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APPLICATION OF COMPUTATIONAL FLUID DYNAMICS IN THE ASSESSMENT OF THE SPREAD OF TOXIC COMPOUNDS EMITTED BY A DIESEL ENGINE INSIDE A VEHICLE

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1. INTRODUCTION

Diesel engines exhaust gases contain volatile substances detrimental to user's health in their composition. In particular, BTX group consisting of aromatic hydrocarbons such as benzene, toluene and xylene can be included in these compounds. These substances enter into the environment of human life, due to their physical-chemical properties (volatility at temperature of human existence), easily enter into the body through the respiratory tracts [1].

During the operation of diesel-engine vehicle especially specific threat to the health of its users are the exhaust gases that enter into the interior, both emitted by a diesel unit, as well as by other road users. This is particularly dangerous in the case of professional drivers (trucks, working machines) [2].

This study covers the assessment of driver's exposure on the contact with hydrocarbons emitted by the diesel engine, which enter into the interior of vehicle through a ventilation system, using the methods of computational fluid dynamics.

The atmosphere of environment inside a vehicle cabin is characterized by relatively high sensitivity to external and internal flow- thermal conditions. Chemical composition of this specific micro - atmosphere is a complex mixture of gas substances deriving both from internal and external sources, with dynamically changing participation, closely associated with the method and conditions of vehicle usage and also equipment morphology of the cabin itself [3].

Dynamics of changes in air-supply and temperature inside the cabin, therefore, will determine chemical composition of the air in its interior, in particular the qualitative-quantitative composition and spatial distribution of low-boiling and volatile organic combinations.

Spatial distribution is particularly important when we take into consideration ways of toxins absorption into the body.

Analysis of changes in the thermal and flow conditions is thus an important factor in the assessment of the importance of vehicle's air quality, particularly in terms of exposure to human health, cannot be ignored. Volatile organic compounds enter into the human body mainly through respiratory tracts. Such factors as physical-chemical properties and exposure time have influence on the assessment of toxic influence on the heath of vehicles' users. Distribution of these substances in the vehicle's interior and in particular their concentration at the height of user's head is of great importance. The methods of computer aided engineering basing on fundamental principles of fluid dynamics (CFD - Computational Fluid Dynamics) are modeling tool for flow modelling of liquids and gases. They allow for modeling of laminar and turbulent flows mainly using RANS method (Reynolds Average Navier - Stokes). Currently used computational programs have the ability to choose a particular turbulence model for accurate modeling of flow phenomena. Modelling programs additionally enable calculations of heat flow, the flow of discrete phase (impurities) stationary and non-stationary. Thanks to computer-assisted engineering work, it is possible in the virtual environment, in a relatively short period of time, to simulate the movement of a number of variants with altered geometry boundary conditions. It also enables optimization of geometry, depending on the selected flow parameter.

2. METHODOLOGY

For computational exemplary simulations of concentrations distribution of volatile organic compounds, in the interior cabins of vehicles, ANSYS-FLUENT software was used.

Computational fluid dynamics methods are often used by researchers in air flow and VOCs modelling in the interior cabins of vehicles [2]. Their use, however, have been limited so far to assess the effectiveness of ventilation systems, evaluation of thermal comfort, efficiency in car windows evaporation and heating the interior from direct sunlight.

According to the adopted proprietary methodology assessing the quality of the internal environment of the vehicle cabin, CFD methods were used to model the spread of volatile organic compounds inside the cabins in various types of vehicles. Tests and analyses were multi-directionally performed to evaluate[2-5]: performance of toxic substances in the interior of vehicle cabin's micro - atmosphere, methods of air distribution inside a vehicle cabin, and the distribution of concentrations of volatile organic compounds, the impact of cabin's geometry on the distribution of VOCs in its interior, the impact of cabin's geometry changes on the distribution of carcinogens in its interior.

The following vehicles were chosen to be tested, which are representatives of different categories of vehicles (including jobs positions): working machine - excavator Doosan DX 190W, tractor - DAF XF 150, passenger car segment B - Fiat Punto.

Geometric models of selected vehicles were prepared in the Catia. Then, on so prepared geometrical models computational grid was applied. The grid was basing on tetra type elements, was compacted in air inlets and outlets contaminated with VOC.

