Numerical simulation of pollutant dispersion in a test ventilated room

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Abstract. The paper presents the numerical study of 3D flow and neutrally buoyant pollutant transport in a model atrium under conditions of test experiment by Thatcher et al. (2004) with a controlled uranine dye spill. For the Reynolds number of 2160 the Reynolds-Averaged Navier-Stokes approach was applied. Analysis of CFD predictability for a steady-state fully-developed regime and a transient process was done in comparison with the experimental data on contaminant concentration fields. For various positions of the contaminant source the ventilation effectiveness was computed and discussed.

1. Introduction

Dispersion of airborne pollutants in indoor spaces is important for risk analysis and emergency response. One of the reasons for that is an increased possibility of a chemical or biological attack, like a release of biological agents indoors [1] or a release of a toxic contaminant in an indoor space [2]. Hazardous events could occur also due to a spread of a flammable gas into a residential space [3]. Most of the toxic or flammable materials are heavy gases [4], and a special heavy gas dispersion model must be used in this case. If light gases dispersion is under study, positive buoyancy largely influences the flow and dispersion fields [5]. However, for some specific conditions it is possible to treat a contaminant as a neutrally buoyant (passive) pollution. An example of such a problem is a potential accident on board the International Space Station (ISS), for example, a pure oxygen release from a respiratory support pack providing aid to a crewmember in respiratory distress [6], a carbon dioxide release into the ISS cabin atmosphere in case a portable fire extinguisher discharge [7], or an accidental leakage of ammonia from the ISS thermal control system into the cabin atmosphere [8].

To ensure that the habitable area could be evacuated in case of a hazard material spill, an accurate Computational Fluid Dynamics (CFD) prediction of the pollutant dispersion is helpful. In engineering practice, CFD models based on the Reynolds-Averaged Navier-Stokes (RANS) equations solution are widely used, and, in particular, RANS models were applied in [6-8]. Despite RANS-based CFD modelling is recognized as a promising tool to simulate various dispersion scenarios, it is necessary to validate the computational data before the predictions can be used in engineering practice. RANS results depend strongly on the particular turbulence model used, and the uncertainty due to the turbulence model influence could be high especially when a fully developed turbulent flow (a turbulent jet) combines with a moderate Reynolds number flow (recirculation zone) in one problem, that is typical for ventilation tasks [9]. The validation of RANS results could be performed using
benchmark experimental data obtained in a test room configuration. Among others, an experiment performed for a scaled atrium by Thatcher et al. have resulted in a well-documented set of data [10, 11] that is suitable for verification of pollutant transport CFD models. These test data have been used already to validate the computational data obtained with a commercial CFD code [11] and an in-house Navier-Stokes code [12]. The objective of this work is to examine the ANSYS Fluent data on dispersion of indoor contaminant released from a point source in a large indoor space.

2. Problem formulation

2.1. Geometry model

The computational domain for the model atrium ventilation analysis is illustrated in Figure 1. The model atrium is a rectangular-shaped volume of \(2.8 \times 10^{-2} \text{ m}^3\). The height of the model atrium is \(H = 0.38 \text{ m}\) (in the \(z\)-direction), other dimensions are \(L = 0.3 \text{ m}\) (in the \(x\)-direction), and \(W = 0.24 \text{ m}\) (in the \(y\)-direction). There is a facet at one of the corners of the atrium, \(W_f = 0.21 \text{ m}\). Five rectangular inlets that simulate ventilation supply diffusers are placed at this facet. The height of each inlet opening, taken as the length scale, is \(H_{in} = 0.01 \text{ m}\), and the inlet length is \(L_{in} = 0.043 \text{ m}\), see Figure 1c. The outlet from the computational domain (Figure 1b) simulates a ceiling-level exhaust duct with the dimensions \(H_{out} = 0.035 \text{ m}, L_{out} = 0.25 \text{ m}\). Three plane cross-sections used for solution visualization are illustrated in Figure 1d. There are two horizontal cross-sections, \(A_1\) at \(z = 0.205 \text{ m}\), and \(A_2\) at \(z = 0.06 \text{ m}\). Section \(A_1\) passes through the middle line of one of the inlets, while the position of section \(A_2\) corresponds to the contaminant concentration measurement plane in the experiments [10, 11]. The vertical cross-section \(B\) is oriented perpendicular to the wall containing the inlets.

