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PERFORMANCE EVALUATION OF CFD CODES IN BUILDING ENERGY AND ENVIRONMENTAL ANALYSIS

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ABSTRACT

Experimental studies in building energy usage and environmental analysis are very time consuming and expensive, and require sophisticated sensors and instrumentation techniques. So, there has been great interest in developing Computational Fluid Dynamics (CFD) computer codes to improve building design and HVAC systems. The majority of these CFD programs are based on the solution of Navier-Stokes equations, the energy equation, the mass and concentration equations as well as the transport equations for turbulent velocity and its scale. The aim of this study is to present the advantages, applicability and potentialities of CFD in building design. The advantages and the performance of (two) commercial CFD codes and an academic CFD code develop for this purpose are evaluated. The codes were applied to predict typical situations of the airflow in buildings and the predictions were compared with experimental results.

INTRODUCTION

The advantages, applicability and general potentialities of CFD for use in building design have been adequately established. This paper intends to go further evaluating and comparing the numerical results obtained with two commercial codes and an academic one with experimental data. Therefore, the scope is to present the validation of the numerical results and discuss the potentialities, complexity and user interface of each code. The growing development of new design standards in indoor air quality, thermal comfort and safety, and awareness of the advances in computer-aided engineering design by means of new technological methods in modelling building airflow and related phenomena has raised interest among architects, building services engineers and environmental engineers in the numerical analysis of building design. Since the birth of CFD codes, the specialists in the area acknowledge the advantages of using this kind of software in several applications related to building engineering. However, most of the developments of these codes were focused on the production of general-purpose codes, which could be applied in many practical engineering situations where the thermo-fluid processes' analysis was requested. Derived from this characteristic, most of these codes were very difficult to use. Nowadays, the advances in computer hardware and software has allowed the development of a new generation of CFD codes which are much more user-friendly in terms of mathematical modelling, numerical techniques and presentation of results. Therefore there have been many studies assessing the potential of CFD for use in building design for a wide variety of applications, concerning the evaluation of external and internal flows. Chow (1996), Ladeinde *et al.* (1997), and Martin (1999) listed problems that have benefited or could benefit from the application of CFD techniques. The research of Zhai *et al.* (2001), Bartak *et al.* (2002) and Djuneady *et al.* (2003) tried to combine CFD with the analysis methods of total building energy. The integration of CFD and energy simulation can be done through several different approaches to satisfy the multiple criteria needed in each method. Therefore, coupling strategies could be used to easily determine the particular boundary conditions imposed in the CFD analysis, provide complementary information about the environmental performance of buildings and obtain more reliable and accurate predictions. The state of the art in integrated building simulation can be found in Clarke (1998). Studies in this domain may be grouped into external and internal flow simulations.

Simulations of ***external flows*** are developed to investigate, for instance, wind loading over buildings, pedestrian level winds and pollutant dispersion. The modelling challenges of CFD in building design are attached to the large domains, the complex geometry with a range of physical scales, the uncertain boundary conditions and to a wide range of physical processes. The most important physical phenomena in the externally built environment are the atmospheric boundary layers, the unsteady flow, the separating bluff body flow and dispersion. Smith *et al.* (2002) developed a model of transport and dispersion of airborne contaminants in an urban environment. These phenomena challenge the capabilities of CFD codes because the chemical and biological releases in the atmosphere induce several impacts over several spatial scales like those exposed by Brown (2001). To demonstrate the applicability of a commercial CFD code, Alamdari (1994) developed a simulation of the external flow around offshore platforms. In this case, the airflow analysis is of great importance both in terms of aero and fluid dynamics considerations in relation to the safety design of production platforms. As exposed by Boris *et al.* (2002) the recent terrorist attacks and the subsequent anthrax outbreaks augment the demand of project measures that can protect the inhabitants or users of a building from chemical and biological attacks. Nevertheless, the prediction of wind flow patterns and the dispersal of chemical and biological agents are difficult, because many factors may influence the dispersal of this kind of agent. Tamura *et al.* (2001) made use of CFD techniques applied to wind engineering to compute wind flow around a low-rise building immersed in the turbulent boundary layer. Previous computational results obtained in the wind engineering field have been limited to the cases of uniform flow imposed for flow conditioning, making the estimation of actual wind loading in buildings and structures difficult because there was no information about the turbulence effects on aerodynamic forces.