RANS method of double-equitation of turbulence k-ε model was used for calculation. At the inlets there was a velocity vector corresponding to ventilator capacity used in the ventilation system. The vector was decomposed into 3 components in order to achieve the objective angle of inlet air to the cabin in relation to the dashboard. At its outlet a boundary condition of free effluent to the atmosphere was used. At the inlet there was VOC injection in form of discrete phase. Two most common compounds toluene and benzene were adopted for modelling. The value of given concentration resulted from measurements. The calculations were carried out to obtain the convergence of results at the level of 10^{-4} for each monitored parameter.

3. RESULTS AND DISCUSSION

Representative of lorries is a truck tractor DAF 105 XF. In the car, the driver who spends at work according to the provisions about 9 - 10 hours driving. After finishing work on the road the driver who also sleeps in it, nourishes and rests. Therefore micro – atmosphere in such a vehicle is very important for the driver.

In the DAF type car there is possibility to divide the air flow onto: legs, central supply and windscreen. A series of calculations with different combinations of air flow at the same flow rates of the central fan were conducted (Fig. 1).

Conducted numerical simulations show that the highest concentrations of BTX compounds of the group are at the level of driver's head when the central air flow was used (Fig. 1b). Similarly high concentration of hazardous substances in the vicinity of the driver's head is when air flow is on windscreen and central (Fig. 1d) and central flow and legs. (Fig. 1e)

