VALIDATION OF SELECTED SOFTWARE IN TERMS OF AIR AGE SIMULATION

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Abstract
The paper pertains to the assessment of indoor air quality in terms of its air age in a ventilated space. It involves a comparison of Computational Fluid Dynamics (hereinafter CFD) simulation software and their validation by an experiment carried out in a test chamber. A total of 14 cases were simulated and compared using the software: OpenFOAM, BlueCFD-AIR, DesignBuilder, and Ansys.The aim is to evaluate the accuracy and usability of the software by comparing selected computational domains and meshes. The results obtained show that the assessed software achieves satisfactory accuracy for air velocities and air ages. Models with simplified inlet geometry and half-domain offer the best balance between accuracy and computational effort.

Keywords
OpenFOAM, DesignBuilder, Ansys Fluent, air age, validation

1 INTRODUCTION

With the progressive development and increasing availability of a great number of CFD software, new possibilities and limitations arise for their use in building environment technology. For example, optimizing the cost of creating indoor environments in terms of air quality and occupant thermal comfort may be a suitable application area for CFD simulations [1]. In contrast to commercial and closed-source software with professional user support (Ansys Fluent, DesignBuilder, Star-CCM+, etc.), freely available or open-source software (like OpenFOAM, BlueCFD-AIR, Code Saturne, etc.) stands out for having little or no user support.

The aim of this paper is to experimentally validate (determined and simulated) data with Ansys Fluent software in other software, namely: OpenFOAM, BlueCFD-AIR (an extension to the OpenFOAM core), and DesignBuilder. For the verification process, the geometry, boundary conditions and data from a previously published paper [2] were used, which dealt with a single inlet (inlet) position and three different outlet positions for three different air exchange rates – half, once and twice per minute. Only one of these nine simulations was selected for validation, namely the configuration of inlet and outlet at the same height with air change rate twice per minute.

2 METHODOLOGY

Used methodology includes the age of air theory, a description of the validation experiment, and a description of the computational CFD model.

Age of air theory

The local mean age of air (LMA) (1) 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 [3]. Such a particle is transported by the flow, which we can be traced or calculated using CFD simulations. Its motion in the computational domain can be traced, for example, with use of scalar transport through a velocity field or kinetic turbulent energy. For the step-up method the local mean age of air can be calculated as:

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

where C_p^{sup} is the concentration added to the supply air and C_∞ is the concentration of gas in time ∞.

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Over time, the particle accumulates various pollutants (such as dust, droplets, viruses, VOCs, etc.) and it is assumed that the older it gets, the more dangerous it is for human health. Experimental validation of mathematical models enhances their reliability and broadens the applicability of CFD models in practical applications and research.

Ventilation efficiency, air change

The ventilation efficiency (2) is specified as the ratio of the nominal air change time τ_n and the mean age of air τ_{LMA}. Nominal air change is defined as the ratio of the room volume V (m^3) to the quantity of supply air Q (m^3s^{-1}).

$$\varepsilon_a = \frac{\frac{V}{Q}}{\tau_{LMA}} = \frac{\tau_n}{\tau_{LMA}} \tag{2}$$

The ratio is defined as the nominal time constant τ_n (s), and its inverse is defined as the air exchange (m^3s^{-1}) [2], [3].

The equation above is valid when used in systems without air circulation [3]. The ventilation efficiency then varies in the interval <0;1> depending on the quality of the designed system and the flow temperature. In some cases, it is possible to achieve a value >1 due to buoyancy forces or primary ventilation of the residence (breathing) zone [4], [5], [6], [7].

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 Fig. 1. 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.

Fig. 1 Experimental chamber [2].

The air flow to the test chamber was supplied by a radial fan with flow controlled by a potentiometer. The air velocity at the measuring points was determined with a Kanomax multichannel anemometer using the hot wire method.