The major applications of CFD in ***internal flows*** are related with HVAC system performance and indoor air quality improvement, exhaust systems optimisation with the simulation of fire and smoke extraction, and to the prediction of natural ventilation rates. The internal physical factors that difficult the building design modelling are the low Reynolds number flow, together with the dispersion, combustion and radiation and the buoyancy effect. Although all these phenomena involved the use of CFD in building design became an increasingly important analysis tool in the building industry, allowing the replacement or support of model tests and was the answer to the need for cost effective and efficient design. It was used as an analysis tool for non-standard designs and a move towards designing for safety. Hagström *et al.* (2000) describe the different distribution methods of room air conditioning and compares the results for the heat, humidity and contaminant distributions obtained by several authors. The investigations developed by True *et al.* (2002) consist of the numerical prediction of natural ventilation in a cross-ventilated room by means of CFD. A commercial CFD code was used, varying the boundary conditions (pressure boundary limits and inlet opening direction) to define the several simulation models. Voigt (2002) presented a study of a 2D CFD calculation of the flow in the Annex 20 test case (Nielsen (1990)). This one makes use of LDA measurements to obtain the velocity distributions, and the results were compared with recent PIV measurements carried out in a water scale model (Pedersen *et al.* (2001)). Müller (1998) evaluated the performance of different turbulence models in room airflow applications. Experimental measurements in a test room were compared with the numerical calculations. The standard k-ε model, a low Reynolds model and a RSM were used to get an overview about their applicability in two different ventilation systems in order to get momentum and buoyancy driven flow fields. Holmberg *et al.* (2000) investigated the indoor air quality and climate control parameters in a standard single-person office unit by CFD calculations and measurements. In order to achieve the goal, a new ventilation assessment method with control parameters for settling particles was developed and tested. Karimipanah *et al.* (2000) did experimental measurements in a mock-up of a full-size classroom with realistic loads and developed CFD simulations. Four different air distribution systems were tested to predict and measure the air velocity; air temperature; ventilation effectiveness and local mean age of air. In general, the features and benefits of CFD application in building design are the reduced cost, the development of unique models, the analysis of various phenomena, as well as the ability to visualise results, answer some failure analysis questions, determine outcomes and promote faster, better and less expensive designs.

PHYSICAL MODEL AND EXPERIMENT

This paper is supported by the studies developed by Pitarma (1998) to evaluate the cold air circulation in closed rooms and the consequent thermal comfort of the occupants, since both issues should be taken into account during the building design. Two methods were developed in that study, one experimental and another computational (development of CLIMA 3D code), for modelling of non-isothermal turbulent flows in closed rooms, including both natural and forced convection. The evaluation of different air distribution systems and the cold conditions provided into the enclosure domain were carried out. One of the air distribution systems evaluated consists of a closed room with a discharge and return grilles (representative of the inlet and outlet of an air-conditioning system) located on the same wall. The predictions of the temperature and velocities distribution in the enclosure domain are important to evaluate air-conditioner efficiency and the thermal comfort of the occupants. The aim of this study is based on earlier investigation that attempted to evaluate the differences in modelling this particular case test using distinct CFD codes. The CLIMA 3D computational model was validated through comparison of the predictions with experimental data. A schematic representation of the 3D-room test section (1,52 × 0,72 × 0,66 [m]) is shown in Figure 1.

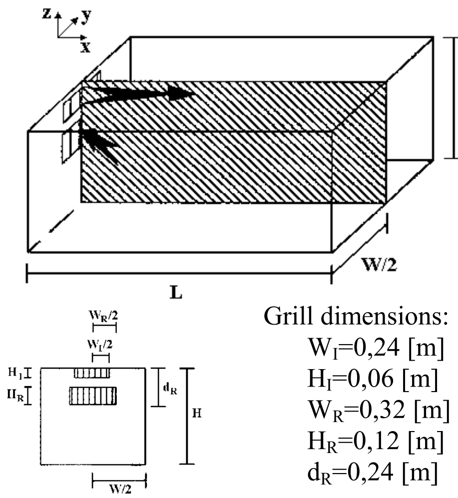

Figure 1 – Geometrical characteristics of the physical model and assumed symmetry.