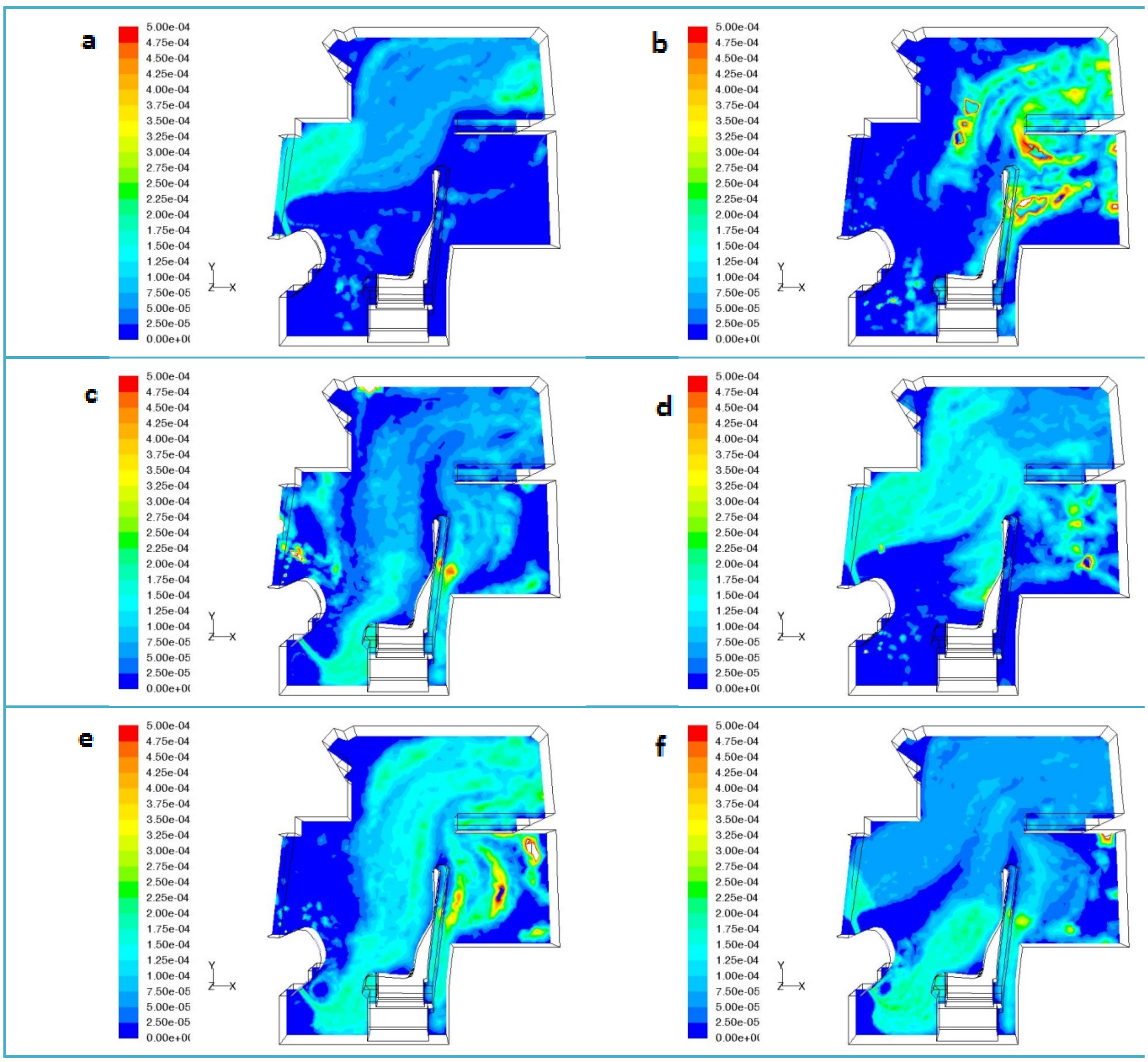


Fig. 1. An example of simulation of benzene, toluene, xylene distribution (BTX) (kg / m3) in the truck DAF FX 105 cabin in the section of driver's position (xy plane) air-supply: a) air-supply on windscreen b) central air-supply c) air-supply on legs d) air-supply on a windscreen and central e) central air-supply and legs f) air-supply on windscreen, central and legs.

According to the CFD results, which aim was to indicate the location in the vehicle cabin places in which there is the highest VOC concentration that is the greatest health risk to vehicle's users, in order to take samples for chromatographic investigations it is necessary to set to central air-supply and collect gas at the driver's head position.

Numerical analysis of CFD showed that air-supply settings are very important in terms of driver's exposure on carcinogens in its interior. It is possible to set the air-supply in such a way so as to allow the driver to work in comfortable working conditions (supply rate and temperature) and to be minimally exposed to VOCs. Numerical modeling shows the location of maximum and minimum concentrations of carcinogens in the whole vehicle's cabin.

Hundreds of samples from the whole vehicle's cabin should be collected in order to obtain similar results in experimental studies . The CFD results can accurately and precisely determine the maximum concentration at particular air-supply settings to collect the maximum concentration of carcinogens.

In order to analyze the effect of vehicle's geometry on the distribution of toxic concentrations of substances in the interior, numerical simulations of air flow inside the original and modified vehicle's cabin were performed. Geometrical model of passenger car's cabin class B was performed and then by modifying the geometry of the interior the impact of these changes on the distribution of dangerous substances was tested (Fig. 2).

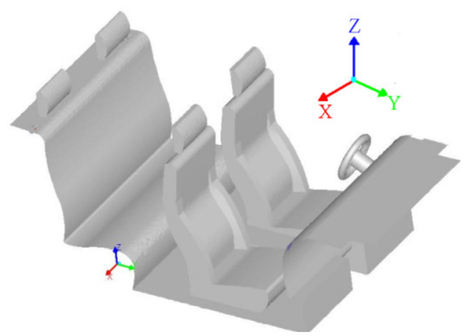


Fig. 2. Geometrical model of cabin's interior of B-segment vehicle

Modifications of the interior were performed by increasing in each of the three models, whole interior dimension of 10% for the individual axes. Apart from the base model, model longer by 10%, wider by 10% and 10% greater were also performed (Table. 1). The calculations take into account selected VOCs carcinogens (benzene and toluene).

Table 1. Description of vehicle's interior modifications.

Symbol	**Geometry variant**	**Diameter**		
		Width	Length	Hight
B	Base geometry	X	Y	Z
E1	Changed geometry (extended): wariant 1	X + 10%	Y	Z
E2	Changed geometry (extended): wariant 2	X	Y + 10%	Z
E3	Changed geometry (extended): wariant 3	X	Y	Z + 10%

Calculations were carried out by setting the air flow in side ventilators (Fig. 2).

The results of numerical simulations have shown that there is an effect of the interior's dimensions changes on distribution of volatile substances with carcinogenic nature (Fig. 3).

