and 3.5 [mm] (inside diameter, i.e. diameter of

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Fig. 1 Gauge section of the aerodynamic tunnel

Fig. 2 Inlet part of the aerodynamic tunnel with turbulent elements

Fig. 3 Pollutant source on the floor and measuring probe

the leak). The air-pollutant gas mixture was generated in simple "System for pollutant generation" that was placed out of the tunnel.

"System for pollutant generation" consists of air pump with constant set flow rate and glass flow chamber where permeation tubes with liquid pollutant were placed inside [2]. Pollutant permeates through the walls of permeation tubes in gaseous state, mixes with flowing air and is drifted through the hose to the nozzle placed in the tunnel gauge section floor. The source of pollutant is defined to be constant (concentration of pollutant in mixture is constant for a few hours until the permeation tube is empty).

There was generated vertically stratified logarithmical profile of a horizontal air flow velocity. The reference value of air flow velocity was 1.5 [m/s]. This profile was measured experimentally using LDA (Laser Doppler Anemometry) method [4]. The flow field in the tunnel is not stratified thermally. Turbulence, generated by turbulent construction elements on the tunnel's floor of the inlet section, simulates real atmospheric conditions (*Fig. 2*). Temperature in the tunnel was about 17 [°C] (the air for gauge section was sucked from outdoors), temperature of the air in laboratory was 22 [°C] ("System for pollutant generation" took the air from indoors), the air pressure was 98 200 [Pa] and air relative humidity was 50 [%]. Values of concentration in points were determined by taking the sample of the air from the gauge section and its analysis by CO_2 laser photoacoustic spectrometry system (Edinburgh Instruments, type WL 8 – GT) [5]. Photoacoustic signal (values of voltage) is detected and transformed into the values of mass fraction (concentration) based on the calibration curve for certain pollutant.

This physical experiment resulted in three series of concentration data measured in several points of space in the aerodynamic tunnel gauge section. The following gas pollutants were measured: Methanol CH_3OH ($\rho = 1.43$ [kg/m^3]); 1,1,2,2-Tetrachlorethylene CCl_2CCl_2 ($\rho = 7.01$ [kg/m^3]); Acetone CH_3COCH_3 ($\rho = 2.46$ [kg/m^3]).

3. CFD Numerical Simulation

Advanced software ANSYS Fluent 12.1.4 belongs to the most widespread CFD codes all over the world [1],[3]. In this case, it was used for the numerical simulation of heavy and light pollutant motion and scattering. The code is based on numerical solution of partial differential equations set by the finite volumes numerical method. Equations represent physical law of weight conservation, law of momentum conservation and law of energy conservation. Software includes wide range of sub-models that enable the investigator to solve wide range of issues considering various differing boundary conditions.

Geometry shape, grid and types of boundary conditions were defined using the software Gambit 2.2.30. Geometry grid consists of 443 850 cells. Cells are smoothed vertically to the floor of the gauge section and horizontally to the pollutant source (nozzle). "RNG k-ε model" of turbulence was chosen for basic stratified flow field calculation and "Species transport model" was used for transport of species calculation. Gauge section inlet boundary condition was defined as "Velocity Inlet", gauge section outlet as "Outflow", floor of the gauge section as "Wall" and sidewalls together with ceiling were marked as "Symmetry". Pressure was set on the value of 98 200 [Pa] and temperature on the value of 300 [K] (16.85 [°C]). Also air flow velocity profile, intensity of turbulence profile, turbulent kinetic energy profile and dissipation rate profile were defined on the gauge section inlet (see equations 1–4):

$$v = 0.2371 \cdot \ln(Y + 0.0001) + 1.3571 \quad (1)$$

$$I = -0.0673 \cdot \ln(Y + 0.0001) + 0.1405 \quad (2)$$

$$k = 1.5 \cdot (v \cdot I)^2 \quad (3)$$

$$\varepsilon = \frac{1.225 \cdot 0.09 \cdot k^3}{1.4}. \quad (4)$$

In these equations, v [m/s] is the air flow horizontal longitudinal velocity (in direction of X-coordinate), I [%] is the intensity of turbulence, k [m^2/s^2] is the turbulent kinetic energy, ε [m^2/s^3] is the dissipation rate and Y [m] is the vertical length coordinate (axis orthogonal to the plane of the tunnel floor).The leak surface of the pollutant source was defined as "Velocity Inlet". The velocity of the flow through the leak surface was set on about 1 [m/s]. Pollutant source leak velocity has always been a bit different for different pollutants because every pollutant permeates differently through permeation tube (the velocity of permeation, i.e. the pollutant amount leaked per time is different). This issue was solved as steady (time-independent). Calculation accuracy (criterion of convergence) was set on the value 0.0001. Results are presented in figure (*Fig. 4*) and in comparative graphs, where final concentration values at points are displayed.

