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Assessment of the Influence of Input Parameters in CFD Simulation of Ventilation in an Experimental Chamber

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Abstract. The aim of this paper is to evaluate the impact of selected input parameters on the accuracy and usability of CFD simulations. This paper compares the achieved results of Computational Fluid Dynamics (hereinafter CFD) simulations of air age with the ventilation results of a specific experimental box. A total of 16 variants were simulated for different simulation settings, including various computational domains and meshes in OpenFOAM, Ansys Fluent, DesignBuilder, and BlueCFD-AIR software. The paper primarily focuses on the importance of meeting the suitability criterion for the yPlus parameter used in the wall function of turbulent models k-ε and k-ω SST, and the resulting air age. Simulation with the best yPlus parameter shows the best agreement in airflow velocity and air age with the experiment. Overall, this led to an improvement in accuracy by 41 % compared to original simulation and 56 % compared to the previous our best OpenFOAM simulation.

1. Introduction

Currently, there is a wide variety of software on the market, including CFD software. Some are freely available (such as OpenFOAM, BlueCFD-AIR, etc.), while others are commercial (such as Ansys Fluent, DesignBuilder, etc.). Commercial software generally offers good user support in the form of forums or electronic books with descriptions and explanations of functions. Freely available software typically relies more on the user community. Both commercial and freely available software have one thing in common: the final configuration is done by the user.

Presenting and optimizing any physical problem without experimental validation can lead to significantly different results from reality [1]. A well-validated model is essential for accurate simulation [2], [3]. Such a simulation can be used in indoor environments, for example, to optimize HVAC systems, improve or maintain thermal comfort for occupants, and enhance air quality, while reducing the amount of supplied air and the energy required for operation [4], [5]. This, in turn, reduces environmental demands and operational costs [6], [7].

The aim of this article is to experimentally validate data obtained and simulated using Ansys Fluent software, comparing it with other software tools such as OpenFOAM, BlueCFD-AIR, and DesignBuilder (similar to the approach taken in [8]) and to emphasize the importance of maintaining appropriate mesh quality for turbulent models, primarily focusing on the yPlus parameter based on achieved results. The geometric model, air exchange, and data for air age and velocity were adopted from reference [9]. It was compared for one inlet position and one outlet position at the same height with air exchange occurring twice per minute.

2. Methodology

The methodology includes a description of the theory of air age, the yPlus parameter, a description of the validation experiment, and the CFD model.

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2.1. Age of air

The local mean age of air (hereinafter LMA) is a statistical value of the time a particle spends from its release from an inlet to a specific position in the room, without accounting for the time the particle has spent in the exterior [10].

The tracked particle (e.g., CO_2) can be calculated in CFD as a gas mixture, multiphase, or using passive scalar transport and the solution of the overall convection-diffusion equation in a steady-state or transient manner. In incompressible flow, the equation holds that T is the transported scalar, U is the flow velocity, and D_T is the diffusion coefficient divided by the density (both must be constants) as in equation (1)[11].

$$\frac{\partial T}{\partial t} + \nabla \cdot (UT) - \nabla^2 (D_T T) = 0 \tag{1}$$

For the step-up method, also used in article [9], the age of air at a measured point can be calculated by the equation (2):

$$\tau_{age} = LMA_p = \int_0^\infty \left(1 - \frac{C_p^{sup}}{C_\infty}\right) d\tau \tag{2}$$

Where C_p^{sup} is the concentration added to supply air and C_∞ is the concentration of gas in time ∞ [8]. As air ages, it accumulates various pollutants and hazardous substances. Validating CFD simulations using experimental data is an essential step if we intend to use these simulations in practice.

Knowing the age of air allows us to calculate ventilation efficiency ϵ_{AC} showed in the equation (3). This is the ratio of the nominal air exchange time τ_n to the age of air τ_{age} [9], [10]. If ventilation efficiency is less than 1, it indicates inefficient air usage in the space, prompting considerations for optimization. Values greater than 1 can be achieved through ventilation of the breathing zone or buoyancy forces [12], [13], [14], [15]. The equation below is valid only for systems without circulation [10].

$$\varepsilon_{AC} = \frac{\tau_n}{\tau_{age}} \tag{3}$$

2.2. yPlus

Dimensionless parameter describing the behavior of flow near a wall. It relates the real distance from the wall (y), the friction velocity near the wall (u_T), and the kinematic viscosity (ν) as in equation (4). For the use of k-ε models with simplified logarithmic wall functions (showed in Figure 1), the recommended range for yPlus (hereinafter y+) is from 30 to 300. The optimal value for y+ ≈ 30 to achieve the best accuracy [16], [17], [18], [19].