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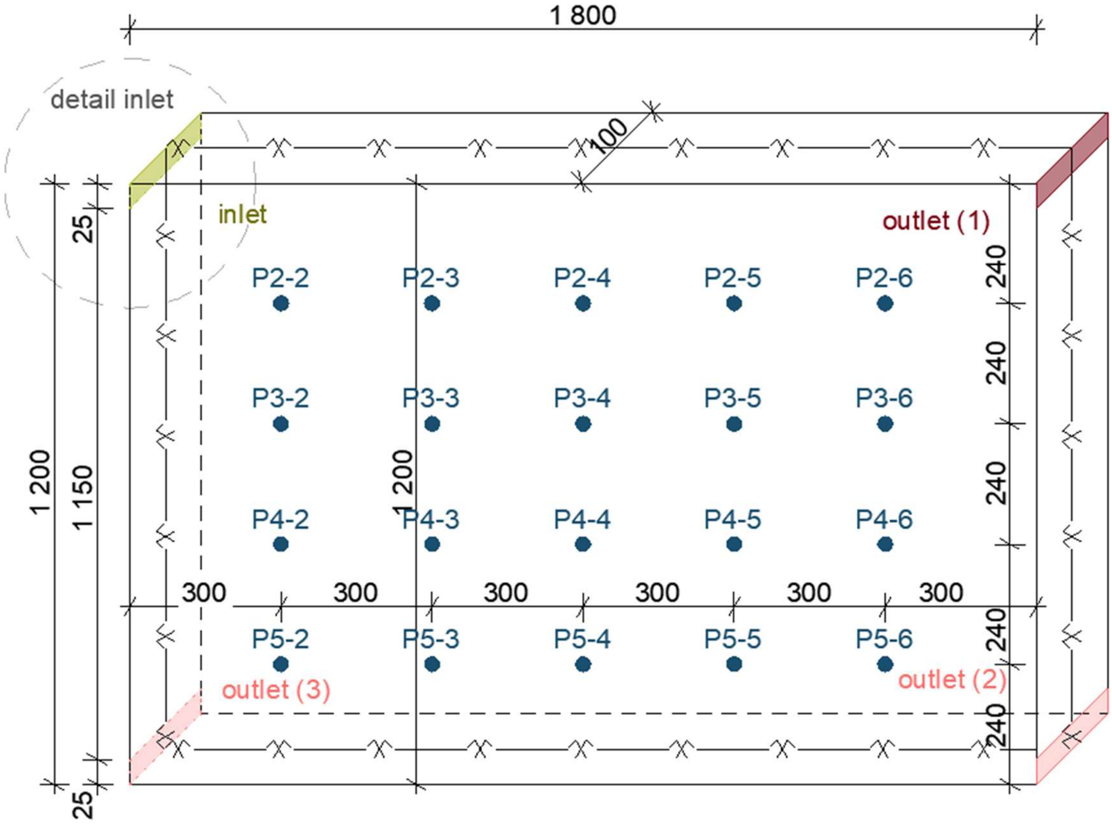

Fig. 2 Geometry, sensor positions.

Tracer gas (CO_2) and a programmed User Defined Function (UDF) were used to calculate the age of the air. At each measured point (illustrated in Fig. 2), the concentration was measured second by second with a MultiRAE detector. Gas injection was performed by using the step-up method, from the initial value to the desired value. The Local Mean Age (LMA) values were calculated using the tracer gas concentration over time obtained from the measuring device [2].

CFD model

The airflow was modelled as isothermal, incompressible, and with both steady-state (SS) and transient (TR) conditions (for 10 min – the duration of the experiment). The dynamic viscosity of air was considered at 15 °C, $1{,}86 \times 10^{-6}$ kg.m^{-1}.s^{-1} as reported in publication [2]. The k-ε a k-ω SST turbulence models were employed. The turbulence intensity at the inlet was chosen to be 10% because the value was not mentioned in the paper [2].
The OpenFOAM software simulations used open-source meshers CfMesh (most simulations – unlabelled) and SnappyHexMesh (labelled "“SHM”) with (shown in Fig. 3) and without prismatic layers on the walls with a scaling factor of 1.2. Various mesh configurations were generated, featuring basic cell sizes of 20, 15, and 10 mm, with total cell counts approximately ranging from 300 (Fig. 3), 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”, both illustrated in Fig. 4.