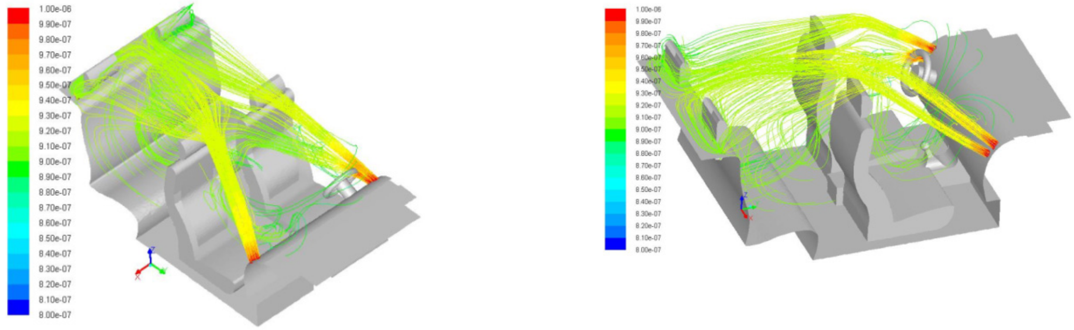


Fig. 3. Flow rate, m^3 / s (central supply) The boundary conditions for the calculation are shown in Table 2.

Table 2. Boundary conditions for CFD calculations

Compound concentration, kg/m^3	
Benzene (and isomers)	$1,58*10^{-6}$
Toluene (and isomers)	$3,14*10^{-6}$
Ventilation settings	
Flow rate, m^3/s	$4,2*10^{-4}$ m^3/s
Model setting of the ventilation system	Side air-supply

In order to analyze the driver's exposure to toxic substances (as the most exposed vehicle's user of due to exposure time) in the analysis the distribution of concentrations in driver's position cross-section was the most important factor to focus on (Fig. 4).