The experiments have been performed under steady state conditions on a reduced physical model developed by dimensional analysis and similarity. The similarity between reduced physical model and prototype was obtained by dimensional analysis applying the Buckingham's π method. Thirteen dimensionless groups were deduced from seventeen significant variables of the physical phenomenon. The geometrical, cinematic (and dynamic) and thermal similarity between the model and the prototype was obtained through the π's equality. In Table 1 are exposed the scaling factors obtained for the variables.

Table 1 – Scaling factors.

VARIABLE	SCALING FACTOR
Length	2,5
Time	2,5
Temperature	1,0

This experimental model was made in Perspex and a laboratorial air-conditioning unit to simulate an air-conditioning split model was used. The experimental measurements of temperature and velocity were done in several spatial locations using a probe positioning system. The probes used for measurement of air temperature were type T thermocouples. The temperature field readings were accomplished by a data acquisition system. For air velocity measurements the constant temperature hot-wire/film anemometry technique was used. One hot-film omni-directional probe and two hot-wire simple probes were used to take into account the flow direction and the effects of the fluid temperature. An exhaustive description of the experiment facilities, measure instrumentation and the experimental methodology through several approach tests may be found in Pitarma (1998).

COMPUTATIONAL MODELS

The computational models are based on a numerical procedure, which solves in finite-difference form using a control volume technique, the three-dimensional (x_j) time-averaged (t) equations of conservation of mass, momentum, thermal energy and chemical species (Derivation of these equations can be found in specific related literature). These *conservation laws* may each be expressed in terms of partial differential equations. These may be written for a dependent variable (ϕ) in the following general form:

$$\frac{\partial \phi}{\partial t} + \frac{\partial (u_j \phi)}{\partial x_j} - \frac{\partial}{\partial x_j}\left(\Gamma_\phi \frac{\partial \phi}{\partial x_j}\right) = S_\phi$$

Where u_j represents the mean velocity on each cartesian direction, Γ_ϕ represents the exchange coefficient and S_ϕ is the general source term. These governing flow equations are highly non-linear and self-coupled with no direct equation available for static pressure that appears in the momentum equations. Therefore, to obtain the solution of the conservative governing equations it is necessary to use numerical techniques, which consist in their discretization using the finite volume method that convert them into a finite set of numerically solvable algebraic equations, completely described by Patankar (1980). Considering that the flow could be driven by buoyancy in specific zones of the domain, the Buossinesq approximation, which ignores the effect of pressure changes on density, is employed. The buoyancy-driven force is treated as a source term in the momentum equations. The air is considered as an ideal gas, where the equation of state relates the properties of the substance at equilibrium gas phase state accurately. This approach implies some simplifications, without modifying the nature of the physical phenomena. Since most real flows are turbulent, the closure of the equation set was achieved by using the standard *two-equation* k-ε turbulence model. The effect of turbulence was modelled on the three computational models by k-ε turbulence model, which involves the solution of two additional partial differential equations for the turbulent kinetic energy (k) and its dissipation rate (ε). This model is analysed in detail by Launder *et al.* (1974). For the three computational models the standard wall functions were used to bridge the viscous effects and the steep dependent variables gradients close to solid surfaces. The complete description and the implementation details both for the wall functions and turbulence model can be found in Rodi (1980). Due to the symmetry of the physical domain, the computational models had a simplified geometry as shown in Figure 1. The flow domain was discretized into an orthogonal uniform staggered grid comprised of $19 \times 9 \times 11$ control volume (V.C.). A grid independent test was carried out to evaluate the accuracy of the solution. The boundary conditions imposed in the computational models are of common practice in numerical simulations as set out in Table 2.

Table 2 – Boundary conditions (B.C.).