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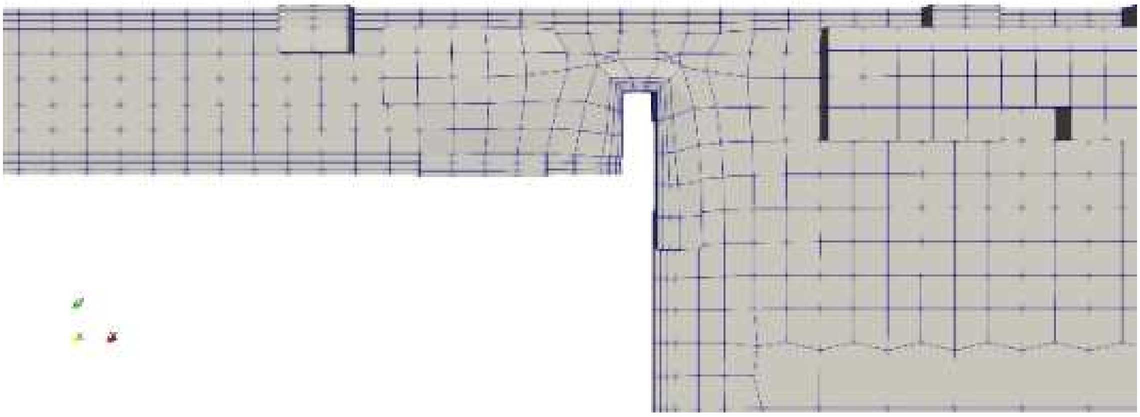

Fig. 3 Mesh of 300 thousand cells, detailed inlet (CfMesh).

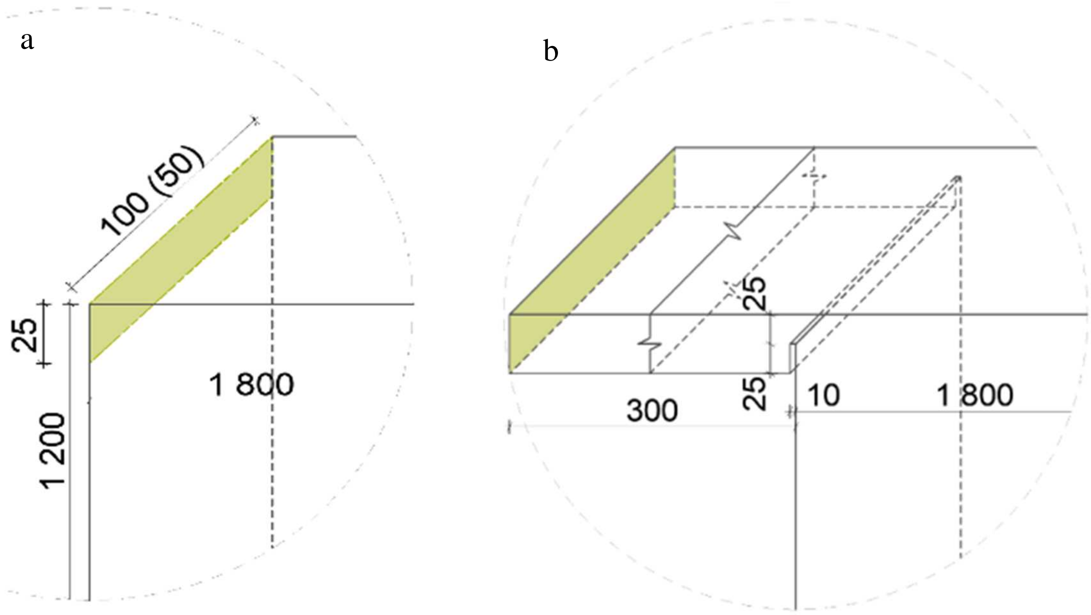

Fig. 4 Inlet types: a) flat inlet b) detailed inlet.

The DesignBuilder (DB) software, designed for simulating larger spaces, imposes a minimum dimension size of the computational cell to 50 mm. The computational mesh can be created in a non-equidistant manner with potential continuous refinement in the desired direction, typically towards the wall. Four computational meshes were generated with cell counts of 2,600, 83,000, 141,000, and 243,000, respectively. The unstructured computational mesh utilized in the original publication [2] was constructed using ANSYS Fluent software and comprises tetrahedra; however, additional details are not provided.