![Figure 1](https://via.placeholder.com/150)

**Figure 1.** (a) Computational domain; (b) exhaust (outlet) opening; (c) supply (inlet) opening, (d) plane cross-sections for solution visualization.

2.2. Problem settings and turbulence modelling

Experiments by Thatcher et al. [10] were performed with water as the carrying medium. The computations were set for water as well, that is considered as an incompressible fluid with a constant molecular viscosity \(\rho = 998.2 \text{ kg/m}^3, \mu = 1.003 \times 10^{-3} \text{ kg/m s}\). The supply flow rate of \(1.68 \text{ m}^3/\text{hour}\), i.e. 60 volume changes per hour, was set that reproduces the experimental conditions completely. It is assumed that the volume flow rate is equally partitioned among five openings, and the uniform velocity distribution of \(V_{in} = 0.217 \text{ m/s}\) is prescribed at each supply section with the inlet velocity
vectors directed normally to the inlet surface. The Reynolds number based on the inlet width and the inlet velocity is equal to 2160, and the flow is treated as turbulent.

The model of a continuous local source specified in one cell of the computational grid was used to simulate the pollutant release. In the experiments, the pollutant spill was simulated using an uranine (sodium fluorescein) dye solution introduced into the model atrium (water tank) just above the floor. The uranine dye, at a constant concentration of 10 mg/l, was supplied through a 5 mm diameter foam ball at a flow rate of \(10^{-4}\) m\(^3\)/s. Four different positions of the source were considered in the computations, namely, the baseline Case #1 with the source near the floor (this configuration corresponds to the experimental conditions), Case #2 with the source beneath the ceiling, Case #3 with the source near the inlet openings under the supply jet, and Case #4 with the source near the inlet openings above the supply jet. The source coordinates are given in Table 1.

### Table 1. The list of cases computed

| Case          | Case #1 | Case #2 | Case #3 | Case #4 |
|---------------|---------|---------|---------|---------|
| \(x_{src}\)   | 0.07    | 0.07    | 0.24    | 0.24    |
| \(y_{src}\)   | 0.095   | 0.095   | 0.035   | 0.035   |
| \(z_{src}\)   | 0.01    | 0.31    | 0.103   | 0.303   |

The molecular Schmidt number value was \(Sc = 10^3\). The zero contaminant concentration was specified at the inlet boundaries of the computational domain that corresponds to the experimental conditions without water recirculation. The zero contaminant flux condition was prescribed at all the wall boundaries.

In addition to the steady-state computations of the fully-developed dye dispersion, a transient contaminant dispersion regime was modelled. Spread of the pollutant after its sudden onset was computed with the “frozen” velocity distribution. Boundary conditions for the transient analysis were the same as for the steady-state computations. The zero value of the initial contaminant concentration was set.

#### 2.3. Computational aspects and solver settings

Two meshes of the same topology clustered to the walls and to the supply and exhaust openings were used in the computations. The initial mesh consisted of 424,704 cells. For this mesh, the normalized wall distance of a cell centre adjacent to a solid wall, \(y^+\), was in the range from 20 to 40 over the majority of the solid walls. The refined mesh consisted of 3,397,632 cells and it was obtained from the first mesh by means of refinement by a factor of two in each direction. On the basis of the preliminary mesh sensitivity analysis it was concluded that the solution obtained with the initial mesh could be treated as non-sensitive to the mesh size.

The commercial CFD package ANSYS Fluent 18.0 was used. The computations were performed based on the Reynolds-Averaged Navier-Stokes (RANS) approach. Four turbulence models were used for simulations: the Spalart-Allmaras model (SA), the standard \(k-\omega\) model by Wilcox with the low-Re correction (KO), the Menter shear-stress transport model (SST), and the standard \(k-\epsilon\) model (KE). The turbulent Schmidt number, \(Sc_t\), was set to 0.7. The inlet turbulence intensity was equal to 10\%, and the inlet ratio of the turbulent to molecular viscosity, \(\nu_t/\nu\), was equal to 25.

To compute the flow, that is the baseline solution for the contaminant transport modeling, the governing equations for conservation of mass, momentum, and turbulence characteristics were solved using the steady segregated pressure-based solver. Fully converged steady-state solutions were obtained for the SA, KO and KE models. However, it was not possible to get a converged steady-state solution when applying the SST model even using the initial mesh. The reason for that is that the version of the model used in ANSYS Fluent by default generates low turbulent viscosity due to limiter operation. Typical viscosity ratio values for the SST solution were less than 30, while other models
predict the \( \frac{v_{turb}}{\nu} \) values up to 150. The SIMPLEC pressure-velocity coupling scheme was used. The second-order upwind spatial discretization scheme was used, both for the momentum and the turbulence model governing equations. The standard pressure interpolation scheme was employed. The Green-Gauss cell based option was set as the method of computing the gradients.