AREA	B.C.	PRESCRIBED PROPERTIES
Discharge grill	Velocity Inlet	U_0=3,1 [m/s] T_0=5 [ºC] $k_0=0{,}0025 \cdot U_0^2$ [m²/s²] $\varepsilon_0=10 \cdot U_0^{1,5}/A_0$ [m²/s³]
Return grill	Pressure outlet	$p_0=1{,}013 \cdot 10^5$ [N/m²] mass balance T_{ext}=25 [ºC]
Enclosure surfaces	Fixed temp.	T_{WEST} = 22,73 [ºC] T_{EAST} = 18,94 [ºC] T_{LOW} = 14,62 [ºC] T_{HIGH} = 10,05 [ºC] T_{NORTH} = 5,48 [ºC] T_{SOUTH} (symmetry plane BC)

For the computational models developed with the commercial codes the boundary conditions implemented by default were used. One of the main differences of the computational models lies on this boundary condition. In the academic code initially developed to simulate the physical phenomenon mentioned, a method of modelling the heat transfer on the outside surface was implemented consisting of the calculation of the inner and outer convection heat transfer coefficient. Then, using the thermal conductivity and thickness of the several materials that compose the walls, the overall heat transfer coefficient was obtained. This coefficient is used in each iteration to calculate the heat flux along the wall through Newton's Law of cooling. Thus, the heat flux imposed may vary from this code to the commercial ones, where a fixed heat flux boundary condition was imposed at the walls. It is necessary highlight that the code development was very time consuming. This was one of the reasons why this method was not implemented on commercial codes computational models, since one of their major advantages is the easiness and fastness in obtaining numerical previsions if the model is based on the default modelling tools. In addition, this method of modelling the heat transfer on the outside surface of the walls could not be applied with the commercial codes because was not possible with the current non-recompilable version of the PHOENICS® code. With the FLUENT® code it could be done developing a set of user-defined functions, but it will increase the computational model development time and reduce the comparative elements between the commercial codes. Therefore, a fixed heat flux boundary condition was imposed at the walls available by default on the two commercial codes.

The scheme used to discretize the convective terms in the general transport equations for all the dependent variables varies from each computational model as exposed in Table 3. Details about the discretization schemes by control volume method can be found in Spalding (1972).

Table 3 – Discretization scheme.

MODEL	SCHEME	NOTES
CLIMA 3D	Hybrid (HDS)	Programmed
PHOENICS®	Hybrid (HDS)	Default
FLUENT®	1st order upwind (UDS)	HDS is not available

The method for pressure-velocity coupling, by a global procedure of numerical integration of the flow domain equations, as presented by Patankar (1980) also differs from each computational model as presented in Table 4.

Table 4 – Pressure-velocity coupling method.

MODEL	METHOD	NOTES
CLIMA 3D	SIMPLE	Programmed
PHOENICS®	SIMPLEST	Method available
FLUENT®	SIMPLE	Also available: SIMPLEC PISO

The algebraic equations are solved by an iterative procedure, which varies from each code as can be seen in Table 5.

Table 5 – Solution method.

MODEL	SOLUTION METHOD	NOTES
CLIMA 3D	line-by-line	Programmed
PHOENICS®	TDMA SARAH	Default
FLUENT®	Gauss-Seidel AGM	Default

To reduce the high variation of the dependent variables during the iterative procedure of calculation, the linear relaxation is used until a prescribed convergence criterion ($\lambda=5 \cdot 10^{-3}$) based on residuals analysis is met. In Table 6 the values of the linear relaxation factors for the several scalars are exposed and vectorial variables used for all computational models.

Table 6 – Linear relaxation factors.