OpenFOAM (OF) and BlueCFD-AIR (BA) used the SIMPLE solver for the steady state (SS), and only one simulation used the SIMPLE.C solver for the k-ω SST turbulence model (kω). In the case of the transient (TR) calculation, the PIMPLE algorithmization was used. For both approaches, second-order upwind discretization schemes were used. DesignBuilder works with upwind, SIMPLE and k-epsilon settings. The Fluent setting is not mentioned in [2], only standard k-epsilon turbulence model is referenced.

The relaxation factors for the SIMPLE solver in the steady-state cases used the same values: 0.3 for the pressure field, 0.5 for k, ε, and ω, 0.6 for the velocity, and 0.7 for the age of air. In one case using the k-ω SST model and the SIMPLE.C algorithmization, 0.2 for velocity and pressure, 0.5 for the other variables. For the PIMPLE solver, all relaxation factors were set to 1. The convergence criterion for the norm. residuals of all variables is 10^{-5}. Unfortunately, Fluent settings are not mentioned in paper [2].

In the case of Fluent [2], the hardware used is unknown. Custom simulations leveraged the computational power of a hexa-core processor operating at a frequency of 3.6-4.2 GHz to minimize computation time through parallelization. DesignBuilder operated on a single core of the same PC.

3 RESULTS

Postprocessing of the 14 simulations calculated in OpenFOAM and BlueCFD-AIR was performed in Paraview software version 5.10.1 or 4.0.1. In the case of DesignBuilder, post-processing was done directly in the programme and by exporting data in .csv format further processed in Excel. In this scenario, data located outside the centres of the exported cells were calculated by linear interpolation. Considering the extensive dataset from all performed simulations, only those with the highest accuracy were chosen for representation in Fig. 6. For simulations that did not converge correctly, the calculation had to be left running long enough to be averaged (labelled AVG). The "Temporal Statistics" tool from the Paraview software was used to average the calculated data, mostly air velocity and age of air. The post-processing of the selected age of air results is depicted in Fig. 5.

a)

b)