The steady-state pollutant transport problems were computed with the “frozen” velocity field, i.e. only contaminant transport equation was solved. For the transient pollutant transport case, unsteady computations were performed using the air velocity fields defined by a corresponding fully converged (steady-state) solution. The second order implicit unsteady formulation was used. The time step of 0.5 s was set, and the length of the sample computed was 180 s.

3. Results and discussion

3.1. Steady-state flow fields and contaminant concentration distributions

First, analysis of the velocity fields is presented to demonstrate the effect of the turbulence model. For vertical cross-section B, Figure 2 illustrates velocity magnitude contours computed with three turbulence models that allowed obtaining the fully-converged steady-state solutions. Qualitatively, the flow patterns look similar: five inlet jets merge near the central region of the atrium. The joint stream reaches the opposite wall where it impacts with the surface, turns upward and downward, and forms two recirculation zones. Though three solutions obtained with the different turbulence models look similar, there are visible quantitative distinctions. For example, the solution obtained with the SA model demonstrates relatively shorter jet length and larger recirculation zones (Figure 2c), while the solution obtained with the KO model has more intensive flow in the recirculation zones (Figure 2b).

![Figure 2. Velocity magnitude distributions at vertical cross-section section B: (a) KE model, (b) KO model, (c) SA model.](image)

Figure 3 shows velocity magnitude contour plots as well as pathline patterns at horizontal cross-section A1. The velocity distribution at this section located approximately at the mid-height of the model atrium is typical for most of the atrium volume. The flow in the plane is divided into two large counter-rotating vortices separated by the inlet jet. As it is visible in Figure 3, the intensity and the length of the jet computed with three different turbulence models is almost the same (though SA model slightly under-predicts the length of the jet), but the recirculation zones shape differs from one plot to another (especially the shape of the smaller zone shown in the upper part of the plots).

For the lower horizontal cross-section A2, Figure 4 illustrates the fully-developed pollutant concentration fields. The computational data extracted from the steady-state solutions (Figure 4a,b,c) are presented in comparison with the measured concentration distribution (Figure 4d). According to [10], the experimental data representation is an ensemble averaged image obtained by combining of
1000 instantaneous images. The plot presented in Figure 4d is the reproduction of the data taken from [11]. The red dot presented in Figure 4d indicates the location of the source (it is placed at the same x- and y-coordinates, but at a vertical distance 5 cm below the measurement plane). It could be concluded that there is a qualitative agreement between the simulation results and the experimental observations. Quantitatively, there are visible distinctions. The computed contaminant concentration is higher than the measured one in the regions of high concentration (dark zones), and it is under-predicted in the regions of lower concentration. Besides distinctions in the concentration level, the computed data demonstrate some drift of the maximum of the contaminant concentration towards the right part of the plot as compared with the measurement data. The effect of the turbulence model on the concentration field in the section considered is more pronounced than on the velocity field in Figure 3 (another cross-section), and the distinctions in the concentration fields computed with different turbulence models are of the same order of magnitude as the difference between the experimental and computational data. It could be concluded that the contaminant concentration fields obtained with the SKE models look more reasonable as compared with the fields obtained with the SA model and KO model.

![Figure 3](image-url)  
**Figure 3.** Velocity magnitude distributions and pathline patterns at horizontal cross-section A1: (a) KE model, (b) KO model, (c) SA model.

![Figure 4](image-url)  
**Figure 4.** Fully-developed contaminant concentration distributions at section A2: (a) KE model, (b) KO model, (c) SA model, (d) experiment [11].
3.2. Results of unsteady computations in comparison with the experimental data

The present section describes the results of transient computations that illustrate the temporal behaviour of the dispersion following the onset of the pollutant release. Figure 5 shows the images created from computational and experimental data [11] during the period of contaminant concentration distribution development at the same horizontal cross-section A2. The plots present images at four successive time instants for which the experimental data on instantaneous concentration fields are available: 12 s, 36 s, 60 s and 180 s after the sudden onset of the contaminant release. The computational data obtained with the SKE turbulence model are analysed (Figure 5a,b,c,d) as this model demonstrated the best predictability of the fully-developed concentration field (Figure 4a). According to [11], the experimental data sets were obtained by means of the averaging of 19 images taken at the same elapsed time after the start of dye release in independent experiments.

