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NUMERICAL PREDICTION OF THE PROPAGATION OF GASEOUS CONTAMINANTS IN THE VENTILATED LABORATORY

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NUMERYCZNE PROGNOZOWANIE ROZPRZESTRZENIANIA SIĘ ZANIECZYSZCZEŃ GAZOWYCH W WENTYLOWANYM LABORATORIUM

Celem zaprezentowanych badań było doskonalenie jakości modelowania numerycznego metodą CFD rozprzestrzeniania się zanieczyszczeń gazowych w laboratorium badawczym ze źródłem znacznika gazowego i odciągiem miejscowym przy wentylacji ogólnej mieszającej, prowadzone przy wykorzystaniu identyfikacji eksperymentalnej przepływu. Przedstawiono krótką informację o metodzie CFD w zastosowaniu do modelowania przepływu powietrza i zanieczyszczeń gazowych. Scharakteryzowano badany obiekt i dotyczące go dane eksperymentalne. Podano sposób budowy jego modelu obliczeniowego ze szczególnym zwróceniem uwagi na modelowanie nawiewnika. Porównano wyniki obliczeń i pomiarów prędkości powietrza i stężenia zanieczyszczenia gazowego. Podjęto próbę poprawienia jakości wyników obliczeń rozkładów stężenia znacznika gazowego przez zwiększenie dokładności odwzorowania nawiewnika, wypływającej z niego strugi oraz pola przepływu powietrza w rejonie źródła zanieczyszczenia i ssawki. Sprawdzono możliwość wykorzystania wyników obliczeń numerycznych do wyznaczania skuteczności działania odciągu miejscowego.

Summary

The aim of the presented investigations was to improve the quality of CFD numerical modeling of the propagation of gaseous contaminations in a test laboratory with a tracer gas source and a local exhaust in general mixing ventilation. The investigations were carried out making use of experimental identification of the flow. Concise information is presented concerning the CFD method applied in the modeling of the airflow and gaseous contaminant. The tested object has been characterized, as well as its respective experimental data. The ways of generating its simulation model has been described, paying special attention to the simulation of the diffuser. The results of prediction have been compared with the results of measurements of the air velocity and the concentration of gaseous contaminant. Attempts have been made to improve the quality of the obtained results of prediction of the distribution of tracer gas concentration by increasing the accuracy simulating the diffuser, the jet leaving the diffuser and the airflow pattern in surrounding the contaminant source and suction nozzle. It has also been tried to utilize the results of numerical prediction for the purpose of determining the effectiveness of the local exhaust.

INTRODUCTION

One of the tasks of rooms ventilation is the removal of generated gaseous contaminants, so that their concentration in occupied zone would not exceed values permissible for human beings. This can be realized mainly by local ventilation and capturing the pollution at the place of its generation. At the same time a general ventilation must be applied in order to dilute those contaminants which had escaped from the area controlled by the local exhaust. It is the aim of the designer of ventilation systems to choose such an air distribution in the ventilated room which would warrant the correct distribution of the contaminant concentration in compliance with the appropriate distributions of the parameters of ventilation airflow. For designing reliable tools are indispensable, permitting the prediction of these distributions. So far the following methods of prediction have been used: investigations in actual objects similar to these being designed or in their physical models. In spite of their doubtless advantages they have not found general application in the process of designing.

There is still some hope to solve these problems by predicting the ventilation airflow by means of *Computational Fluid Dynamics* (CFD) which determines the numerical methods permitting to solve models describing the flow of fluids connected with the exchange of heat. Such methods were already successfully applied earlier in other fields of science and technology, e.g., in meteorology or processing engineering. Recently researchers dealing with ventilation flows also use this method [2]. It is less expensive and requires less time than physical experiment. It does not require use the complicated testing equipment for measurements. It can be applied in investigations to be carried out in buildings in which measurements are rather troublesome, due to, for instance, large dimensions, elevated temperature, the presence of contamination affecting human health, and too small, not measurable or to large airflow velocities.

Beside the increased possibilities and availability of computer-aided calculations it is more and more often used as the designer's tool helping to choose and to check the concept of the air distribution in ventilated rooms. Therefore, beside complicated CFD packets, containing various options of modeling, applied for investigations in various fields of knowledge, commercial codes with standard options have come into being, concerning merely the ventilation flow, which however may be applied in practical engineering.

CFD programs are more and more often used in testing and designing of contaminant removal from ventilated rooms. This method has already been applied in the case of industrial halls in general ventilation, e.g. in chemical plants [2], in clean room in food-processing industry [9], but also in rooms with local exhaust, e.g. in kitchens [5], operating rooms [3]. Investigations based on numerical methods concerned also the concentration of gaseous contaminants in buildings of public utilities emitted by human body, e.g. in classrooms [11], or by the equipment of these enclosures [1].

Comparative tests indicate a rather good agreement of the results of numerical prediction of the contaminant concentration with the results of measurement carried out in actual objects or their physical models [4, 6], particularly in the case of a simple airflow in ventilated rooms. Problems may turn up only if we have to do with a complicated flow field. In such cases there may occur considerable discrepancies and the results of numerical calculations must be corrected. The first step is then to find out the source of the errors and imperfections encountered in the prediction by controlling the quality through making use of the results of physical experiments. Only in the next step these errors can be eliminated.

The aim of the investigations presented in this paper was to improve the accuracy of numerical prediction of the distribution of gaseous contaminants in the test laboratory with the pollution source and local exhaust, operating in the general mixing ventilation. These investigations were run basing on the experimental identification of the flow.

CONCISE INFORMATION ON THE CFD METHOD AS APPLIED IN MODELING VENTILATION FLOWS

Computational Fluid Dynamics methods at the stage of testing or designing ventilation and air conditioning may have the following applications: prediction of airflow patterns in rooms and determination of the predicted distributions of air parameters such as velocity or temperature. The starting points for the model are the differential equations offering a mathematical description of conservation laws:

– mass – equation of the continuity of flow,
– momentum – Navier-Stokes equation,
– energy – energy equation.

However, if such model is to be used for testing ventilation, the specific nature of the physical phenomena involved should be considered. First of all, accurate description of the structure of diffusers and representation of jets supplied from them. It is also essential to make a proper choice of the discretization grid suitable for the geometry of the structure. The non-uniformly refined orthogonal Cartesian grid is commonly used, often in combination with localized grid, as well as *Body Fitted Coordination* grid.