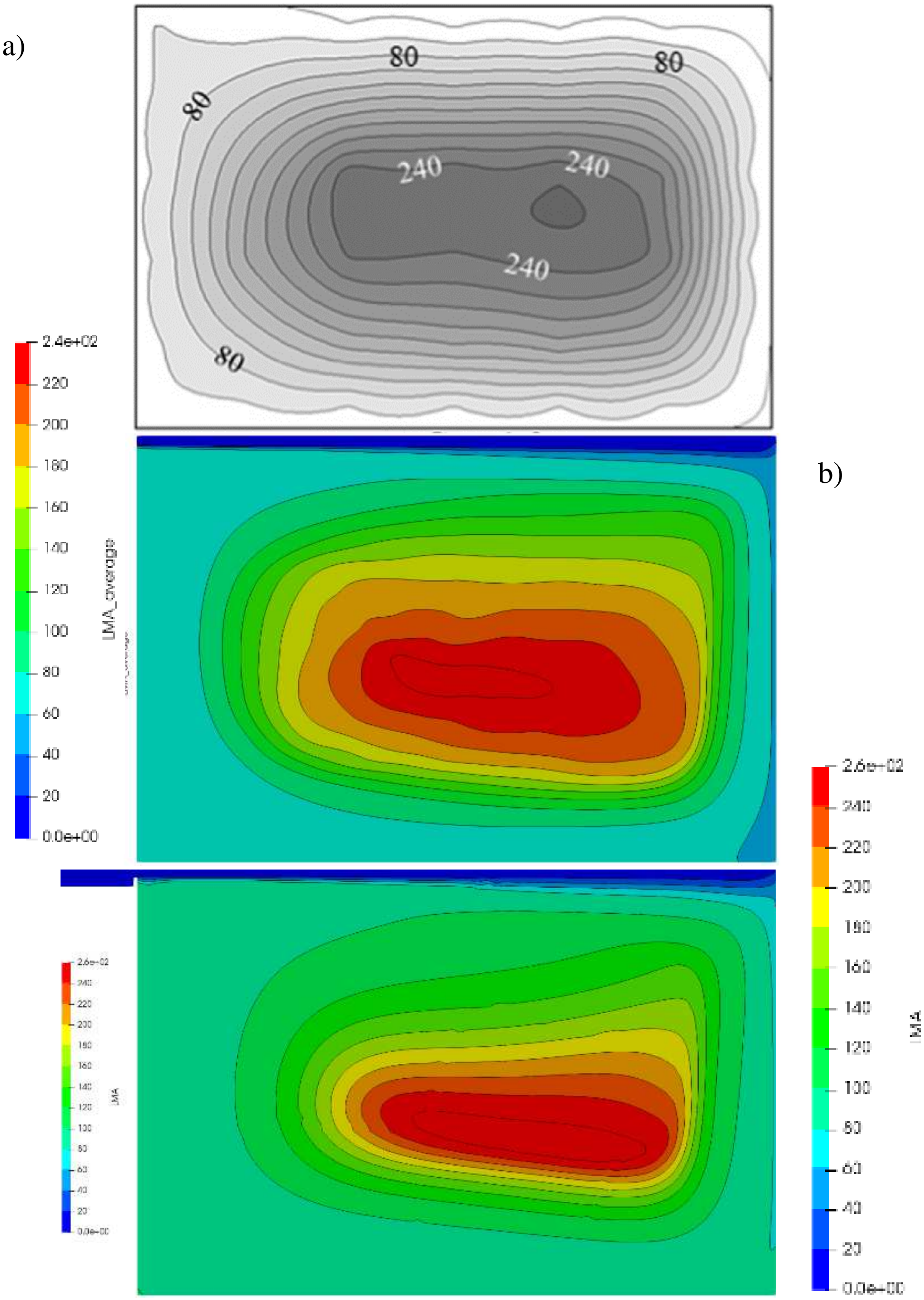

Fig. 5 LMA: a) from article [2]; b) averaging – 300 thousand cells; c) averaging – 1,200 thousand cells.

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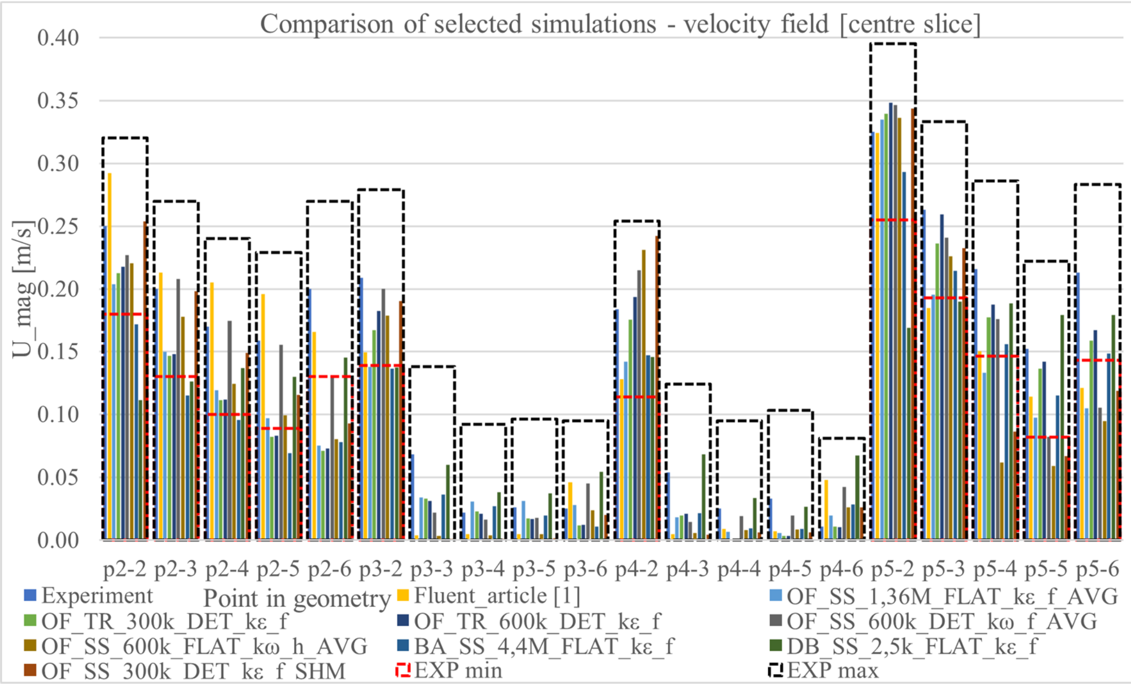

Fig. 6 Velocity field results comparison.

