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# Evaluation of CFD codes by comparison of numerical predictions of an air-conditioned room case study

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## Abstract

Nowadays, the advances in computer hardware and software allowed the development of a new generation of Computational Fluid Dynamics (CFD) codes which are much more user-friendly in terms of mathematical modelling, numerical techniques and presentation of results. The aim of this study is to present the evaluation and comparison between the numerical results obtained with two commercial codes, an academic one and experimental data for a of a typical ventilation case study. Therefore, the scope includes the validation of the numerical results and discussion of the potentialities, complexity and user interface of each code.

*Keywords: computational fluid dynamics, commercial codes, FLUENT<sup>®</sup>, CFX<sup>®</sup>, ventilation.*

## 1 Introduction

There have been many studies assessing the potential of CFD for use in engineering for a wide variety of applications, concerning the evaluation of external and internal flows. In addition, we notice an increasing trend in the usage of computational simulation, through the numerical solution of the conservation equations as a support tool to the development of engineering projects. Chow [1], Ladeinde *et al.* [2], and Martin [3] listed problems that have benefited or could benefit from the application of CFD techniques. The CFD

commercial codes have now come to represent an effective method of study by its higher simplicity of use, graphical versatility and capabilities. However, being not open enough to the programmer incites some controversy relatively to its true potential. This study is an extension of the work developed by Gaspar *et al.* [4] with the following objectives: (1) evaluate the general capabilities of two of the most widely used CFD commercial codes (FLUENT<sup>®</sup> and CFX<sup>®</sup>), (2) compare their numerical predictions with those obtained with an academic code and (3) validate the numerical predictions obtained with the different CFD codes comparing them with experimental results. The case study of the codes' application consists in a typical situation of an air-conditioned room to predict three-dimensional turbulent airflow with thermal buoyant effects and air temperature distribution. The validation of the mathematical model was done comparing the numerical predictions with the experimental data for a 1/2.5 laboratory scale model obtained by dimensional analysis, designed to provide similarity with a prototype. The numerical results suggest that this modelling technique allows the study of a wide range of problems, with simplicity and low costs and it is highly desirable as a preliminary assessment of indoor environmental conditions during the design phase. Effective optimization of building designs requires an integrated interdisciplinary approach to the planning of buildings technical systems. This means generally a simultaneous design work performed by architects, civil engineers and engineers specialized in heating, ventilating, air conditioning (HVAC) and other building systems with the objectives to plan, to build and to operate a both energetically and functionally optimized building while respecting all required comfort and safety criteria. The research performed by [5, 6, 7] tried to combine CFD with whole building energy analysis methods. The state of the art in integrated building simulation can found in Clarke [8]. The major applications of CFD in this field are related with HVAC system performance and indoor air quality improvement. In this field, several numerical studies have been developed with the commercial codes under evaluation. These numerical models allowed the prediction and evaluation of the airflow and heat transfer, which are references to the present study. Among them stands out the studies [9, 10, 11] that used the code FLUENT<sup>®</sup> and [12, 13] which applied the code CFX<sup>®</sup>. 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 the ability to visualise results, answer some failure analysis questions, determines outcomes and promotes faster, better and less expensive designs.

## **2 Experimental model**

The case study of the codes' application consists in a typical situation of an air-conditioned room to predict three-dimensional turbulent airflow with thermal buoyancy effects and air temperature distribution supported in the studies developed by Pitarma [14]. These works concerned the evaluation of 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 the code CLIMA 3D), for modelling of non-isothermal turbulent flows in closed rooms, including both natural and forced convection. The air distribution system consists in a discharge and return grilles (representative of the inlet and outlet of an air-conditioning system) located on the same wall of the closed room. The CLIMA 3D computational model was validated through comparison of the predictions with experimental data. The experimental tests had 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  $\pi$  method. An exhaustive description of the experiment facilities, measurement instrumentation and experimental methodology tests can be found in Pitarma [14].