4. Numerical Data Verification

In *Fig. 5*, *Fig. 6* and *Fig. 7*, XY-coordinates of measured points are displayed. All of them were measured in single vertical longitudinal plane, in which the source of pollutant (nozzle) is located. In *Fig. 8*, *Fig. 9* and *Fig. 10*, comparative graphs of concentration values in points obtained by physical experiment, as well as by numerical model, are displayed. Serial number of each measured point was established with respect to the consecutive order of measurement.

Comparative graphs show similarity between the results of physical experiment and numerical model. The maximum difference between both data sets is one order. The greatest variance can be observed at points that are located close to the pollutant source.

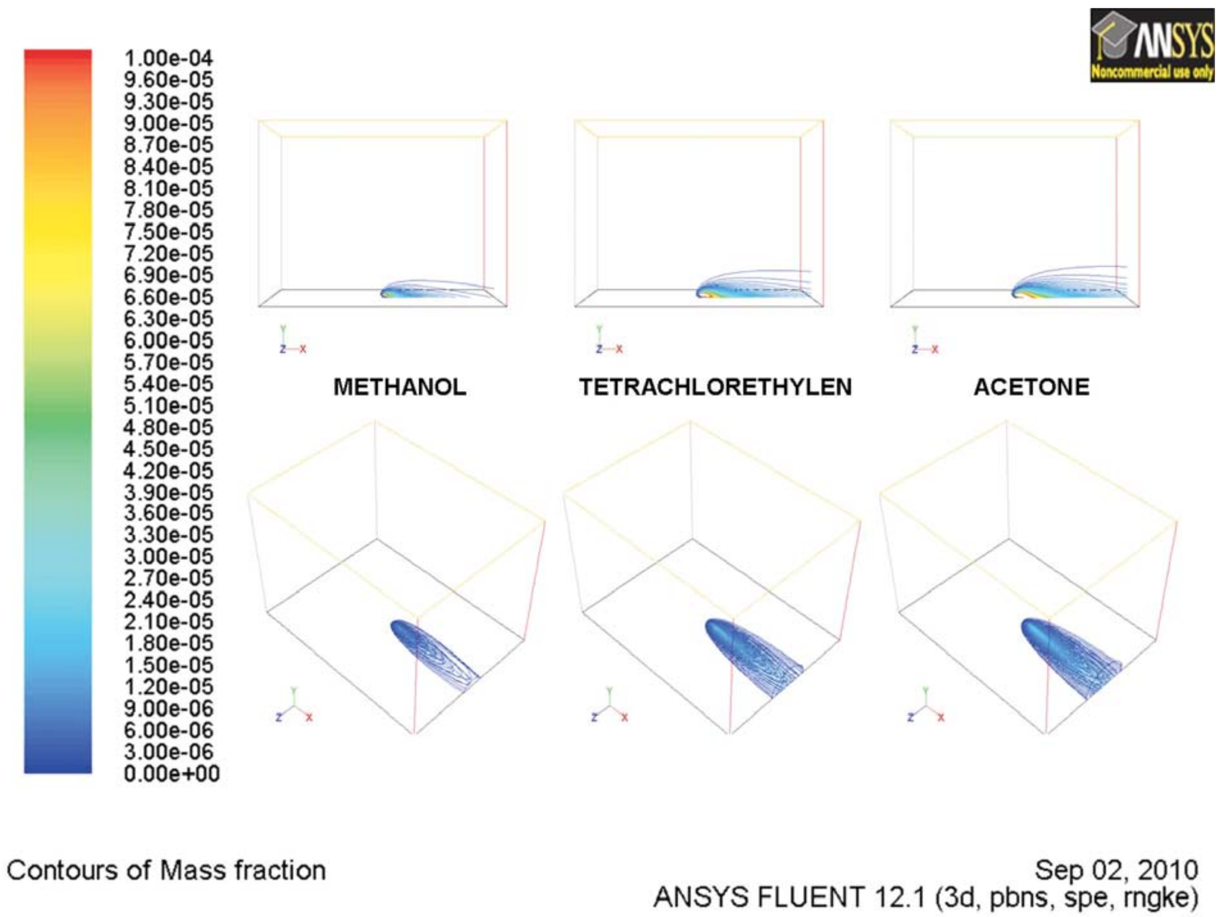

Fig. 4 Contours of mass fraction of Methanol CH3OH, 1,1,2,2-Tetrachlorethylen CCl_2CCl_2 and Acetone CH3COCH$_3$ (ANSYS Fluent 12.1)