To determine the velocities at the measured points of the chamber, the authors in [2] used an unspecified Kanomax anemometer using the hot wire method. The minimum and maximum values, denoted in the graph by the dashed black and red lines, represent a deviation ±0,07 m/s, estimated for the method.

For each experimentally measured and Ansys Fluent simulated point, a deviation arises from the conducted simulations, expressed using Root Mean Square Error (RMSE) (3) – the root of the mean square error of all measurements. The value ŷ represents the expected value from the experiment/Fluent, while y is calculated using the validation simulation, n is the evaluated point (e.g., P2-2, P4-3, etc.), and M represents the total number of measurements.

$$RMSE = \sqrt{\frac{\sum_{n=1}^{M}(\hat{y}_n - y_n)^2}{M}} \tag{3}$$

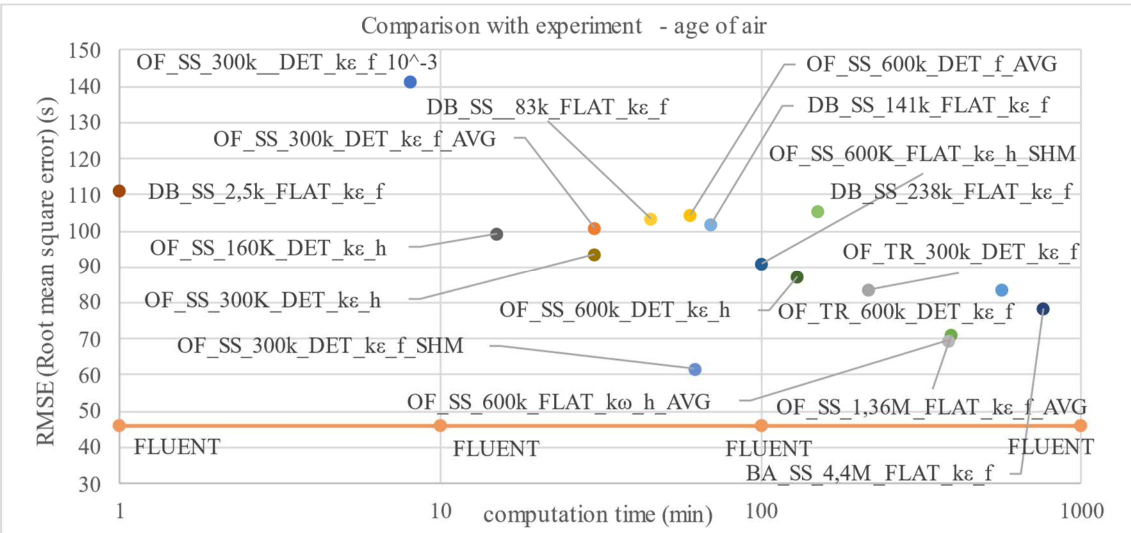

Fig. 7 RMSE for LMA – comparison with experiment.