### **3 Mathematical and numerical model**

#### **3.1 Mathematical Model**

As other CFD codes, the academic one (CLIMA 3D) relies on the statement that all thermo-fluid problems are governed by the principles of conservation of mass, momentum, thermal energy and chemical species. These *conservation laws* may each be expressed in terms of partial differential equations (Derivation of these equations can be found in specific related literature). Considering that the flow could be driven by buoyancy in specific zones of the domain, the Boussinesq approximation is employed. The buoyancy-driven force is treated as a source term in the momentum equations. The air is considered as an ideal gas. Since most real flows are turbulent, the closure of the equation set was achieved by using the standard *two-equation* k- $\epsilon$  turbulence model, analysed in detail by Launder *et al.* [15]. 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 detail both for the wall functions and turbulence model can be found in Rodi [16]. 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, the solution of the conservative governing equations is obtained using numerical techniques.

#### **3.2 Numerical model**

The computational model consists on a numerical procedure, which consists in the discretisation of the conservative equations by the finite volume method into a finite set of numerically solvable algebraic equations representative of the mentioned three-dimensional time-averaged conservative governing equations as described by Patankar [17]. Due to the symmetry of the physical domain, the computational models had a simplified geometry as shown in Figure 1. The flow domain was discretised into an structured grid with  $19 \times 9 \times 11$  control volume [  $(\Delta x, \Delta y, \Delta z) = (0.08, 0.06, 0.04)$  [m] ].

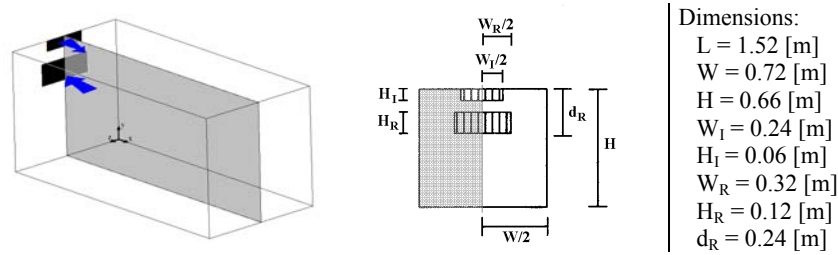


Figure 1. Geometrical characteristics of the computational model.

The boundary conditions imposed in the computational models are of common practice in numerical simulations as present in Table 1.

Table 1: Boundary conditions.

Area	Boundary Condition	Prescribed properties
Discharge grill	Velocity inlet	$U_0=3.1$ [m/s] $T_0=278.15$ [K] $k_0=0.0025U_0^2$ [m <sup>2</sup> /s <sup>2</sup> ] $\epsilon_0=10U_0^{1.5}/A_0$ [m <sup>2</sup> /s <sup>3</sup> ]
Return grill	Pressure outlet	$p_0=1.013 \cdot 10^5$ [N/m <sup>2</sup> ] Mass balance $T_{ext}=298.15$ [°C]
Enclosure surfaces	Fixed heat flux	$q''_{WEST} = 5.4$ [W/m <sup>2</sup> ] $q''_{EAST} = 4.5$ [W/m <sup>2</sup> ] $q''_{LOW} = 8$ [W/m <sup>2</sup> ] $q''_{HIGH} = 5.5$ [W/m <sup>2</sup> ] $q''_{SOUTH} = 5.5$ [W/m <sup>2</sup> ]

One of the most significant differences of the computational models lies on the boundary condition. In the academic code initially developed to simulate the physical phenomenon mentioned, the method of modelling the heat transfer was based in the calculation of the inner and outer convection heat transfer coefficients. 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 (available by default) was imposed at the walls. It is necessary to highlight that the development of the academic code 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. But these two codes also allow modelling simultaneously the physical phenomenons underlie the heat transfer: conjugate heat transfer (conduction and convection) and thermal radiation. In this last mode of heat transfer each code contain different mathematical models. The

scheme used to discretise the convective terms in the general transport equations for all the dependent variables varies from the academic code that used the Hybrid scheme, to the commercial codes that used the Upwind scheme. Details about the discretisation schemes by control volume method can be found in Spalding [18]. The method for pressure-velocity coupling, by a global procedure of numerical integration of the flow domain equations differs from each computational model. The academic and the FLUENT<sup>®</sup> code used the SIMPLE method, as presented by Patankar [17] while the code CFX<sup>®</sup> uses a Rhie-Chow [19] interpolation scheme. The algebraic equations are solved by an iterative procedure exposed in Table 2.