For k-ω SST models, the initial y^+ should not exceed values greater than 10 (typically starting around 1) with a sufficient number of prism layers to resolve the entire viscous and transitional layer [16], [17], [18], [19].

$$y^+ = \frac{y \cdot u_T}{\nu} \tag{4}$$

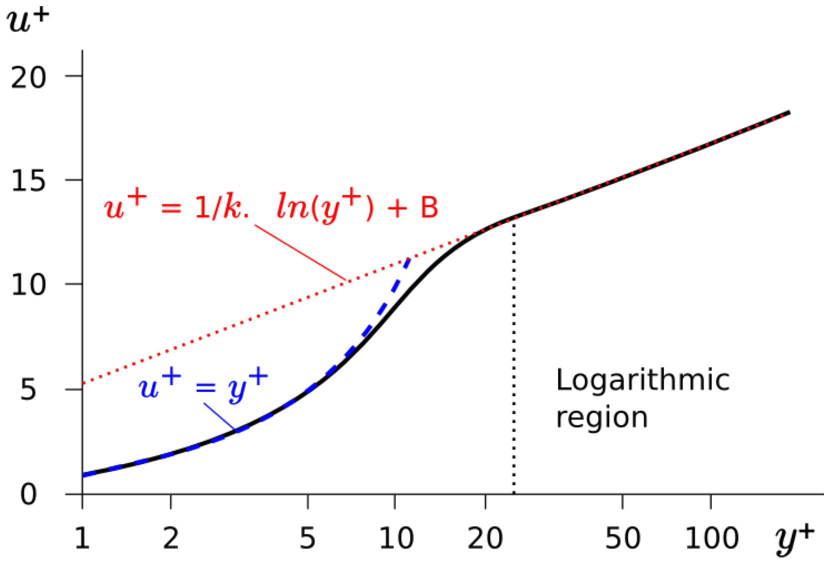


Figure 1 Law of the wall [20].

2.3. Description of the validation experiment

The experimental chamber, with dimensions of 1.8 × 1.2 × 0.1 m, was constructed with single-layer clear acrylic glass shown in Figure 2. An inlet with dimensions of 100 × 25 mm was located in the upper left corner. There were three outlet positions, namely: top right corner, bottom right corner, and bottom left corner – one for each case. The dimensions of the outlets were the same as the inlet. Figure 3 shows the measuring point positions. Further detailed in publications [8], [9].

Figure 2 Experimental chamber [9].