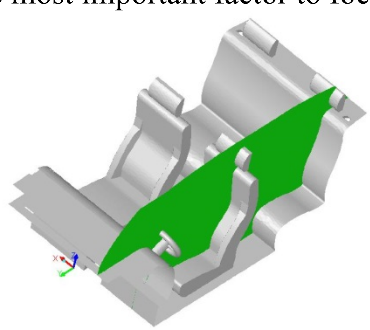
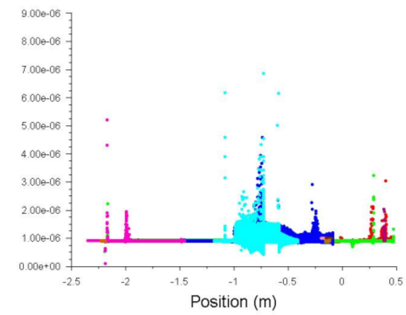
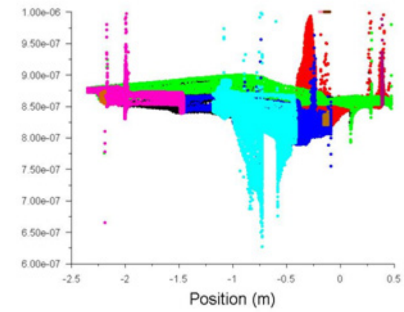
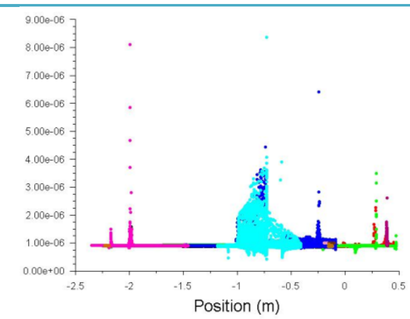
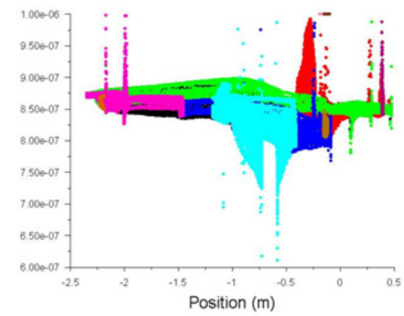
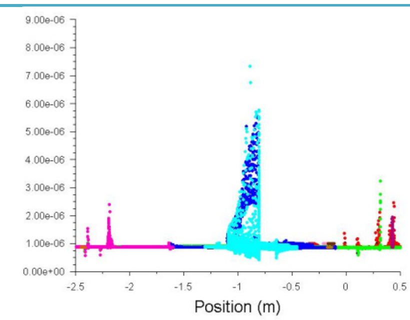
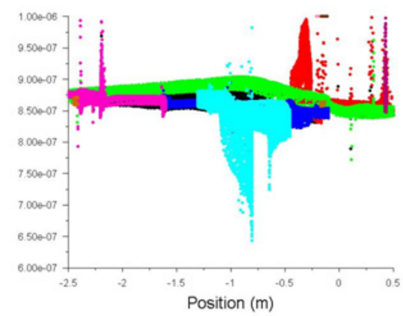
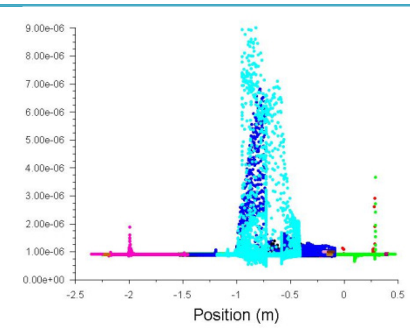
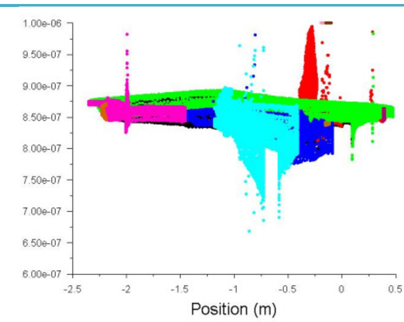
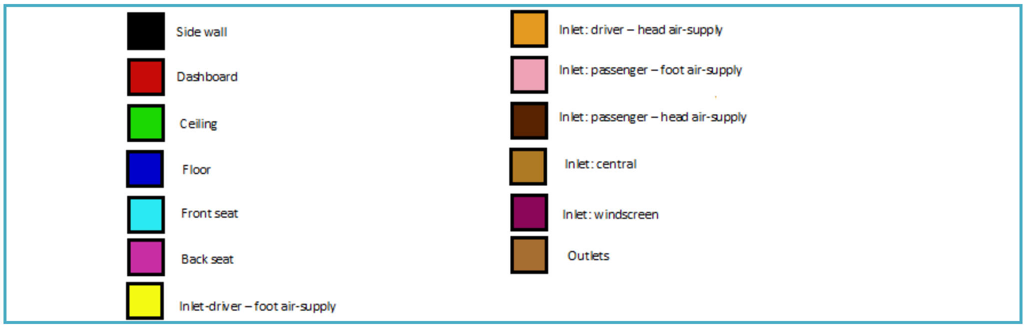


Fig. 4. The cross-section in driver's plane

The test results of simulation of particle distribution of benzene and toluene in the interior of the vehicle tested at baseline and after changes of geometry are summarized and shown in Table 3.

Table 3. Results of the numerical analysis of particle distribution of selected aromatic compounds in the vehicle's interior before and after the changes in geometry

Volume fraction	
Benzene	Toluene
B	
	
E1	
	
E2	
	
E3	
	



According to the model results it can be seen that even a relatively small change in geometry of the vehicle's interior changes the distribution of carcinogens in the cabin of the car, which is best exemplified by benzene (Table 3). The highest concentration of benzene in the driver's seat occurs when the geometry of the E3 variant (10% elongation of the vehicle's cabin). Base variant seems to be the most advantageous if we take benzene concentration distribution into consideration. Analyzing toluene distribution the most favorable seems to be variant E2 (10% length elongation). Analyzing concentrations graphs, it is visible that change in geometry affects the distribution of VOCs concentrations inside the vehicle's cab. The calculations assume a small change in the geometry. Tests were carried out on proportionally increased geometry in all three directions. Not analyzed Changes in the geometry of the shape of individual components as seats, dashboard, windows; curves, air-supply distribution, position of a steering wheel etc. were not analyzed. It is necessary to carry out a series of calculations which take into account the release of VOCs directly from cabin's equipment elements.