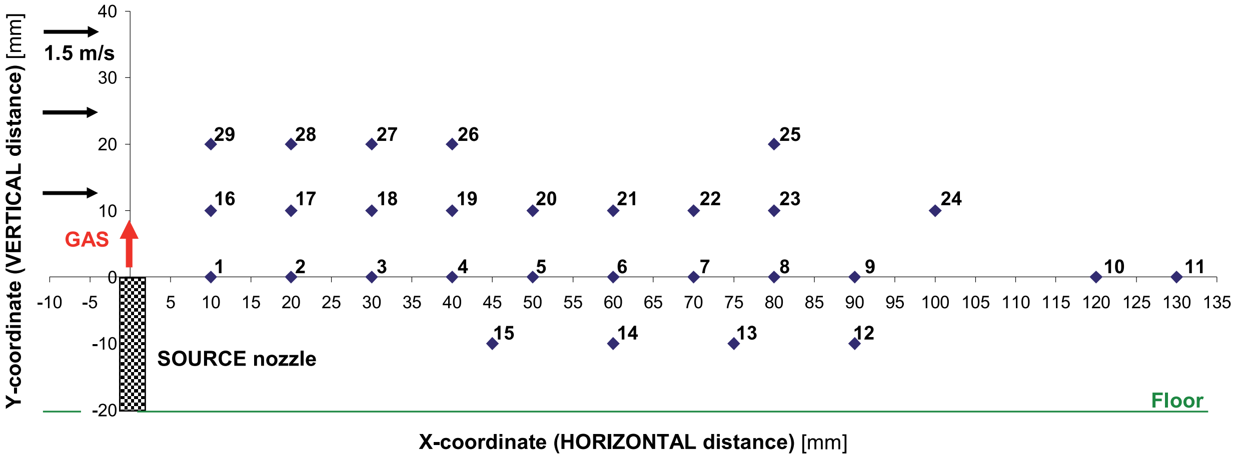

Fig. 5 Methanol CH_3OH (X, Y-coordinates of measured points)

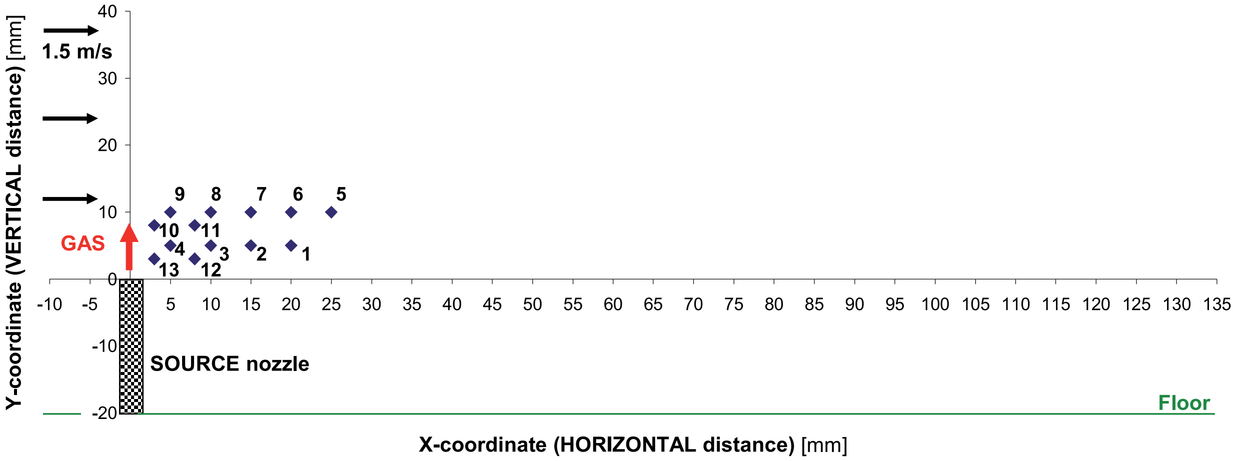

Fig. 6 1,1,2,2-Tetrachlorethylen CCl_2CCl_2 (X, Y-coordinates of measured points)