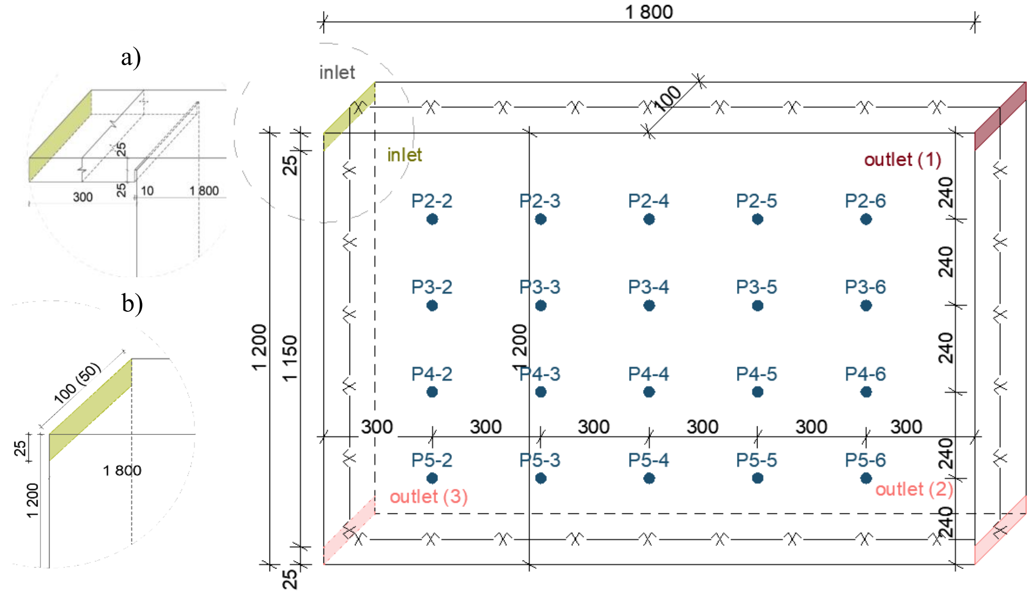


Figure 3 Sensor positions; geometry with: a) detailed inlet; b) simplified inlet [8].

2.4. CFD models

The airflow was modelled as isothermal and incompressible, either in steady-state (labelled as "SS") or transient (labelled as "TR") conditions with the same boundary conditions as in the article [9]. Various mesh configurations were generated, featuring basic cell sizes of 20, 15, and 10 mm, with total cell counts approximately ranging from 300, 600 to 1,200 thousand cells (labelled as "f"). Additionally, symmetric halves were considered and labelled as "h". Two methods of modelling the air supply to the experimental chamber were also compared: the detailed approach, labelled "DET", and the simplified approach, labelled "FLAT", illustrated in Figure 3.

The OpenFOAM (OF) software used the k-ε and k-ω SST turbulence models with an estimated turbulence intensity of 10 %, as this value was not specified in the article [9]. The meshers cfMesh (most simulations – unlabelled) or snappyHexMesh (labelled as "SHM") were used. For the mesh employing the k-ω SST turbulence model, a prismatic layer with a growth factor of 1.2 was also employed. Two models were further optimized using the y^+ parameter, which was met in areas of highest velocity. The meshes for this simulation contain 70,000 cells (labelled as "70k") for the full mesh and 76,000 cells (labelled as "76k") for the symmetric half-mesh.

The DesignBuilder (DB) software used a steady-state simulation with the finest setting of a 50 mm base computational cell.

Ansys Fluent (AF) used a more unspecified 20 mm hexahedral mesh mentioned in publication [9] for the transient simulation. In the measuring points regions, significant refinement with a tetrahedral mesh was employed.

BlueCFD-AIR (BA), based on OpenFOAM, uses the snappyHexMesh mesher with refinement of for cells near wall with a base cell size of 20 mm and only steady-state solutions.

More detailed settings are mentioned in [8].

3. Results

The differences between the simulation results and experimentally determined data for air age and airflow velocity are presented in the following graphs below. Deviations were calculated using statistical tools such as the arithmetic mean, median, and Root Mean Square Error (RMSE). The value $\hat{y}_i$ represents the predicted value (experimentally determined), y_i represents the actual value (determined via simulations), and n is the total number of measurement points. The deviations were calculated as shown in equation (5) for the arithmetic mean:

$$\bar{y} = \frac{1}{n}\sum_{i=1}^{n} y_i \tag{5}$$

As the median for an even number of values in equation (6):

$$\tilde{y} = \frac{y_{\left(\frac{n}{2}\right)} + y_{\left(\frac{n}{2}+1\right)}}{2} \tag{6}$$

And also as shown in equation (7) for the Root Mean Square Error (RMSE):

$$RMSE = \sqrt{\frac{1}{n}\sum_{i=1}^{n} (\hat{y}_i - y_i)^2} \tag{7}$$

Table 1 Differences between experiment [3] and simulations (absolute values) at selected points

Model/Mesh	p2-2	p2-6	p3-2	p3-3	p4-4	p3-5	p5-2	p5-4	AVG	MED
Fluent_article [1]	12	10	108	132	38	23	25	2	29.5	14.5
OF_SS_300k_DET_kω_h_SHM_AVG	11	12	43	40	59	63	31	56	42.8	34.9
OF_TR_300k_DET_kε_f	18	2	207	216	8	27	29	50	56.1	28.1
OF_TR_300k_DET_kε_f	18	2	207	216	8	27	29	50	56.1	28.1
OF_TR_600k_DET_kε_f	14	4	207	216	8	27	29	50	56.1	28.1
OF_SS_1.36M_FLAT_kε_f_AVG	1	3	169	191	31	1	44	13	46.3	28.5
BA_SS_4.4M_FLAT_kε_f	4	1	205	183	19	81	55	62	58.6	47.6
DB_SS_2.5k_FLAT_kε_f	2	40	237	228	104	87	49	75	91.5	73.5
OF_SS_160K_DET_kε_h	11	2	178	171	221	150	36	40	70.1	38.0
OF_SS_70k_DET_kε_f	6	19	1	19	47	3	31	28	22.7	20.7
OF_SS_76k_DET_kε_h	5	9	107	204	74	28	29	20	46.3	19.2

Table 1 shows the differences in air age [s] between the experimental measurements and simulations in absolute values, with the calculated mean and median for all points.