In accordance with the measurements, the computational data reproduce the monotonous growth of the region with high values of contaminant concentration. This zone is located at higher values of the x-coordinate near the back side wall. As pointed in [11], there are some fluctuations in the instantaneous experimental data sets because 19 replicate experiments seem to be not enough to obtain a stable ensemble averaging. However, the comparison presented in Figure 5 allows demonstrating qualitative agreement between corresponding experimental and computational frames.

![Figure 5. Instantaneous (developing) contaminant concentration distributions at section A2 at instants (a),(e) 12 s, (b),(f) 36 s, (c),(g) 60 s, (d),(h) 180 s; (a-d) computational data in comparison with (e-h) experimental data [11].](image)

3.3. Evaluation of ventilation effectiveness

To provide safety and comfort, a ventilation system needs to provide an adequate supply of fresh air to the occupants and to remove the hazard contaminant successfully. Qualitatively, the possibility of a ventilation system to remove internally generated pollutants could be illustrated by a bubble where the
pollutant concentration is higher than some predefined value. For four different positions of the source considered in the current study, Figure 6 presents the isosurfaces of contaminant concentration $C = 0.0039$; the concentration is higher inside the isosurface. The source positions are marked with red circles. It is visible that the largest bubble is obtained in Case #2 with the source located near the ceiling, while the smallest bubble is in Case #4 with the source located above the supply jet.

![Figure 6. Isosurfaces of the contaminant concentration $C = 0.0039$: (a) Case #1, (b) Case #2, (c) Case #3, (d) Case #4; red circles point to the source locations.](image)

The ventilation effectiveness proposed by Sandberg [13] is a quantitative characteristic of a possibility of a ventilation system to remove internally generated pollutants from the ventilated space. The ventilation effectiveness is defined in terms of the concentration of the pollutant in the room and can be expressed either as a local effectiveness demonstrating the ventilation system performance variation between different parts of a room or as an overall effectiveness for the whole room.

Figure 7 illustrates the distributions of the local ventilation effectiveness, according to [14] expressed as $\varepsilon_c = (C_{\text{out}} - C_{\text{in}})/(C - C_{\text{in}})$, where $C_{\text{in}}$ represents the contaminant concentration in the outdoor supply air, $C_{\text{out}}$ – the contaminant concentration in the exhaust air, and $C$ – the local concentration. To avoid division by zero in the vicinity of the supply sections, the inversed quantity, $\varepsilon_c^{-1}$, is presented in the plots, so that large values correspond to the regions with poor ventilation effectiveness.

![Figure 7. Distributions of the reversed local effectiveness of ventilation, $\varepsilon_c^{-1}$: (a) Case #1, (b) Case #2, (c) Case #3, (d) Case #4; red circles point to the source locations.](image)

The values of the overall ventilation effectiveness for the removal of pollutants expressed as $<\varepsilon_c> = (C_{\text{out}} - C_{\text{in}})/(<C> - C_{\text{in}})$ [14], where $<C>$ is the mean concentration in the ventilated zone are given in Table 2. The variation of the size of the high-concentration bubble (Figure 6) is in accordance with the overall effectiveness values.

|   | Case #1 | Case #2 | Case #3 | Case #4 |
|---|---------|---------|---------|---------|
| $\frac{C_{\text{in}}}{C_{\text{out}}}$ | 0.7     | 1.5     | 2.2     | 3.0     |
4. Conclusion
RANS modeling of flow and contaminant transport in the model ventilated atrium with five supply openings have been performed using the ANSYS Fluent 18.0 CFD package. The computations were set at conditions of the benchmark test experiments with dye release into the water-filled tank at Re of 2160. The focus of the study was on the contaminant dispersion in the occupied zone where high spatial and temporal resolution digitized images of dye concentration were available. It was found that the effect of the turbulence model on the concentration field is pronounced, and the distinctions in the concentration fields computed with different turbulence models are of the same order as the difference between the experimental and computational data. Detailed comparison of the RANS computational results with the experimental observations showed that there is qualitative agreement between corresponding experimental and computational frames. For various source positions, evaluation of the ventilation effectiveness was performed, and it was shown that the worst scenario is realized when the source is located in the upper part of the atrium far from the supply jet.

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