The greatest difficulty encountered in the solution of the above set of equations is the fact that ventilation airflows are mostly turbulent. *Direct numerical simulation* of the differential equations representing completely turbulent ventilation airflow still remains impossible. Accordingly, different models of the turbulence are proposed to enable the description of this phenomenon. The equations of the models are created for the parameters of averaged flows, with two types of averaging: in time and in space (spatial filtration).

After the equations of the model are averaged in time, apart from the independent variables: time τ and location x_i, they also contain dependent variables averaged in time: components of mean velocity vector $\overline{V_i}$, mean temperature $\bar{T}$ and mean concentration of gaseous contaminant $\bar{c}$. The form of these equations in tensor note is following:

– equation of the continuity of flow:

$$\frac{\partial \rho}{d\tau}+\frac{\partial\left(\rho \overline{V_i}\right)}{\partial x_i}=0 \tag{1}$$

– Navier-Stokes equation (Reynolds equation):

$$\frac{\partial\left(\rho \overline{V_i}\right)}{\partial \tau}+\frac{\partial\left(\rho \overline{V_i}\,\overline{V_j}\right)}{\partial x_j}=-\frac{\partial \bar{c}}{\partial x_i}-\rho \cdot g_i \beta \cdot\left(\bar{T}-T_o\right)+\frac{\partial\left(\nu \cdot \rho \cdot \partial \overline{V_i} / \partial x_j\right)}{\partial x_j}+\frac{\partial}{\partial x_j}\left(-\rho \overline{v_i' v_j'}\right) \tag{2}$$

– energy equation:

$$\frac{\partial\left(\rho\cdot c_p\cdot\overline{T}\right)}{\partial\tau}+\frac{\partial\left(\rho\cdot c_p\cdot\overline{V_j}\cdot\overline{T}\right)}{\partial x_j}=\partial\left(\lambda\cdot\frac{\partial\overline{T}}{\partial x_j}\right)+\frac{\partial}{\partial x_j}\left(-\rho\cdot c_p\cdot\overline{v'_j\cdot T'}\right)+S_T \quad (3)$$

– diffusion equation:

$$\frac{\partial\left(\rho\cdot\overline{c}\right)}{\partial\tau}+\frac{\partial\left(\rho\cdot\overline{V_j}\cdot\overline{c}\right)}{\partial x_j}=\frac{\partial}{\partial x_j}\left(-\rho\overline{v'_j\cdot c'}\right)+\frac{\partial}{\partial x_j}\left(\rho\cdot D\cdot\frac{\partial\overline{c}}{\partial x_j}\right) \quad (4)$$

where: g_i - the earth acceleration,

β - the coefficient of air cubical expansion,

c_p - the specific heat of air,

l - the thermal conductivity of air,

r - the air density,

S_T - source term,

D - the diffusion coefficient.

In addition, correlations of fluctuation components occur for these dependent variables that make this equation set unclosed. Particular models differ in the manner of creating the equations that close the set. In view of this, they are divided into two groups: *Reynold's Stress Models - RSM and Eddy Viscosity Models - EVM.*

The *EVM* models differ in the manner of designating the eddy viscosity coefficient v_t. It describes the local state of the turbulence and contrary to laminar viscosity v it is a variable dependent on location and time. The name of the models is related to the number of the transport equations of parameters, on the grounds of which the coefficient is calculated. They may be zero-equation models, most commonly algebraic and one-, two- or three-equations. The most popular one is the two-equations model k-ε (kinetic energy of the turbulence - its rate of dissipation). The parameters of this model are bounded to eddy viscosity by the following equation:

$$\nu_t = c_\mu\cdot k^2/\varepsilon \quad (5)$$

Their respective values in the modeled zone are determined from the following differential transport equations:

– transport equations of kinetic energy of the turbulence:

$$\frac{\partial k}{\partial\tau}+\overline{V}_j\frac{\partial k}{\partial x_j}=\nu_t\frac{\partial\overline{V_i}}{\partial x_j}\left(\frac{\partial\overline{V_i}}{\partial x_j}+\frac{\partial\overline{V_j}}{\partial x_i}\right)+\frac{\partial}{\partial x_j}\left[\left(\nu_t+\frac{\nu_t}{\mathrm{Pr}_k}\right)\cdot\frac{\partial k}{\partial x_j}\right]+g_j\beta\frac{\nu_t}{\mathrm{Pr}_t}\frac{\partial\overline{T}}{\partial x_j}-\varepsilon \quad (6)$$

– transport equations of dissipation rate of this energy:

$$\frac{\partial\varepsilon}{\partial\tau}+\overline{V}_j\frac{\partial\varepsilon}{\partial x_j}=C_1\frac{\varepsilon}{k}\nu_t\frac{\partial\overline{V_i}}{\partial x_j}\left(\frac{\partial\overline{V_i}}{\partial x_j}+\frac{\partial\overline{V_j}}{\partial x_i}\right)+\frac{\partial}{\partial x_j}\left[\left(\nu+\frac{\nu_t}{\mathrm{Pr}_\varepsilon}\right)\frac{\partial\varepsilon}{\partial x_j}\right]-C_2\frac{\varepsilon^2}{k}+C_3\frac{\varepsilon}{k}g_j\beta\frac{\nu_t}{\mathrm{Pr}_t}\frac{\partial\overline{T}}{\partial x_j} \quad (7)$$

The values in Prandtl's constant equations Pr_k, Pr_ε and coefficients C_1, C_2, C_3 and C_μ were determined by means of experiment or computer optimization for various types of airflow.

On principle, the standard k-ε model should be used in the description of flows with isotropic turbulence for high values of Reynolds numbers. In other cases, it may be a source of some calculation errors. The completion of the k-ε model with the analysis of flows with low values of Reynolds' number is possible thanks to *Low Reynolds Number* models. There is also a version of the k-ε model for flows with anisotropic turbulence.

An example of the model based on spatial filtration is the *Large Eddy Simulation (LES)* model, which is considered to give very promising prospects for ventilation flows. It takes advantage of the hypothesis that turbulent airflow may be divided into big and small eddy so that such division does not exert a big impact on the propagation of big eddy.