For simulations that did not converge correctly, the calculation had to be left running long enough to be averaged (labelled as "AVG"). The y^+ parameter was also evaluated for selected simulations that allowed for post-processing. It was found that a large portion of the simulations did not meet the required values for turbulent models; therefore, two corrective simulations were conducted with a smaller number of cells to improve this parameter. Simulations with a large number of cells using the k-ε turbulence model achieve an average $y^+_{AVG} < 3$. The maximum value from all simulations is 42.27. In the case of the k-ω SST turbulence model, $y^+_{AVG} > 10$ is exceeded in only a few cells. Corrective simulations achieve an average $y^+_{AVG} < 20$, with a maximum y+ of 154.17 or the full computational mesh of 70k cells and 113.43 for the symmetrical mesh. Using Paraview 5.10 software, the wall area for y+ >20; 25; 30 in the case of the k-ε model and y+ <1;5;10 for the k-ω SST model was determined, and the ratio to the total area of the test chamber was calculated.

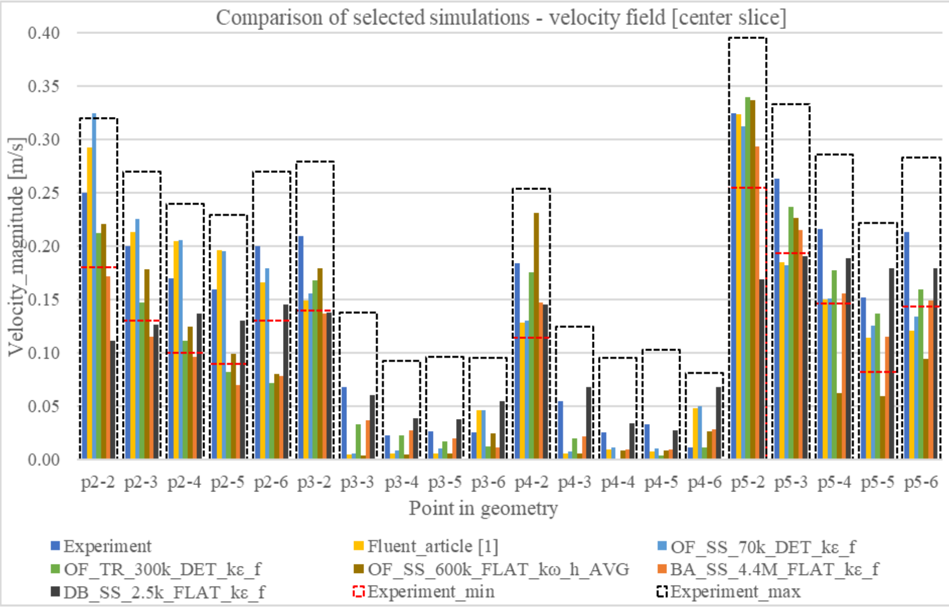


Figure 4 Velocity comparison at measured points

Figure 4 shows a comparison of the velocities of selected simulations at points measured in the experimental chamber using a Kanomax hot wire anemometer. The dashed lines represent the estimated deviations for the method used in the hot wire anemometry, ±0.07 m/s. The greatest deviations are found between the inner points p3-3 to p4-5.