ϕ	p	u_j	k	ε	ρ	H	T	m_v
α_ϕ	0,9	0,4	0,4	0,4	0,3	0,9	0,9	0,9

CODES DESCRIPTION

As with other CFD codes, the academic one (CLIMA 3D) relies on the statement that all thermo-fluid problems are governed by the above mentioned principles of conservation. All the numerical techniques described for the solution of the exposed mathematical models were programmed in FORTRAN. The next step will be to present and compare the generic characteristics of each commercial code. It is important to relate that the non-recompilable, version 3.1 of PHOENICS® code, acquired at 1997, with an academic and perpetual license in a hardware and software platform: PC type with Windows NT operative system was used. In relation to FLUENT® code, version 6.0 recompilable, available from 2001, with an annual and academic license for hardware and software platform: PC type with Windows NT operative system was used. At first sight, the difference most significant between the codes consists of its structure. While PHOENICS® code is composed of three distinct linked functionalities (pre-processing, solver and post processing), the code FLUENT® only incorporates the last two. In PHOENICS® code, the pre-processing consists in the problem definition, which involves the specification of the objects geometry and the intervening spaces, the thermodynamic and transport properties and other types of fluid and involved solid properties, as well as the selection of the mathematical models that describes the diverse physical phenomena. In addition, the orthogonal computational mesh is prescribed, allowing meshes to be formed (orthogonal or BFC) through compatible commercial external software packages, a situation that also occurs with FLUENT® code. This last one does not posses an incorporated pre-processor, but it makes use of GAMBIT® software, where the geometry is created through the definition of vertices, edges or volumes, with diverse degrees of complexity in 2D or 3D. In addition, it allows the creation of the respective structured or non-structured mesh, and the definition of boundary conditions type. Both the geometry and mesh could be imported from different external software. Comparing potentialities of pre-processing, structured mesh generation is much more simple in the first code mentioned since the limits of created objects in the geometry define boundary regions of the computational mesh. However, the mesh generation software that is incorporated in the FLUENT® code allows the mesh generation through various schemes, which could be beneficial in function of the physical phenomena which should be studied in a given geometry. Therefore it is indispensable to generate a computational mesh of great quality to obtain success in the CFD simulations. In PHOENICS® code, the solver solves iteratively the equations formulated in the finite differences (control volumes) form, discretized through one of the 1st or 2nd order available schemes. In FLUENT® code the geometry/mesh is imported and the mathematical models are defined that describe the physical phenomena. In addition, it is carried the definition of the fluid and material properties, the operative conditions and the boundary conditions specifications. In the solver are available diverse discretization schemes for the differential equations, distinct methods of pressure-velocity coupling, the relaxation factors, the initial values and the type of solution monitorization. The numerical solution method is also different as presented in Table 5, and both codes have convergence accelerator algorithms. PHOENICS® has an algorithm of automatic adjustment of the relaxation factors (SARAH), while the FLUENT® code has an algebraic method of mesh refinement (AGM). Relatively to the solvers, the codes can be considered at an equality situation because some of the possibilities are identical. However, each one contains distinct mathematical models, discretization schemes and other functionalities. The two codes incorporate in the source program the post processing functionalities. However, the FLUENT® code has a higher visualisation capacity, has an easier results (local values) management and acquisition due to the innumerable available options. For each code, it can be found in respective user manual details concerning all the specification issues.

RESULTS ANALYSIS

The convergence of the numerical solution is accomplished when the residual error of the several dependent variables goes under 0,5%. In Table 7 is shown the number of iterations needed by each code to obtain the converged solution.

Table 7 – Number of iterations of the solution.

COMPUTATIONAL MODEL	ITERATIONS
CLIMA 3D	946
PHOENICS®	1059
FLUENT®	1168

Although the difference between the speed convergence is not significant, it could be associated to the numerical method of solution. At this point, the computational model developed with the PHOENICS® code presents better performance. To evaluate the simulation capabilities of codes and to establish the validation of the numerical results, below is presented the comparison of experimental and numerical results of air velocity and temperature. Since a hot-film omni-directional probe in the experimental measurements was used, the comparison between the experimental air velocity and numerical results obtained with the three codes is done with the velocity magnitude. In Figure 2 several velocities profiles for different planes intersections are presented. In all the comparative profiles of the numerical results obtained with the CLIMA 3D, PHOENICS® and FLUENT® are represented by ×, ◆, ▲ respectively. The experimental data are represented by ○.