The issue of modeling of the turbulence also involves the choice of the manner of setting the boundary conditions on the walls and in their direct vicinity, the most popular method being the wall function method or the method based on k-ε model *Low Reynolds Number*.

Multiple CFD modeling options are nowadays used in complex research codes, whereas commercial codes usually use standard options: the model of turbulence k-ε, Prandtl's standard wall functions, the orthogonal, Cartesian discretization grid and assuming the boundary conditions directly in the supply openings. To this group of CFD computer programs, the code Flovent used to calculations in present work in the version 4.2, 5.1 and 6.1 is included.

DESCRIPTION OF THE MODELED ENCLOSURE AND ITS SIMULATION MODEL

For the purpose of investigations an actual test laboratory in the technological hall of the Department of Heating, Ventilation and Dust Removal Technology at the Silesian University of Technology was chosen, in which Mierzwiński *et al.* [8] carried out a series of observations and measurements in order to check the effect of a local exhaust, applying various kinds and parameters of the working of mechanical ventilation. The numerical tests, presented in this work, concerned mixing ventilation in isothermal conditions. The results of the analyses concerning mixing ventilation in non-isothermal conditions and displacement ventilation in isothermal and non-isothermal conditions have been presented in [7].

The scheme of the modeled room is to be seen in Figure 1. Its overall dimensions (taking into account also the niches) amounted to: length - 6.15 m, width - 5.8 m, height - 3 m. One of the partitions was an external wall with a window. Inside the laboratory on a table sized 0.75 x 0.8 m there was a point source of the tracer gas of sulphur hexfluoride SF_6, which mixed with air provided gas with a density of ρ = 3.12 kg/m^3. Its emission rate, determined in the course of physical experiment, amounted to 5 cm^3/s. Above the source of tracer gas there was a local exhaust in the form of a suction nozzle with a diameter of d_w = 115 mm, through which q_{vw} = 0.139 m^3/s polluted air was removed. The general ventilation of the room was accomplished by means of an inlet and removal of air in he ceiling. The air was supplied by a square flat diffuser sized 300 × 500 mm with an adjustable angle of the positioning of the blades at an air volume flux of q_{vN} = 0.278 m^3/s. The polluted air was removed through an outlet in the ceiling, sized 250 × 400 mm, shaped as a grille, with a free area ratio of 73%; the amount of removed air being q_{vu}= 0.139 m^3/s.

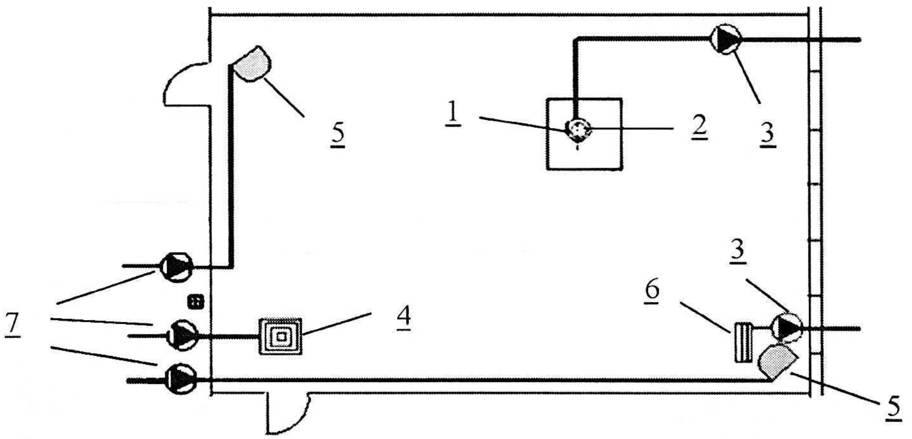


Fig. 1. The scheme of the test laboratory [8]
1 - contaminant source, 2 - suction nozzle, 3 - exhaust fan, 4 - square ceiling diffuser (mixing ventilation), 5 - quasi-laminar diffuser (displacement ventilation), 6 - outlet, 7 - supply fan

For this room was available the results of demarcation of the flow and measured values of air parameters: mean speed (mean module of instantaneous velocity vector, cf. [7]) and temperature, measured by means of a thermometer-thermo anemometer with a multidirectional velocity sensor and concentration of the tracer gas, measured by a gas analyzer. Measurements were taken at points distributed along the central axis of the room at various heights and in the four corners at a height of 1.1 m, marked in Figure 2 by respective numbers. Basing on the results of measurements of the instantaneous speed in the respectively chosen interval of time the values of the kinetic energy of turbulence and its rate of dissipation were estimated for these points. The results of observations, measurements and calculations were used in this work to check the accuracy of numerical predictions.

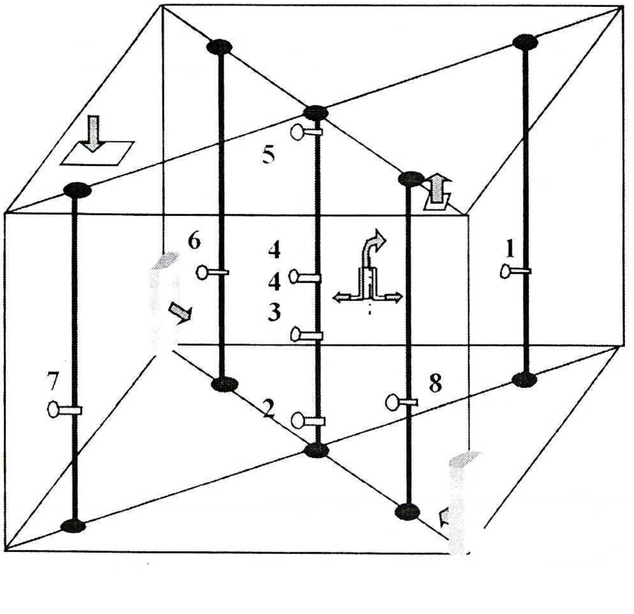


Fig. 2. Localization and numeration of air speed and temperature and contaminant concentration test points (designated by numbers from 1 to 8) in the test laboratory in mixing or displacement ventilations [8]

A simulation model for the test laboratory was developed (Fig. 3), turning to full account all the possibilities of the Flovent code. The data and geometrical, kinetic and thermal boundary conditions, required for calculations, were obtained by stock taking of the room and physical experiment. While developing these models some assumptions simplifying the object, required by the program proved to be indispensable, viz.:

- the suction nozzle was replaced by a square grid outlet, each side being 10 cm long, constituting a ready element of the library of the Flovent code, so that the area of the real exhaust would be maintained,
- the suction conduit carrying off the air from the nozzle was simulated as a closed cuboidal area, cut out from the numerical calculation,
- in the first version of calculations the square diffuser was modeled basing on a ready element of the code, which ought to simulate this type of inlets; the air flowed out of it perpendicularly to the surface of the supply opening, i.e. the flow angle was equal to 0°.