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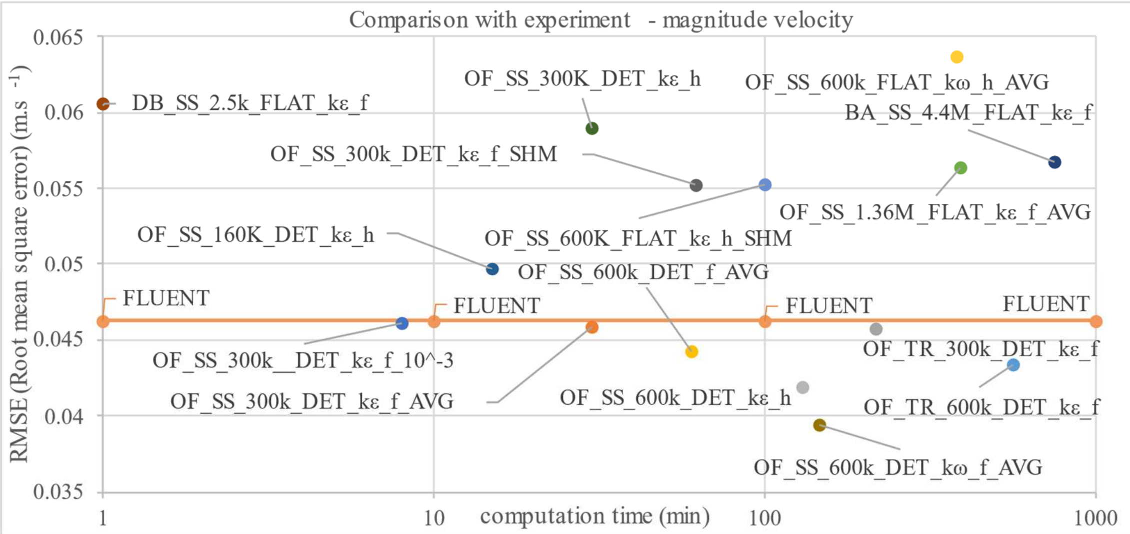

Fig. 8 RMSE for velocity – comparison with experiment.

In the initial simulations, the chosen convergence criterion of 10^{-3} proved to be insufficient, especially for coarser grids, and therefore the residual limit was shifted to 10^{-5}.

Research findings:

- Implementing a stricter convergence criterion produces more accurate results without significant refinement in the velocity field. However, refinement in the age of the air is on the order of tens to hundreds of seconds. A finer convergence criterion is crucial, especially for coarser grids.
- To achieve convergence on the finer grid, refining it in the outlet region helped. For the k-ω SST model, even such refinement was not meaningful and the simulation did not converge sufficiently further and the results had to be obtained by averaging over several iterations. The prolongation of the computational time later had an unfortunate effect on the evaluation of the mean square error as a function of computational time.
- Prolongation of the computational time for averaging does not affect the velocity, but it does affect the age of the air. In the cells with the lowest velocity, the air ages add up to infinity.
- The results show that the match in the velocity field is very good for all software, grid types and turbulence models employed. The maximum average deviation of all simulations from experiment is 0.02 m/s, and the largest root mean square error is 0.063 m/s – Fig. 8.
- The match of the air ages is very good, except for a few completely unsatisfactory points (mainly points P3-3, P3-4 and P3-5) which have a significant impact on the root mean square error comparing the simulation with the experiment – 141.47 s (Fig. 7). The average worst error for selected grids is 70 s.
- Calculating only the symmetric half results in a deviation of 5 to 50 seconds, depending on mesh quality and convergence criteria, compared to the entire domain with a mesh of the same fineness.
- In the case of BlueCFD-AIR, which does not allow much user intervention, an extremely fine mesh of 2 mm with a refinement of the nearest four rows around the walls to 1 mm and 4.4 million cells later proved most successful.
- The BlueCFD-AIR software has very limited ability to produce a good quality mesh, leading to oscillations or divergence of results. The refinement of the mesh partially helps, which is compensated by the extreme increase in computational time. When using only first order discretization schemes, although the desired convergence is achieved, the results are almost double.
- BlueCFD-AIR faces difficulties when importing models (only .stl or .xml (gbXML) can be used). When using .stl, the entire model becomes a single boundary condition, it is not possible to combine multiple .stls into a single model as in other software. The .xml format is very sensitive to the quality of the input geometry, when exporting from CAD (ArchiCAD – BIM) software, boundary conditions (windows, doors) can be shifted by units less than 1 mm, which are not visible in CAD but have a great impact in the creation of the computational mesh ("error cells"). This issue is applicable at lower speeds and larger building openings but becomes critical at higher speeds and smaller cross-sections (degraded or completely erroneous calculation). When using the gbXML export from DesignBuilder, the model is fine (accurate geometry).