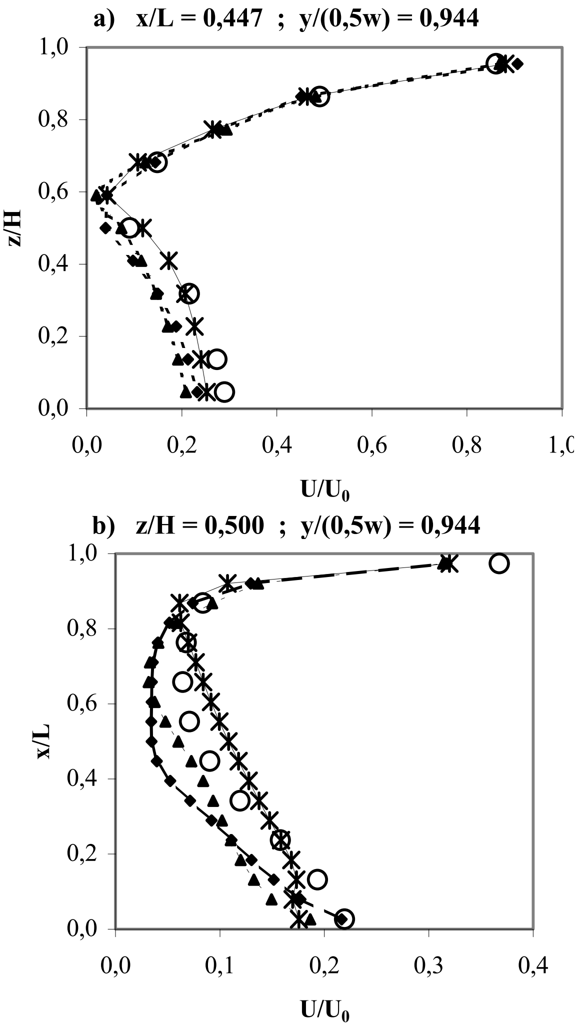

Figure 2 — Velocity profiles.

The comparison between the experimental data and the different velocities numerical profiles shows a similar trend. The numerical results closer to the experimental data are those that had been obtained with the academic code CLIMA 3D. The numerical velocities predictions obtained with the codes PHOENICS® and FLUENT® at some points are closer to the experimental data than those that had been obtained with CLIMA 3D, but globally the numerical results obtained with those commercial codes sub– or over–predict the phenomenon. Comparing only the predictions obtained with the two commercial codes, although the different trends of the velocity profiles, the simulation capabilities are similar. With the same representation as before, in Figure 3 several temperature profiles for different planes intersections are presented.

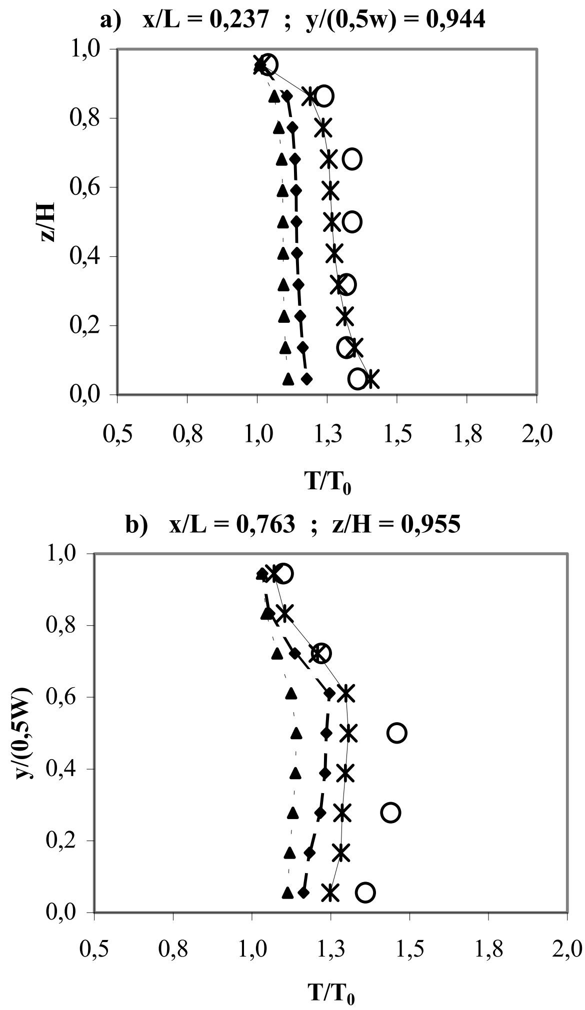

Figure 3 — Temperature profiles.