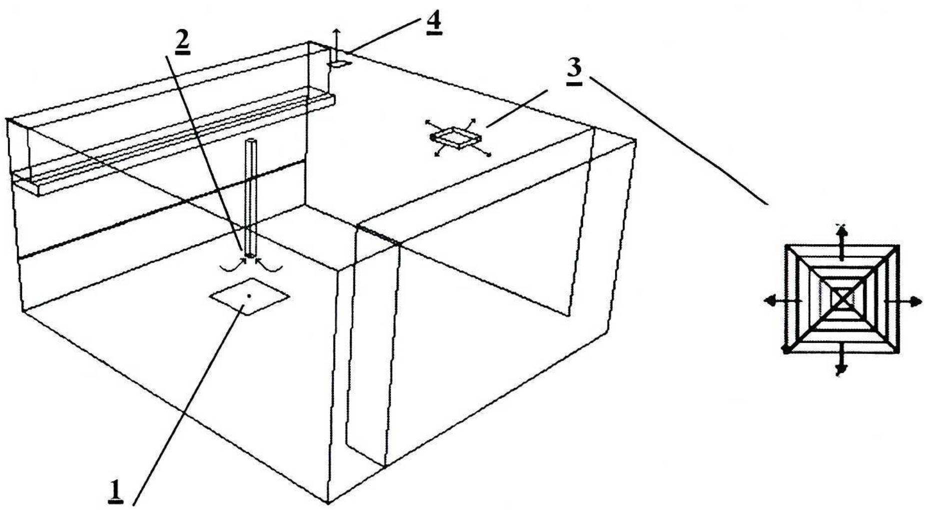


Fig. 3. Simulated model of the test laboratory in mixing ventilation obtained from CFD code Flovent 4.2
1 - contaminant source, 2 - suction nozzle, 3 - diffuser, 4 - outlet

The average air velocity in the ventilation openings, assumed in the calculations, resulted from the air volume flux flowing into the room. The kinetic energy of the turbulence and its rate of dissipation in the inlet were determined by presetting the value of the intensity of turbulence just in the opening. Initially this value was typical for the jet leaving the square diffuser Tu = 60%. Later the calculations were corrected, taking into account the results of measurements of this parameter in the vicinity of the actual inlet.

Numerical calculations were carried out applying the revised LVEL k-ε turbulence model [7] in steady-state conditions for a discretization grid non-uniformly refined, containing in the fundamental variant of calculations 65 x 78 x 70 = 354 900 nodes. For all the variants convergent solutions were obtained.

RESULTS OF NUMERICAL PREDICTION OF THE FLOW OF AIR AND GASEOUS CONTAMINANT AND THE CONTROL OF THEIR ACCURACY BY COMPARISON WITH EXPERIMENT

The results of numerical calculations concerning a laboratory room in mixing ventilation have been presented in Figure 4 as iso surfaces of the mean velocity and concentration of SF_6. According to predictions, the supply jet flowed out of the inlet horizontally under the ceiling in four directions, drifting then down along the walls. This caused the formation of a stagnation zone in the central part of the room, where the source of the tracer gas and the suction nozzle were positioned. The lack of a distinct airflow contributed to the prediction of an undisturbed suction of polluted air by the exhaust. Most of the emitted pollutants were, therefore, entrained by the suction nozzle, so that the calculated values of the contaminant concentration in the laboratory at major distance from the inlet were rather small.

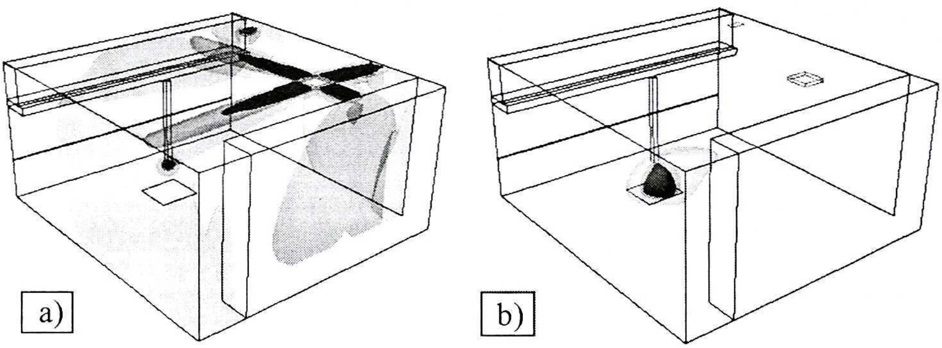
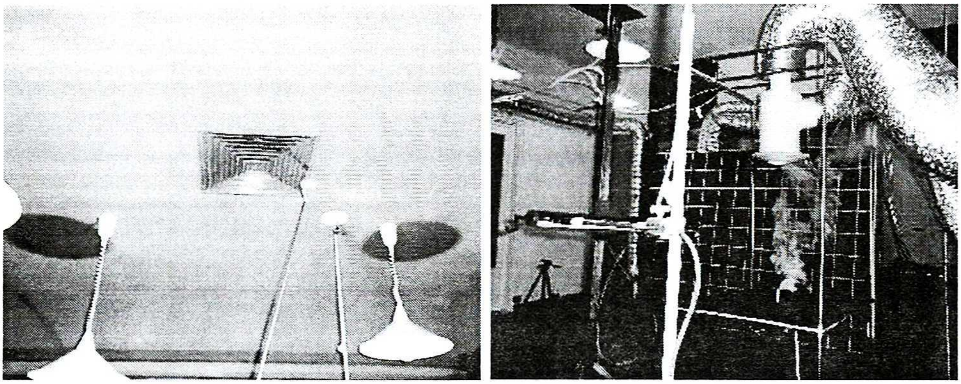