Doosan dx 190w wheel excavator was chosen as a representative of heavy machine. Similarly to DAF and Fiat Punto a 3D model of wheel excavator was prepared (Fig. 5).

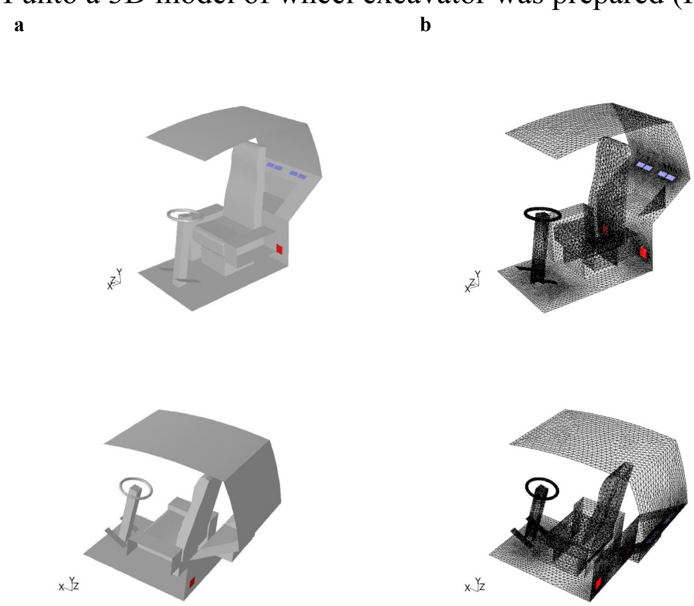


Fig. 5. The geometry of working machine's cabins in Doosan dx 190w

Similarly to the previous calculations the purpose of the study was to identify maps of concentrations of selected toxic volatile aromatic hydrocarbons: benzene, toluene and xylene (BTX) inside the cab, in working conditions of that machine.

BTX concentrations were measured in the air supply to the cabin and the flow rate of air flowing through the ventilation system was measured.

As boundary conditions for calculation, the results of actual measurements were taken into account: total concentration of VAH (volatile aromatic hydrocarbons) at 223.4 μg/m^3 and flow rate settings of the air supplied from the outside on measured average level of: 75 m^3/h and maximum of: 150 m^3/h. The results of numerical analyzes are shown in Figure 6.

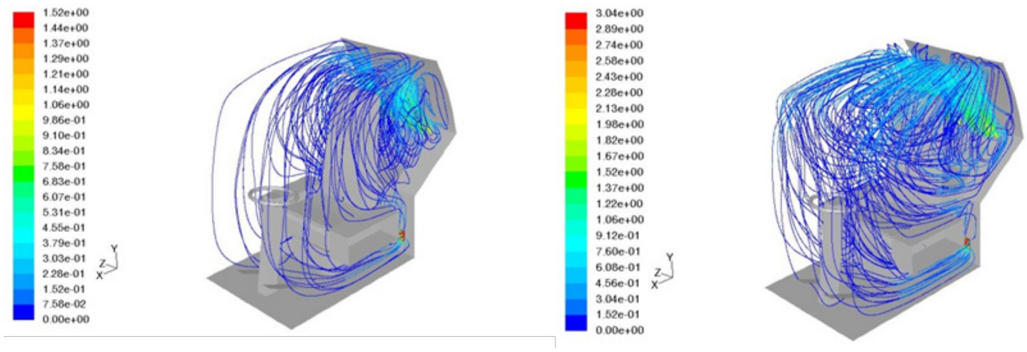


Fig. 6: Distribution of air flow speed, m/sec, for different flow settings a) 75 m^3 / h, b) 150 m^3 / h

Analyzing the results, the most important was the head position of the working machine's operator. The results of the simulation are shown in Figure 7.