Table 2 y^+ values of the simulations

k-ε model simulations	y^+_{min}	y^+_{max}	y^+_{avg}	A [m²]	A_y+ >20 [m²]	A_y+ >25 [m²]	A_y+ >30 [m²]
Fluent_article [1]	-	-	-	-	-	-	-
		A_y+/A [%]			-	-	-
BA_SS_4.4M_FLAT_kε_f	0.07	42.27	2.981	4.92	0.003	0.002	0.000
				A_y+/A [%]	0.06	0.03	0.00
DB_SS_2.5k_FLAT_kε_f	-	-	-	4.92	-	-	-
		A_y+/A [%]			-	-	-
OF_TR_300k_DET_kε_f	0.03	20.3	2.4	5.01	0	0	0
				A_y+/A [%]	0.000	0.000	0.000
OF_SS_1.36M_FLAT_kε_f_AVG	0.02	30.7	1.1	2.46	0.002	0.001	4e-5
				A_y+/A [%]	0.08	0.03	0.00
OF_SS_70k_DET_kε_f	0.03	154.2	18.2	5.01	1.70	1.05	0.69
				A_y+/A [%]	33.95	20.87	13.68
OF_SS_76k_DET_kε_h	0.57	113.4	16.9	2.51	0.742	0.444	0.348
				A_y+/A [%]	29.62	17.72	13.89
k-ω SST model simulations	y^+_{min}	y^+_{max}	y^+_{avg}	A m²]	A_y+ <1 [m²]	A_y+ <5 [m²]	A_y+ <10 [m²]
OF_TR_600k_DET_kω_f	7e-5	9.5	0.6	5.01	4.37	4.90	5.01
				A/A_y+ [%]	87.22	97.86	100.00
OF_SS_300k_DET_kω_h_SHM_AVG	3e-5	26.6	0.5	2.50	2.2	2.49	2.50
		A_y+/A [%]			87.93	99.52	99.92

Table 2 shows the minimum, maximum, and average y^+ on the wall of selected simulations. It also includes the total wall area A [m²], the wall area A_y^+ [m²] with y^+ >20; 25; 30 for the k-ε turbulence model and y^+ <1;5;10 for the k-ω SST turbulence model, along with the calculated ratio of area A_y^+ meeting the condition to the total area A. Detailed models have a larger area due to the inlet region.

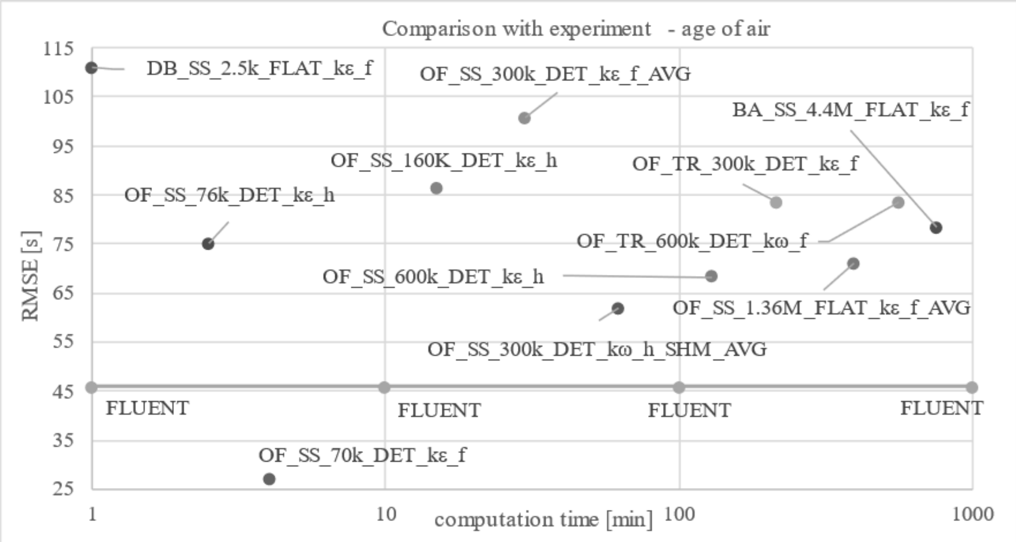


Figure 5 RMSE for LMA - comparison with experiment.