Fig. 4. Iso surfaces distribution in the test laboratory in mixing ventilation, calculated from CFD code Flovent 4.2
a) the mean velocity (1 m/s, 0.5 m/s, 0.15 m/s), b) the concentration of SF_6 (100 ppm, 20 ppm, 0.5 ppm)

A visualization of the airflow carried out in the laboratory applying demarcation by the fume did not confirm the predicted pattern of the airflow from the diffuser, which actually flowed in the room regularly in all directions (Fig. 5a). Such airflow is considered to be characteristic for square ceiling diffusers [10]. Neither was a stagnation zone observed in the vicinity of the suction nozzle. Investigations in situ indicated also disturbances in the working of the suction nozzle caused by the airflow and the diffusion of contaminants in the laboratory.

Such qualitative assessment of the accuracy of modeling of the flow of air contaminated by gas was confirmed by comparing quantitatively the calculated and measured values of the parameters of the flow of air and tracer gas at the test points, (cf. Fig. 2). The comparison of the values of the mean speed, the kinetic energy of turbulence and its rate of dissipation, as well as the concentration of SF_6 are to be seen in the diagrams presented in the next chapter in Figures 6 and 7. The results of measurements and prediction presented in Table 1 permitted to compare the average values of the afore-said parameters in the central axis, on the level 1.1 m and in the suction nozzle. An analysis of these comparisons indicates that:



a) b)

Fig. 5. Airflow demarcation by the fume in the laboratory in mixing ventilation under isothermal conditions [8]
a) square diffuser, b) contaminant source, local exhaust zone

– in the central axis the values of the mean speed of air were lower than the values obtained by measurements (on the average by 5 to 10 times), whereas the calculated values of the concentration were considerably much lower than the measured ones (on the average by 15 to 20 times),
– the predicted values of the gas concentration in the suction nozzle exceeded twice the value measured in this opening on the average,
– therefore, the calculated values of concentration in the exhaust in the ceiling, which only by small amounts of contaminants was reached, were considerably lower than measured ones.

a)

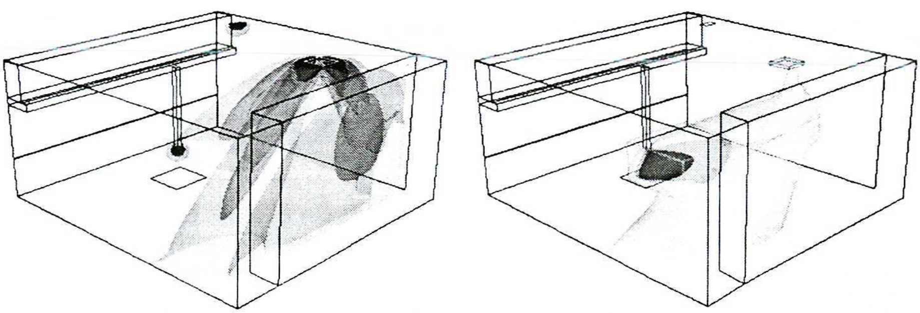
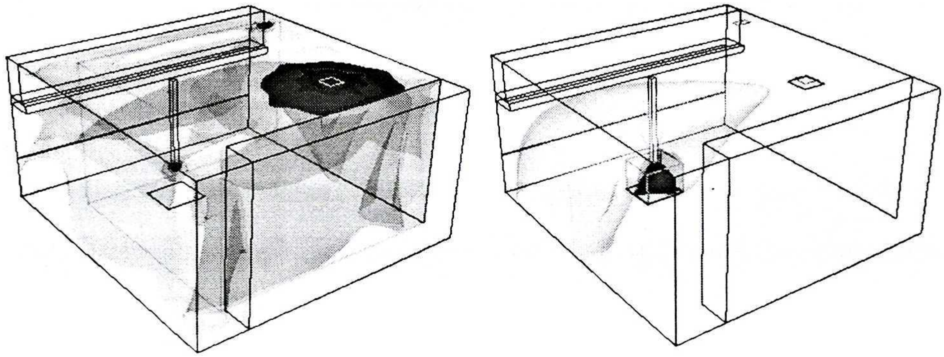


Fig. 6. Iso surfaces distribution of the mean velocity (1 m/s, 0.5 m/s, 0.15 m/s) (on the left) and concentration of SF_6 (100 ppm, 20 ppm, 0.5 ppm) (on the right) in the test laboratory in mixing ventilation, calculated from CFD code Flovent by various ways of the inlet simulation
a) square diffuser with inlet angle 35°,

b)



c)

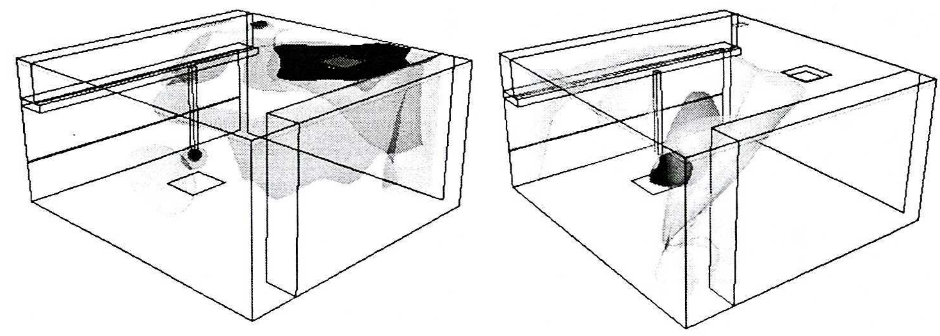


Fig. 6. Iso surfaces distribution of the mean velocity (1 m/s, 0.5 m/s, 0.15 m/s) (on the left) and concentration of SF_6 (100 ppm, 20 ppm, 0.5 ppm) (on the right) in the test laboratory in mixing ventilation, calculated from CFD code Flovent by various ways of the inlet simulation b) square plate diffuser, c) square plate diffuser modified