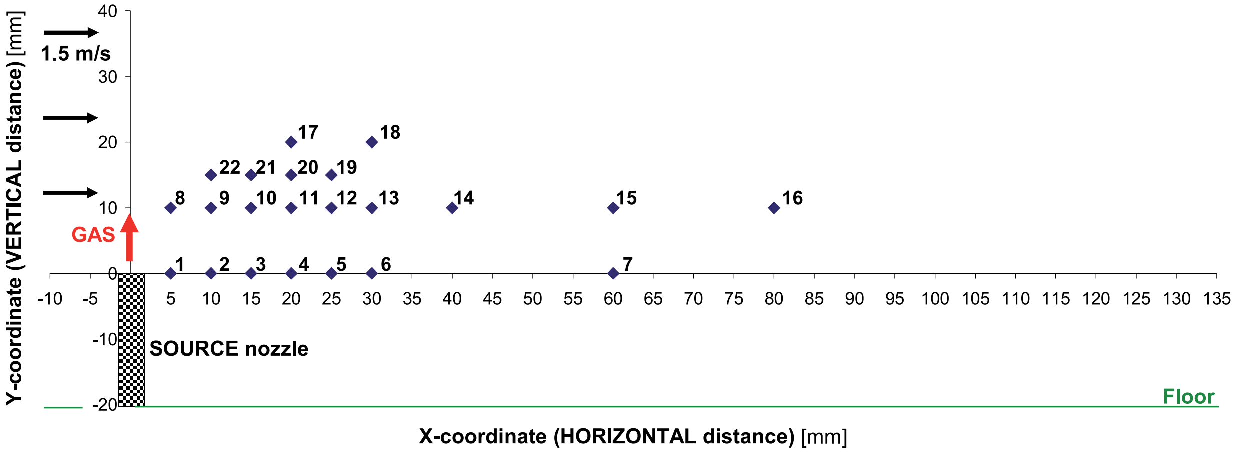

Fig. 7 Acetone CH_3COCH_3 (X, Y-coordinates of measured points)

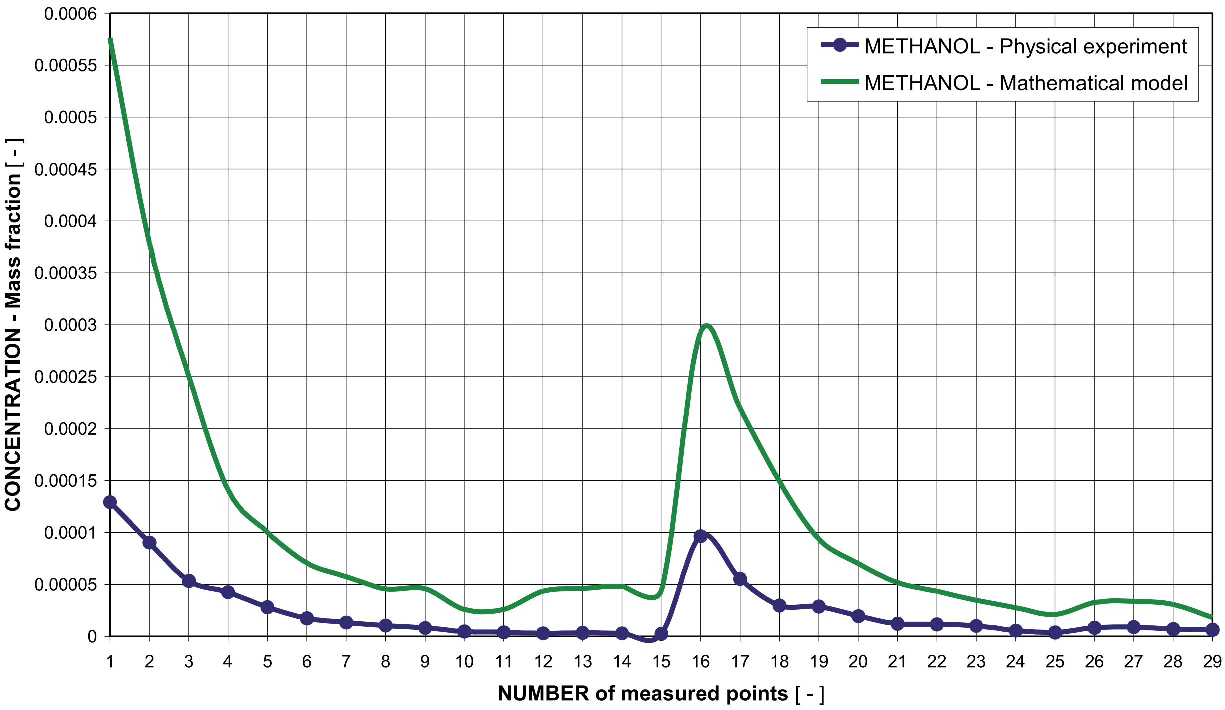

Fig. 8 Methanol CH3OH (comparative graph of physical experiment and numerical model results)