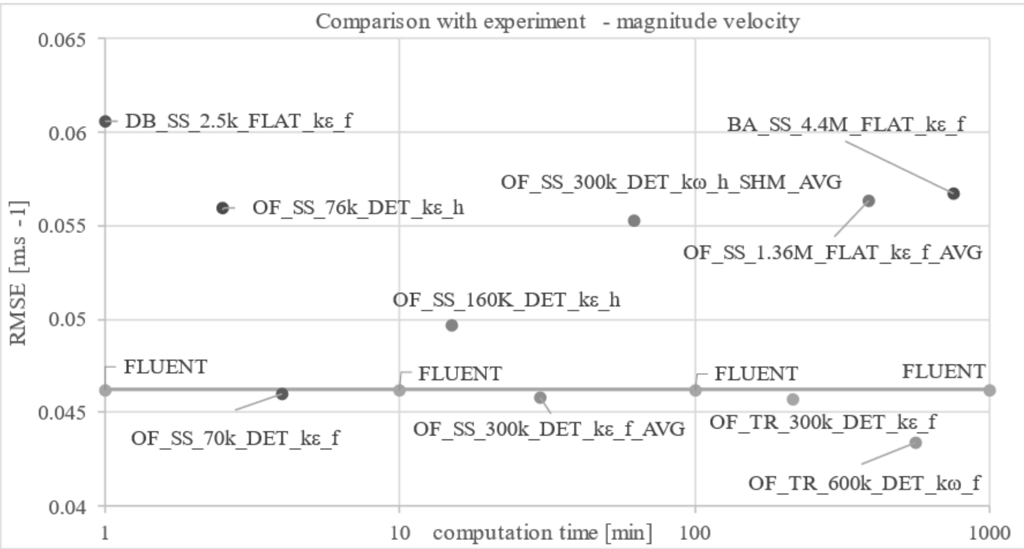


Figure 6 RMSE for velocity - comparison with experiment.

Figure 5 and Figure 6 show the error values of air age and velocity calculated using the RMSE for each simulation in relation to the computation time.

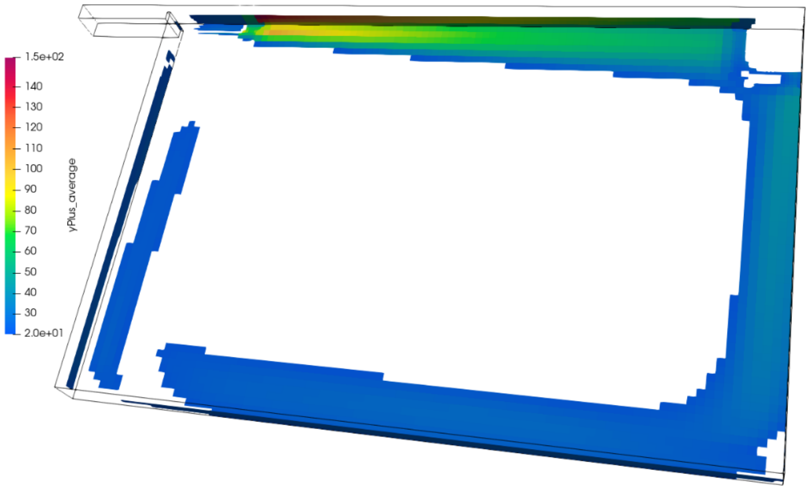
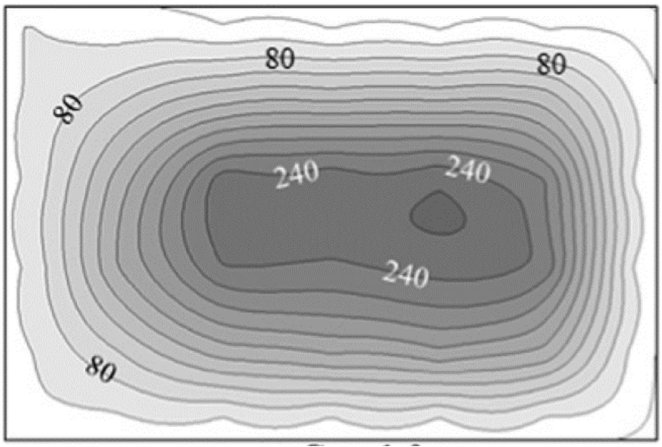


Figure 7 Simulation with 70,000 cells with y^+>20, full domain, k-ε

Figure 7 shows a cross-section of half the computational domain of the simulation with 70,000 cells and the achieved y^+ values >20 in areas with the highest velocity (velocity gradients). The black lines outline the entire computational domain.

a)



b)