Table 1. Measured and calculated average value of parameters in the central vertical axis, on the elevation of 1.1 m and in suction nozzle in the laboratory

	In vertical axis		On elevation 1.1m		In suction nozzle
	Mean speed	Concentration of SF_6	Mean speed	Concentration of SF_6	Concentration of SF_6
	m/s	ppm	m/s	ppm	ppm
Measurement	0.21	2.708	0.18	2.31	13.59
CFD 0°	0.049	0.012	0.037	0.025	35.65
CFD square diffuser 35°	0.055	1.16	0.098	0.92	30.56
CFD square plate diffuser	0.224	0.429	0.112	0.21	45.67
CFD square plate diffuser modified	0.144	1.396	0.10853	1.08853	27.07

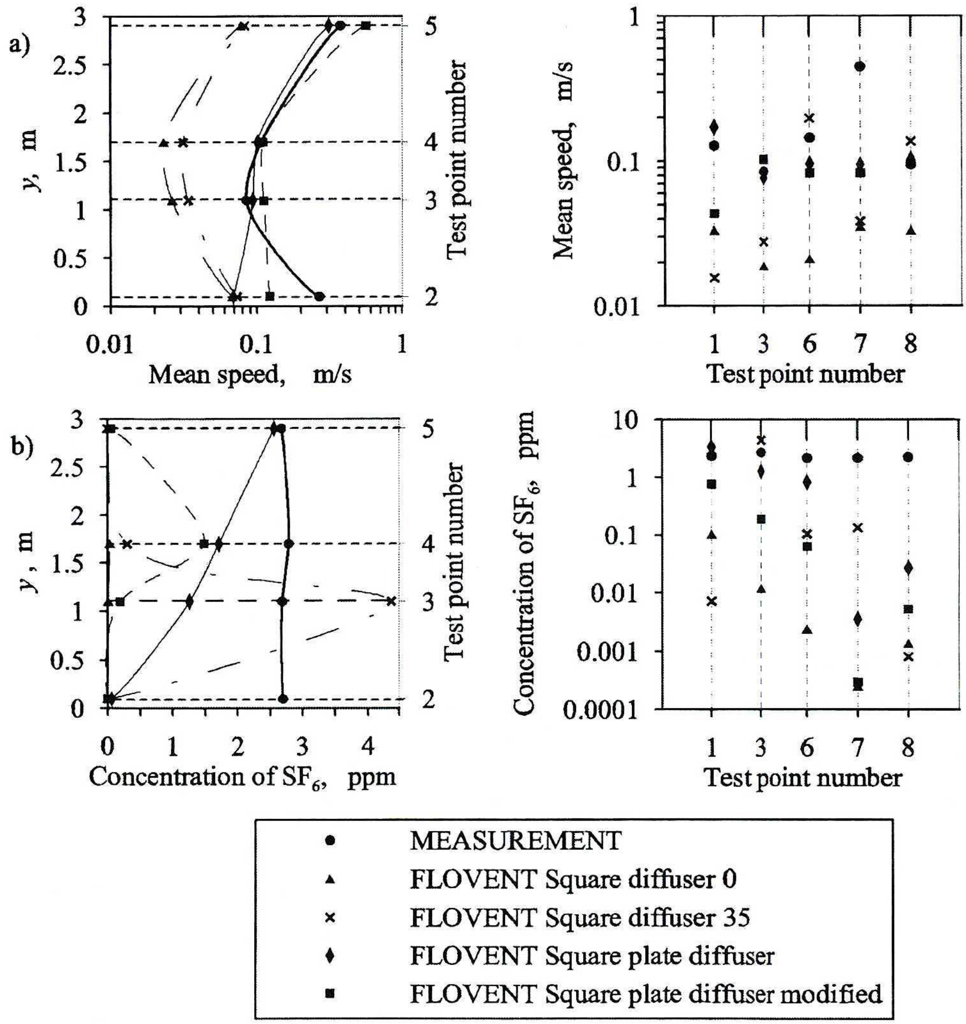


Fig. 7. Comparison between the measured and predicted (by various ways of the diffuser simulation) values of air mean speed and concentration of SF_6 in the laboratory in mixing ventilation in isothermal conditions at the test points in the laboratory (in Fig. 2): a) in the central axis along the height, b) on the elevation of 1.1 m

Thus discrepancies were found between the predicted and the measured distribution of parameters characterizing the flow of air and gaseous contaminants in the laboratory.

APPLICATION OF THE EXPERIMENTAL IDENTIFICATION OF THE FLOW FOR THE IMPROVEMENT OF THE NUMERICAL MODELING QUALITY OF THE PROPAGATION OF GASEOUS CONTAMINANTS

The aim of investigations related in the present chapter was to find the reason of inaccuracies in the numerical modeling of the propagation of gaseous contaminants and to eliminate or at least to reduce them.

Within the frame of the validation of modeling, undertaken by Lipska [7] some discrepancies have been noticed between numerical predictions in compliance with the CFD method and the results of measurements of profiles of the concentration of gaseous contaminations in a ventilated room. The encountered differences were, however, not as large as in the investigated case of the laboratory. There seemed to be an additional reason for such discrepancies. Taking into account the experimental identification of the airflow in this room, carried out by Mierzwiński *et al.* [8], the conclusion was deduced that there may have been an erroneous numerical simulation of the conditions of working of the suction nozzle, caused by the incorrect simulation of the mean air velocity field in the room, particularly in the zone of the emission of contaminant and this local exhaust. This field was generated by the diffuser, and therefore the way of modeling this ventilation opening and the supply jets were considered to be the main reason for the inaccurate prediction of the distribution of the parameters of air and gaseous contaminants in the laboratory.

For this reason it had to be checked if a change in the way of modeling the diffuser might improve the accuracy of predicting the velocity distribution in the entire room. While choosing the proper trend of activities, the results of visualization and measurements in situ were taken into account, as well as the limited possibilities of the Flovent code in this range.

First, it had to be checked whether the giving reality to boundary conditions in the supply opening by their experimental supplementation contributes to an improvement of the prediction. For this purpose the numerical calculations were repeated, assuming as the boundary condition in the diffuser the average value of the turbulence intensity, determined on the basis of measurements in the vicinity of an actual square diffuser, amounting to $Tu_N = 20\%$. An analysis of the results of calculations not quoted in this paper indicated the lack of the distinct effect of this change on the field of airflow in the laboratory.