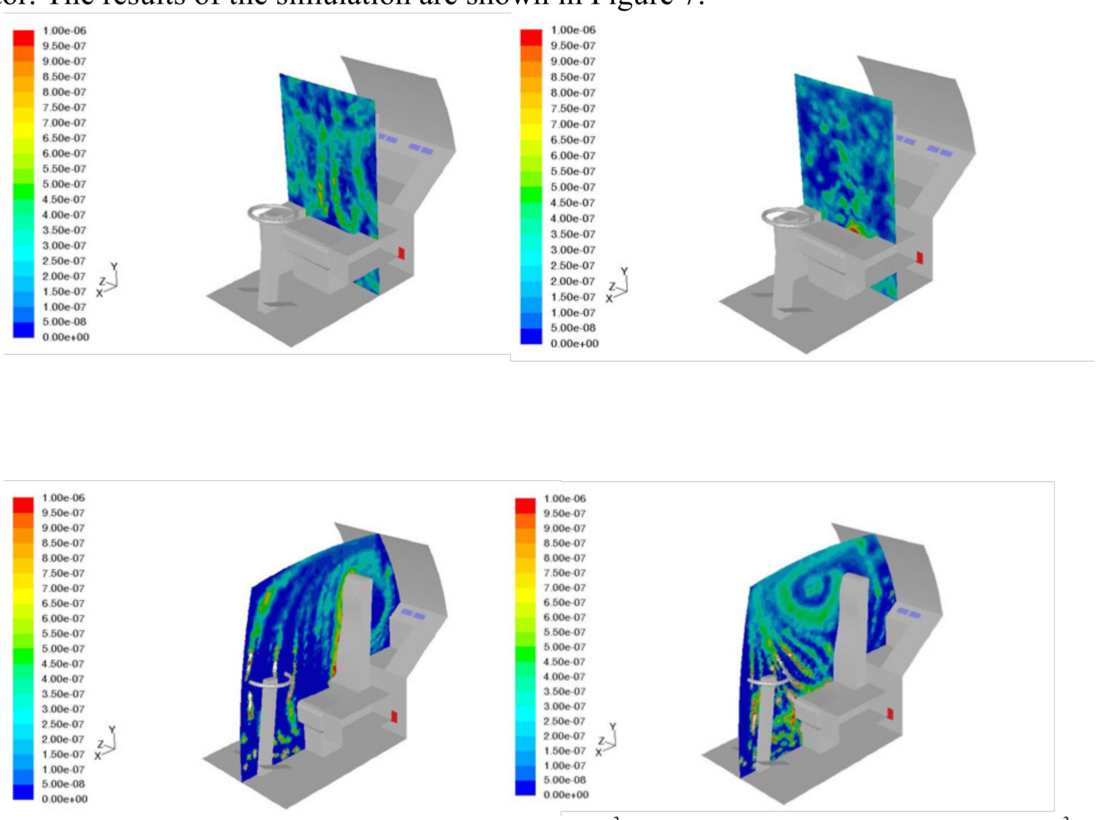


Fig. 7. BTX concentrations: a) yz cross-section, flow rate: 75 m^3/h, b) yz cross-section, flow rate of 150 m^3/ hour, c) xz cross-section, flow rate: 75 m^3/h, b) xz cross-section, flow rate of 150 m^3/h

Distribution of tested compounds in yz cross section shows that higher flow rate is more favorable if it goes for carcinogens distribution inside the cabin and results in better pollutants dispersion inside the cabin (7b). In the case of lower, of set point, value of the flow rate, there are the areas of elevated concentration of the body axis of the driver (operator) (7a). A similar phenomenon is seen in the xy cross section. According to the numerical simulation results in the case of air flow rate of 75 m^3/h elevated concentrations of analyzed VOCs are shown in the vicinity of the seat's user (7c).

Swirled areas of elevated concentrations can be seen in the case of larger than the set point flow rate at the level of the operator legs which is important in terms of human respiratory system - main road of VOC absorption into the body.

4. SUMMARY AND CONCLUSIONS

Using computational fluid dynamics methods it is possible to perform virtual exposure assessment of vehicle users in contact with carcinogens emitted from diesel engine inside a vehicle's cab.

Possibilities of the methods allow to find a correlation between the occurrence of areas with higher concentrations of hazardous compounds and ventilation system settings or geometry of the vehicle's cabin.

In future, these methods can be used in vehicle cabin's interior design, or ventilation system modules, in a way that minimizes risk to the health of vehicles' users.

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