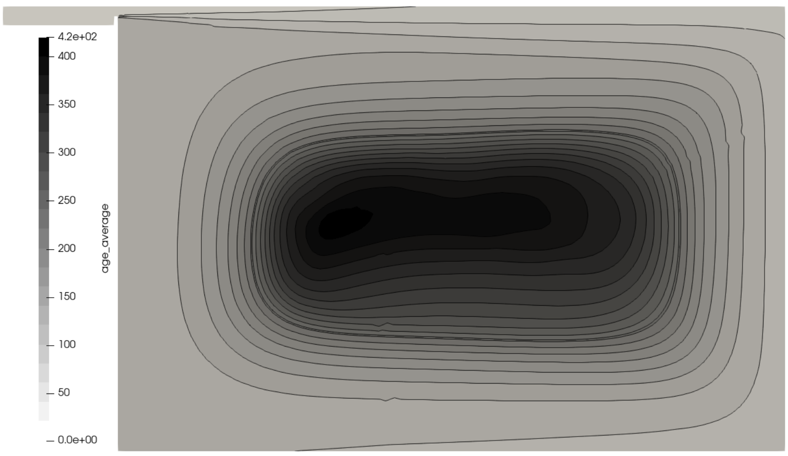


Figure 8 LMA results: a) from article [9]; b) OpenFOAM, 70.000 cells

The comparison of achieved air age results is shown in Figure 8. Part a) which is taken from [9], shows a maximum air age of approximately 260 seconds on the right side, while part b) shows our own steady-state simulation with a maximum average air age of approximately 410 seconds, with the maximum on the left side.
Reseach findings:

- In the simulation using the k-ω SST turbulence model, the use of only 3 prismatic layers proved insufficient for successful convergence and achieving accurate results, despite meeting the recommended y^+ value.
- The DB software does not allow any post-processing of mesh quality and parameters. It is not possible to export or calculate y^+ or any other mesh quality criteria, which significantly complicates optimization.
- BA automatically calculates y^+ upon exporting results. However, it does not allow for detailed user settings of the computational mesh. The software automatically refines the boundary conditions area (inlet, outlet, walls) into four layers of finer cells, making y^+ impossible to control.
- BA automatically reset the basic cell size from 20 mm to 5 mm. The finest cells near the wall are 2.5 mm. Both steps significantly disrupt the smooth progress of the simulation.
- In this case, symmetrizing the simulation with 70,000 cells in OF worsened the agreement with experimental data. The full mesh had 70,000 cells, but its symmetric half unexpectedly had 76,000 cells. This discrepancy occurred because the cells at the symmetry plane were adjusted to ensure correct geometry, causing the cells in the middle to split and increase the total cell count. Consequently, the cells near the boundary conditions became finer, leading to a higher total number of cells and deteriorating y^+, which depends on the cell size near the wall.

Many factors can influence the discrepancy between experimental and simulation results. In the case of the experiment, inaccuracies can be caused by the hot wire method of measuring flow velocity or the cooling of the wire through contact with the structure. Additionally, factors such as the type, internal construction, deviation, calibration, or response time of the CO_2 sensor, as well as unstable or not entirely accurate airflow from the fan, or slight shifts in measuring points, can have an impact. Geometric imperfections of the test chamber may also play a role.
In simulations, errors can be caused by incorrect types or definitions of boundary conditions, inappropriate use of the turbulence model, intensity of turbulence and turbulent characteristics, wall functions, discretization schemes, insufficient convergence, poorly chosen Courant numbers, and similar issues.
Authors of the original article [9] mention that for the unsteady simulation, a hexahedral mesh with a base cell size of 20 mm was used, combined with a fine tetrahedral mesh in the area of measurement points, aiming for an "effective and economical design" [9]. The total computational mesh size exceeded 1.2 million cells, employing the standard k-ε turbulent model. It remains uncertain whether the tetrahedral mesh intruded into the wall region and had at least one prismatic layer to avoid inaccuracies in wall function calculation, while ensuring sufficient use of correctors for this combined mesh. It is thus possible that refining around the measurement points resulted in refining part of the computational domain, potentially failing to meet the required y^+ in regions with the highest velocity gradients.
Differences between simulation and experiment might be, excluding errors on the experimental side, attributed precisely to this step, causing incorrect wall function calculation and thereby compromising result accuracy. The same issue arises in most our simulations using OF, BA, and likely DB.
Therefore, a plausible explanation appears to be the use of incorrect cell size and shape (tetrahedral) near the wall without employing a prismatic layer, or failing to adhere to all mesh quality criteria and the y^+ requirement as specified in article [9].
DB lacks an advanced tool for mesh quality check tool, making it impossible to ascertain the accuracy of flow computation.
BA's mesher operates automatically without user-adjustable settings, automatically refining the mesh at boundaries. The software conducts a checkMesh using OF tools and exports only the y^+ automatically. It exports only the last computational step, making it impossible to average results.
Refining around all walls is not advisable when simulations involve highly variable velocities. Neither DB nor BA can handle complex computational model geometry (detailed inlet).