The next step towards making the velocity distribution real was a change of the airflow angle from the inlet. In the calculations an angle of 35° was assumed, corresponding to the angle of inclination of the cones in the actual diffuser. The result was a change of airflow pattern in the laboratory in comparison with the results of calculations concerning the angle 0°. This is to be seen in Figure 6a (on the left), presenting the distribution of the iso surface of the mean velocity. Four jets leaving the diffuser did not stick to the ceiling, but quickly dropped down, developing considerable velocities in the zone under the diffuser. This did not contribute, however, to an improvement of the quality of modeling the velocity field in vicinity of the suction nozzle and measurement points, as was noticed when the results of predicting were compared with the results of measurements of mean speed in Figure 7 and the average values of these parameters in Table 1. As has been observed, a change of the air flow angle for the square diffuser does not affect a change of the values of mean speed in central axis of the room, but the values of this parameter increased or decreased in various points at a height of 1.1 m.

The geometry of a ready element of the Flovent code, which in compliance with the diagram included in the program (Fig. 3 on the right) ought to simulate a flat square diffuser, has been scrutinized in more detail. Its construction proved to be considerably simplified if compared with the structure of an actual inlet of this type. As a matter of fact this was merely a four-sided inlet with rectangular openings. Therefore, attempts were made to model the geometry of the inlet in some other way, maintaining its free area, in order to achieve a superior aim, i.e. a proper flow pattern of the supply jet and a airflow in the room, particularly in the region of the source of contaminants, and the suction nozzle. The possibilities, offered by the Flovent code, were however in this range rather limited.

Basing on numerous attempts made it was found out that the expected effect can be reached by means of a diffuser modeled in the form of a square inlet grid positioned in the ceiling and a thin square obstacle situated under this opening at some distance from it and corresponding to the dimensions of an actual diffuser. Scrutinizing the iso surfaces of the mean velocity (cf. Fig. 6 on the left) it was found out that it generated a radial wall jet similar to that flowing out of a real diffuser. Further on it is called a square plate diffuser, analogously to a round disc (plate) diffuser with a similar construction, from which such a type of jet flows in the room.

The supply jet propagated uniformly in every direction along the ceiling, but soon dropped down. For this reason the values of the mean speed differed in the measurement points from the measured ones less than in the previous calculations, although there still were some discrepancies near the floor and in the point 7, under the supply opening (Fig. 7a). The average values of the mean speed (Tab. 1) were more close to those obtained in measurements, too.

It was checked how far an improvement of the accuracy of simulation of the mean speed influences the quality of modeling the distribution of the concentration of SF_6; if a square plate diffuser is applied (Fig. 6 on the right). Due to disturbances in the working of the suction nozzle caused by the airflow, the situation changed for the better, but was still not quite satisfactory. Some part of the contaminants was not captured by the suction nozzle and escaped to the room. The calculated values of concentrations in the room were still too low in relation to the measured values (Fig. 7b), and the values in the suction nozzle exceeded considerably the actual ones (Tab. 1).

The accuracy of simulation parameters of the model of the turbulence: the kinetic energy of the turbulence and its rate of dissipation also proved to be much better when the diffuser was simulated in such a way than in the case of applying various versions of a ready element of the code.

Moreover, it was decided to improve the prediction by correcting the geometry of the square plate diffuser. Making use of the trial-and-error method a modified diffuser was obtained in which the air flowed in the room from the plate towards the ceiling. Numerical calculations carried out for such a diffuser required a considerable refinement of the discretization grid in the region of its direct influence. Thus, a grid of $69 \times 65 \times 71$ nodes was used with a local refinement of $122 \times 5 \times 131$ nodes, i.e. altogether there were 388 547 nodes. Thanks to the application of this diffuser a rather uniform propagation of the air along the ceiling and a good adjacency of the jet to the ceiling was obtained (Fig. 6c on the left), as has been proved by an experimental identification of the airflow in an actual object. And, similarly as in reality, the air jets affected the suction nozzle, causing disturbance in its working and the diffusion of contaminants into the room (Fig. 6c on the right). The result was an improvement of the accuracy of predicting the distribution of the concentration of gaseous contaminant, particularly in the central and upper part of the laboratory (Fig. 7b). In comparison with the previous predictions also the average values of this parameter increased considerably in the central axis, on the level 1.1 m and in the suction nozzle. The results of calculations of the air parameters at the measuring points (Fig. 7a and 8) and their average values, gathered in Table 1 may be considered as satisfactory, too.

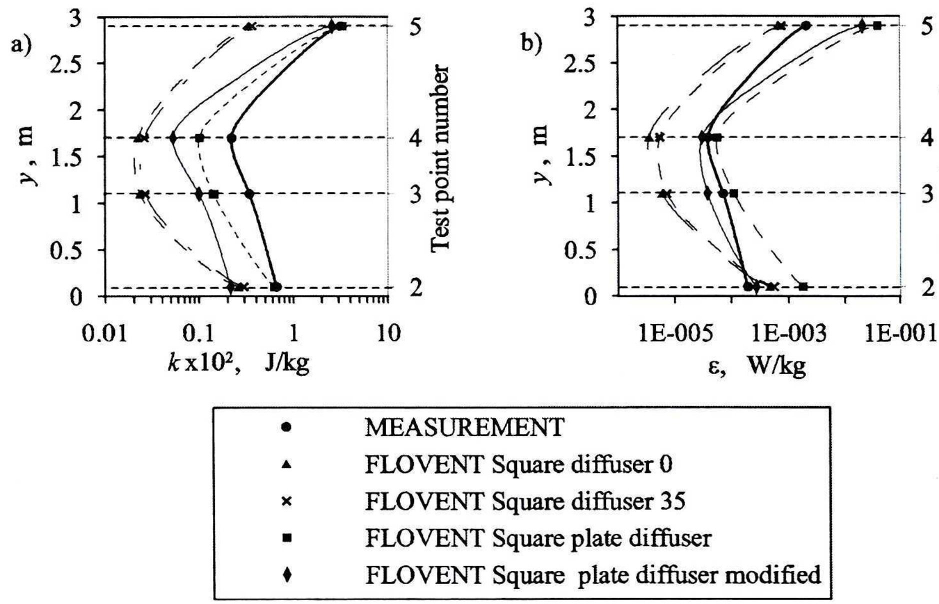


Fig. 8. Comparison between the measured and predicted (by various ways of the diffuser simulation) values of air parameters
a) the kinetic energy of the turbulence, b) the dissipation rate of the kinetic energy of the turbulence at the test points in axis along the height (in Fig. 2) of the laboratory