The main conclusions of the comparison between the experimental data and the different temperature numerical profiles are: the academic CLIMA 3D code is that which predicts more accurately the temperature profiles within the closed room. The numerical results obtained with the two commercial codes are very similar, and both sub-predict the temperature profiles. The numerical predictions for temperature obtained with the code FLUENT® are worse than those obtained with the code PHOENICS®. The code FLUENT® sub-predicts the temperature profile for all the domain points. The comparison between experiment measurements and the numerical results of temperature obtained with the two commercial codes shows a good qualitative agreement, but not for the quantitative values. This difference could be attributed to the different boundary conditions imposed at the walls. In Table 8 the mean absolute (U [m/s] ; T [ºC]) and relative errors for the velocities and temperature predictions is presented.

Table 8 – Mean absolute and relative errors.

ERROR	CLIMA 3D	PHOENICS®	FLUENT®
$\|U_{num}^{*}-U_{exp}^{*}\|$	0,032	0,043	0,043
$\|U_{num}-U_{exp}\|$ [m/s]	0,100	0,132	0,134
$\|T_{num}^{*}-T_{exp}^{*}\|$	0,101	0,200	0,250
$\|T_{num}-T_{exp}\|$ [ºC]	0,507	1,002	1,248

The evaluation of the different profiles shows general, qualitative and, at some points, quantitative agreement between the simulations and the measurements. The comparison between the codes shows quantitative deviations from each other, at some points with considerable value. These discrepancies could be the result of the mathematical and numerical models used by the codes, and especially to the internal code definitions of prescribed boundary conditions. Besides, it is important to take into account that the experimental measurements are not exempt of errors. However, comparing the experimental data with the numerical results obtained with the different codes, the most realistic numerical predictions were obtained with the academic CLIMA 3D code. The comparison between only the two commercial codes shows that the PHOENICS® code better predicts the physical properties distributions than does the FLUENT® code.

CONCLUSIONS

The comparison between numerical and experimental results evidences much more agreement for the velocities than for the temperatures. The velocities comparison presents some minor quantitative discrepancies while the temperature deviations are high due to the different method of modelling the heat transfer on the outside surface of the walls. Thus, in general some effectiveness could be attributed to the computational models developed despite the code that is used. Generally, it is verified that both commercial CFD codes make use of the same specifications related with the mathematical and numerical models. Even so, each one possesses by default several different mathematical models of physical phenomena, numerical techniques and validation cases. Relative to these items, the code PHOENICS® possesses a greater amount of mathematical models and validation cases. The codes present differences in the structure and methodology of calculation that distinguish them by the easiness of use as a function of the versatility and simplicity of the user-program interface. In this field, the FLUENT® code possesses greater potentialities. This last one, incorporating different mathematical models and numerical techniques for a wider range of physical phenomena, possesses a higher solution convergence speed as the complexity of the phenomena increases and an easier user interface. The PHOENICS® code presents greater easiness on the construction of structured computational meshes. Evaluating the codes by the numerical results for the tested practical case, the mean errors of the numerical predictions in relation to the experimental values is lower on the simulation performed with the PHOENICS® code, demonstrating its simulation capacities. The elaboration of an isolated code for the prediction of a physical phenomenon is complex and time consuming which justifies the preferential use of commercial codes. However, the numerical results obtained with the academic code developed for the simulation of this specific type of physical problem, has is much closer to the experimental data. As previously mentioned, it is necessary to point out the discrepancy between the acquisition dates of the commercial codes, and so, between the tested versions and from the development of the academic one. By this statement, it can be stated that the codes are practically in an equal situation to the simulation of these kind of physical phenomena. The errors obtained with all the computational models should be attributed to several simplifications, as well as to mathematical and numerical models and fundamentally to the considered boundary conditions. The main intention of this work is to investigate the difference in modelling physical phenomena with academic self programmed and commercial codes despite the errors of the experimental in the measurements. These commercial codes, by its easiness, simplicity and versatility of use, constitute a powerful tool for the simulation of the most diverse engineering physical phenomena. However, the numerical predictions obtained by these codes are associated with a degree of uncertainty, resulting from the definition of the problem, to the specifications and subsequent simplifications of the mathematical and numerical models considered for the description of the physical phenomenon. Thus, the user experience in CFD is still fundamental and determinative to guarantee the realism of the numerical predictions.

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