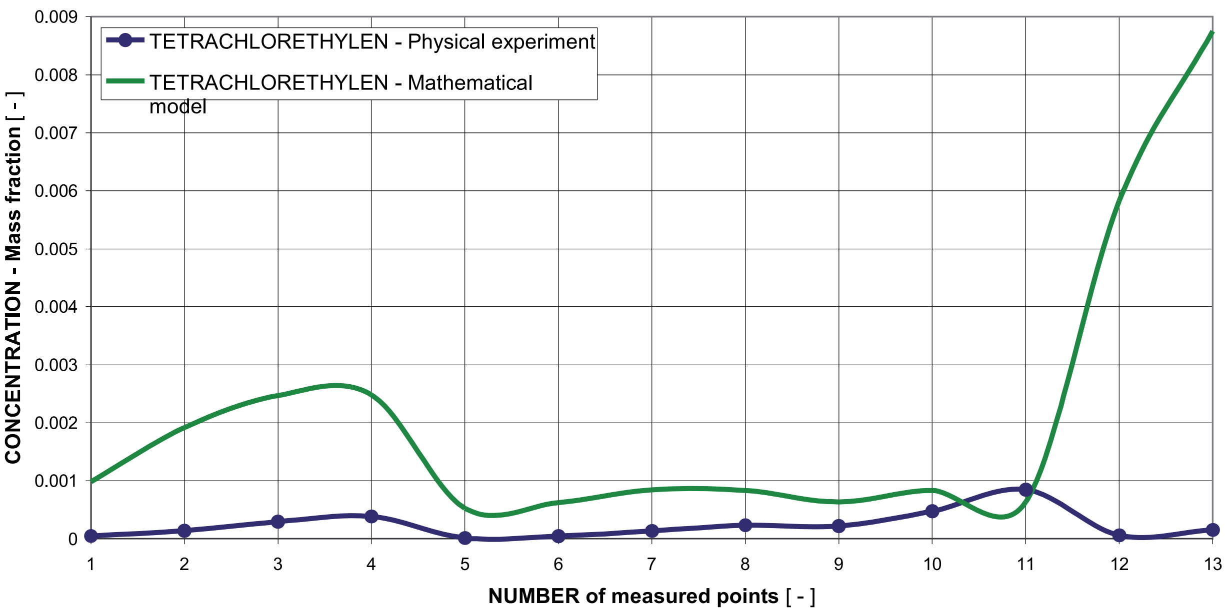

Fig. 9 1,1,2,2-Tetrachlorethylen CCl_2CCl_2 (comparative graph of physical experiment and numerical model results)

In case of Methanol CH_3OH, the greatest variance is visible at points No. 1 – 3 (Fig. 5 and Fig. 8). Air-pollutant mixture plume was probably slightly elevated due to the turbulence behind the source nozzle. At all other points, the variance is minimal. It is still impossible to model the turbulence accurately as it works in the real atmosphere. There has always been some degree of inaccuracy following from the physical experiment as well as from the mathematical model.

In case of 1,1,2,2-Tetrachlorethylene CCl_2CCl_2, both result data sets are very similar. The only exception is represented by the points No. 12 and 13 (*Fig. 6* and *Fig. 9*). Concentration in these