Correcting the way of modeling the diffuser it was possible to improve considerably the accuracy of predicting the distribution of gaseous contaminants in the investigated laboratory. The possibilities of the Flovent code did not permit, however, a more detailed simulation of the square ceiling diffuser and the supply jet. And so the achieved accuracy of modeling the mean velocity field and turbulent parameters inside the room was the most possible reason for applying this program. Moreover, the model of turbulence k-ε, applied in these calculation, was prepared for an isotropic turbulence and mean eddies, not allowing for simulation of large eddies, causing periodically changing circulations of the flow, which were observed in an actual laboratory by Mierzwiński *et al.* [8]. The results were discrepancies between measurements and calculations of the mean speed, affecting the accuracy of modeling the propagation of gaseous contaminants.

THE APPLICATION OF NUMERICAL PREDICTIONS IN THE DETERMINATION OF THE EFFECTIVENESS OF A LOCAL EXHAUST

It was checked whether in spite of occurring inaccuracies in the simulation of the propagation of gaseous contaminations, numerical predictions may be used to determine the effectiveness of a local exhaust. A positive result of such a test would extend the application of CFD codes in the design of local ventilations in enclosures. The investigations were carried out on the example of a suction nozzle installed in the laboratory for all the analyzed variants of mixing and displacement ventilation in isothermal and non-isothermal conditions concerning various ways of modeling the diffusers [7]. The present paper has been restricted to the analysis of the case of mixing ventilation in isothermal conditions.

The effectiveness η was calculated by means of the equation:

$$\eta = \frac{q_{mgo}}{q_{mge}} \tag{8}$$

where:

q_{mgo} – mass flux of contaminant captured by the local exhaust, determined on the known air volume flux drawn off by the suction nozzle and known profile of the contaminant concentration, calculated numerically in the outlet plane of the suction nozzle;

q_{mge} – mass flux of contaminant emitted by the source, being the boundary condition for numerical calculations, based on measurement data; in this given case it amounted to q_{mge} = 15.6 mg/s.

The predicted values of the effectiveness of the suction nozzle have been gathered in Table 2 and compared with the values of this quantity determined by measurements in situ. When analyzing these results it was found out that in most calculations concerning the mixing ventilation nearly all the contaminants were removed by the suction nozzle. Thus, its effectiveness had been predicted much higher than indicated by the data resulting from measurements. An exception was the variant with a modified square-plate diffuser, attaining the predicted value of the effectiveness of the suction nozzle similar to the measured one. This variant had been acknowledged even earlier as the best one for the modeling of the air and gas flow in room. It may, therefore, be concluded that the reliability of calculations concerning the effectiveness of the exhaust basing on the results of numerical CFD modeling is conditioned by a correct simulation of the working conditions of the suction nozzle and the distribution of contaminants over the entire ventilated object.

Table 2. Comparison between measured and predicted values of the effectiveness of the local exhaust in laboratory

Variant	q_{mgo} in suction nozzle predicted	Effectiveness of suction nozzle predicted	Effectiveness of suction nozzle measured
	mg/s	%	%
Square diffuser 0°	15.44	99.0	Serie 1: 75.0 Serie 2 : 86.9
Square diffuser 35°	13.24	84.9	
Square plate diffuser	14.46	92.7	
Square plate diffuser modified	11.39	73	

CONCLUSIONS

Numerical CFD modeling may be applied to predict the propagation of gaseous contaminants in ventilated rooms. A comparison of the results of numerical calculations with the results of measurements in one and the same object has, however, revealed discrepancies between the calculated and the measured distribution of the parameters characterizing the flow of air and gaseous contaminant. The occurrence of such discrepancies due to the possibilities and simplifications of the numerical model should always be taken into account.

Such differences may be somewhat reduced by introducing boundary conditions of the air distribution process resulting from experimental investigations, particularly aerodynamic and thermal boundary conditions in the inlet opening or supply jet, on the walls, in thermal sources and in the sources of contaminants.

In the case of applying the commercial Flovent code, comprising standard options of CFD modeling, the main reasons of the occurrence of discrepancies between the results of calculations and measurements in situ seem to be:

- the assumed k-ε model of turbulence developed for isotropic turbulence and mean eddies that cannot be simulated large eddies which cause periodically changing circulations of the flow to be observed in conditions of an actual laboratory,
- the simplified way of presetting the geometrical and kinematics boundary conditions in the supply opening, particularly simplifications in the construction of the diffuser, influencing the simulation of the momentum profile, and the parameters of air in the supply jet;
- the impossibility of taking into consideration various disturbances affecting the airflow in the room in real conditions, e.g., the infiltration of air through leakages in the doors and windows due to the changing distribution of the static pressure of air outside and inside the room.

In order to improve the accuracy of numerical prediction, the flow of air and contaminants in a room with a local exhaust in general ventilation, it is of essential importance to simulate correctly the flow field in the vicinity of the suction nozzle brought about mainly by the supply jet. Therefore, it is expedient to visualize experimentally and to identify representative cases of the airflow. This will facilitate the proper recognition of the character of the airflow and the assessment of correctness of its prediction.

The options of calculations offered by the Flovent code do not permit to simulate accurately the properties of the supply jets. It was an important cause of inaccuracy of the simulation. An essential drawback proved to be the impossibility of using the box method or prescribed velocity method, which would make it possible to apply in the calculations data concerning the parameters of the supply jet obtained experimentally or from the universal profile.

The analyses have shown that the CFD program, based on standard options of modeling, can be applied successfully for the purpose of assessing the effectiveness of local exhausts, but under the condition of a correct simulation of the aerodynamic conditions of working of the suction nozzle and distribution of the concentration of contaminants in its vicinity.

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