- BlueAIR is preset to export only the last computational step. In case of oscillations and insufficient convergence, the results cannot be averaged and thus possibly more correctly evaluated.
- With a well-set-up computational model and a high-quality mesh, BlueAIR computes more efficiently than the standard version of OpenFOAM.
- DesignBuilder shows relatively acceptable deviations from the experiment (RMSE = 111 s) with the basic mesh setting (50 mm, 2,600 cells). Other, finer, meshes – 83,000, 141,000 and 238,000 – achieve similar deviations (RMSE = 104, 102 and 106 s, respectively). Refining the mesh yields almost no improvement in precision.
- With refinement of the mesh, the calculation of the solved geometry in DesignBuilder resulted in oscillations of the residuals in terms of their size and quantity. However, these oscillations disappear with higher quality mesh types. This phenomenon is also evident in OpenFOAM solvers.
- The choice between a simplified inlet (FLAT) or a detailed one (DET) with inflow does not significantly impact the accuracy of the calculation.

4 DISCUSSION

The achieved results of the simulations (OF, BA, DB) have a very good agreement with each other, with minor differences in some measured points in the comparison with the experiment and Fluent. However, the original paper [2] does not mention what the computational mesh looked like, we do not know the intensity of the initial turbulence or the original computational geometry, and the visual documentation is not well documented.

At first, the authors mention an inlet velocity of 0.36 m/s for the half air change, which corresponds to an inlet of 100 × 50 mm due to the size of the fan, but in the next section they mention a slot of 100 × 25 mm, but it is not shown in the schematic sketch. At the end, they talk about a computational mesh of 20 mm, which would not correspond to 1,280,000 cells, except for extremely finely remeshed inlet or a large number of prismatic layers. On such a coarse grid, a significant deviation could arise. We also do not know on how many experimental measurements and over what time interval the experiment was averaged, nor how long the flow was allowed to settle. It is possible that the authors ended up using a different turbulence model in the simulation.

5 CONCLUSION

If the original simulation matches the boundary conditions, model, and turbulence intensity, we can say that Ansys Fluent performs very well and still achieves better accuracy than OpenFOAM, which is not bad at all. Yet, the experience in configuring and creating an effective computational mesh can significantly influence the outcomes. DesignBuilder exhibits acceptable inaccuracy even with an extremely coarse mesh. However, with refinement, the results tend to become less accurate, albeit at the cost of increased computational effort due to the utilization of only one core. Despite DesignBuilder not permitting more detailed model and solver settings, its results closely align with those of OpenFOAM. All considered tools seem to provide acceptably accurate evaluations of airflow and air age. Overall, models featuring simplified input geometry and half-domain demonstrate the best accuracy-to-computational-effort ratio.

Future research will emphasize assessing the impact of quality criteria on the computational mesh, as well as exploring the influence of the Courant criterion on accuracy and computational effort.

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References

[1] ETHERIDGE, David and Mats SANDBERG. Building ventilation: Theory and measurement. Chichester: Wiley. 1996. ISBN 047196087X

[2] KWON, K.-S., I.-B. LEE, H.-T. HAN, et al. Analysing ventilation efficiency in a test chamber using age-of-air concept and CFD technology. Biosystems Engineering [online]. 2011. 110(4), 421–433. Available at: https://doi.org/10.1016/j.biosystemseng.2011.08.013

[3] SANDBERG, Mats and Mats SJÖBERG. The use of moments for assessing air quality in ventilated rooms. Building and Environment [online]. 1983. 18(4), 181–197. Available at: https://doi.org/10.1016/0360-1323(83)90026-4
[4] ASHRAE Handbook 2009: Fundamentals. SI ed. Atlanta: American Society of Heating, Refrigerating and Air-Conditioning Engineers. January 15, 2009. 880 p. ISBN 978-1933742557
[5] SKÅRET, Eimund and Hans Martin MATHISEN. 1982. Ventilation efficiency. Environment International [online]. 8(1–6), 473–481. Available at: https://doi.org/10.1016/0160-4120(82)90065-4
[6] SANDBERG, Mats. 1981. What is ventilation efficiency? Building and Environment [online]. 16(2), 123–135. Available at: https://doi.org/10.1016/0360-1323(81)90028-7
[7] Age Of Air And Air Change Effectiveness. DesignBuilder [online]. [accessed 2023-11-16] Available at: https://designbuilder.co.uk/helpv7.0/Content/AgeOfAirAndAirChangeEffectiveness.htm

Nomenclature

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