It has been found that unsteady simulations are more accurate than steady simulations on the same mesh with an unresolved y^+, but at the cost of extremely longer computational time. The results clearly indicate that disregarding the correct y^+ at critical locations in the mesh (areas with the largest velocity gradients) leads to less accurate solutions across all compared software platforms - OF, BA, DB, and AF. Another significant issue is likely the large ratio of wall area to volume.
It can be assumed that adherence to the correct y^+ for a larger surface area would increase agreement with experimental data. However, this would necessitate enlarging cells in areas with lower velocities, potentially exceeding the actual thickness of the test chamber walls in regions with the lowest velocities. Thus, maintaining the y^+ parameter across all surfaces in this case is not possible.
Despite the unknown specifics of the hardware used and the incomparability of computational time lengths between our own simulations and those of AF [9] , it can be presumed that computing 1.28 million cells in an unsteady manner took orders of magnitude longer than the 4-minute steady-state computation of 70 thousand cells in OF (which achieved better results).

4. Conclusion

It was found that simulations in OF show better agreement with experiment [9] compared to simulations in AF [9] based on the calculation of RMSE and arithmetic mean. The values are as follows: for OF, RMSE is 27 s and the average error is 23 s, whereas for AF, RMSE is 46 s and the average error is 30 s. The model with the highest surface area ratio complying with y^+ at critical areas shows the best agreement. Improvement compared to the best previous simulation in OF is 55.97%, and improvement compared to the AF simulation in article [9] is 40.69%.
Results of DB cannot be interpreted as poor. Using a minimal number of cells (approximately 2500), simplified geometry of the inlet, and computation time <1 minute, the RMSE results of 111 seconds with an average deviation of 91.5 seconds can be considered very good for interpreting the flow behavior and air age in the studied space. OF achieved the best agreement, but it is necessary to realize that preparing geometry, computational meshing, and working with ParaView for post-processing take time, which the user must invest and especially learn.
BA stands between DB and OF. The software is free, the input geometry needs to be created in another software, setting boundary conditions and meshing is very fast, and after computation, the results can be immediately viewed in its own GUI and exported as an OF case. We also obtain results immediately with maximum values of air age and flow velocity with cross-sections at a predefined height typical for room height. Further post-processing is possible. The software is usable when a simple and uniform adaptation of the computational mesh on all walls suffices.
From the perspective of design speed and result visualization, (DB) and (BA) appear very effective. For more precise computations, (OF) is preferable due to its free availability compared to DB and its robust post-processing capabilities with ParaView.
When designing and evaluating the accuracy of simulations, it is crucial to consider many requirements regarding specific turbulent models and the quality of the computational mesh. These include parameters such as skewness, non-orthogonality, aspect ratio, volume ratio, scaling factor or y^+. However, this article specifically focused only on the y^+ aspect.

Acknowledgement
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Nomeclature

DET	detailed model of inlet
f	whole volume mesh
h	symmetric half of the mesh
10^{-x}	used convergence limit
AVG	average value (non-converged calculation)
BA	BlueCFD-AIR (OF core)
C_p^{sup}	supply air concentration of contaminant
C_∞	concentration of contaminant in time ∞
Conv.	Convergence limit
CFD	computational fluid dynamics
DB	DesignBuilder
FLAT	simplified inlet (2D surface)
OF	OpenFOAM
LMA	local mean age of air
LMA_p	age of air at point "p"
SHM	snappyHexMesh (meshing tool)
TR/SS	transient/steady-state
UDF	user defined function
VOC	volatile organic compound
Xxxk	thousands of cells
xxxM	millions of cells
AF	Ansys Fluent
GUI	Graphical User Interface