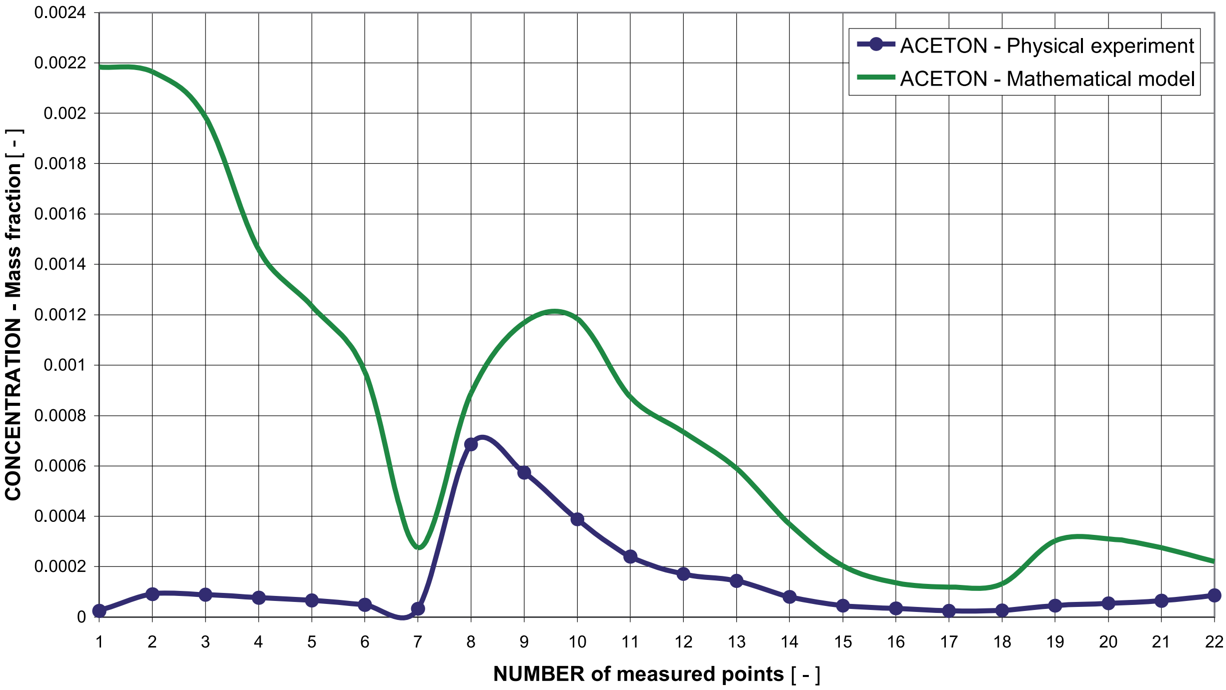

Fig. 10 Acetone CH_3COCH_3 (comparative graph of physical experiment and numerical model results)

two points was measured by the end of the experiment and it can be clearly seen that the permeation tubes (source of pollutant in "System for pollutant generation") were almost empty. That is why the final amount of pollutant was strongly reduced. This fact can be considered to be a methodical mistake during the execution of physical experiment.

In case of Acetone CH_3COCH_3, both result data sets are very similar again except points No. 1 – 6 (*Fig. 7* and *Fig. 10*). Air-pollutant mixture plume was probably again slightly elevated due to the turbulence behind the source nozzle, and declined back after passing greater distance behind the nozzle. At all other points, the variance is minimal.

5. Conclusion

It was proved by physical experiment and numerical simulation that velocity of permeation differs depending on the kind of pollutant. Assuming the constant amount of air in the mixture given by air pump, the amount of pollutant permeated through the walls of permeation tubes is always different depending on the kind of pollutant. This fact is confirmed by pollutant plumes of different sizes and areal ranges (*Fig. 4*). For the reason of pollutant amount variance in every kind of mixture, it is hardly possible to draw comparisons of motion and scattering between heavy and light pollutants based on their density. Heavy pollutant plume (the value of pollutant density is higher than that of air density at constant temperature and pressure) should descent to the ground. Light pollutant plume (the value of pollutant density is lower or approximately equal to that of air density at constant temperature and pressure) should climb. In this case it is impossible to observe any pollutant plume descent or climb. For example, it could be caused by small value of pollutant concentration in the mixture, as well as by the high air velocity in the tunnel gauge section.

Results of physical experiment could be used with success for the verification of numerical model that has been included in software ANSYS Fluent 12.1.4. Based on executed verification, there is an opportunity to work up an analysis leading to physical experiment optimization using CFD tools.

According to both modeling approaches result (see section 4), it can be deduced that numerical model verification by means of physical experiment data was successful, and this kind of numerical model can definitely be used for mathematical modelling of similar issues, considering even more difficult geometry, different pollutant source location and different boundary conditions.

In the future this work can be developed by further similar comparative studies and studies of turbulence, pollutant's motion and scattering theories in real atmosphere, leading to better and more complex understanding of these phenomena.

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