Table 2: Solution method.

Computational model	Solution method	Additional notes
CLIMA 3D	line-by-line	Programmed
CFX <sup>®</sup>	ILU (with MG)	Default
FLUENT <sup>®</sup>	Gauss-Seidel (with 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 ( $\lambda = 5 \times 10^{-3}$ ) based on residuals analysis is met. In Table 3 are exposed the values of the linear relaxation factors for the several scalars and vectorial variables used for all computational models.

Table 3: Relaxation factors.

$\phi$	p	$u_j$	k	$\varepsilon$	$\rho$	H	T	$m_v$
$\alpha_\phi$	0.9	0.4	0.4	0.4	0.3	0.9	0.9	0.9

All the described numerical techniques for the solution of the exposed mathematical models had been programmed in FORTRAN for the development of the academic code (CLIMA 3D).

#### 4 Commercial codes description

Next it will be presented and compared the main generic characteristics of each commercial code. It is important to state that was used the version 5.6 of the code CFX<sup>®</sup>, supplied in 2003, with an extended capabilities trial license. In relation to the code FLUENT<sup>®</sup>, it was used the version 6.0, available from 2001, with an annual and academic license. These licenses were produced for a hardware and software platform: PC type with Windows NT operative system. At first sight, the difference most significant between the codes consists of its structure. While code CFX<sup>®</sup> is composed of four distinct linked modules (geometry and mesh builder, pre-processor, solver and post-processor), the code FLUENT<sup>®</sup> only incorporates the last three. This last one doesn't has an incorporated geometry and mesh builder, but it makes use of the integrated

software GAMBIT<sup>®</sup>, where the geometry is created through the definition of vertices, edges and volumes, with diverse degrees of complexity in 2D or 3D. In addition, this software allows the creation of the respective structured or non-structured mesh, and the definition of boundary conditions type. The geometry creation and the mesh generation procedure are similar in the CFX<sup>®</sup> code, but this one is more user-friendlier. While in software GAMBIT<sup>®</sup> are defined the location and type of the boundary conditions, for CFX<sup>®</sup> are only defined their location. Both mesh builders within the codes allow the generation of non-structured mesh through various schemes, which could be beneficial in function of the physical phenomena that should be studied in a given geometry. Until the present day and as the authors still do not handle all capacities of mesh generation included in code CFX<sup>®</sup>, the comparison of the geometry and mesh builder is advantageous with the code FLUENT<sup>®</sup>. Although the code CFX<sup>®</sup> possesses greater easiness of use, the software linked to the other commercial code enjoy of a simple method to generate structured meshes and an easy manner for evaluating the mesh quality. This last characteristic is essential to generate a computational mesh with quality to promote a successfully simulation. For both codes, the problem is defined in the pre-processor, 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. Also, are defined the numerical techniques to solve iteratively the equations formulated in the finite differences (control volume) form, discretised through one of the 1<sup>st</sup> or higher order available schemes. The geometry/mesh is imported and are defined the mathematical models that describe the physical phenomena. In addition, it is carried out the definition of the fluid and material properties, the operative conditions and the boundary conditions specifications (While in code FLUENT<sup>®</sup> it is only needed to specify the value, in code CFX<sup>®</sup> it is necessary to specify the type and value). In each one are available various discretisation schemes for the differential equations; distinct methods of pressure-velocity coupling (only for code FLUENT<sup>®</sup>, who has available: SIMPLE, SIMPLEC and PISO); relaxation methods; values initialization procedures and the type of solution monitorization. The numerical solution method is also different as presented in Table 2, and both commercial codes have convergence accelerator algorithms based in an algebraic method of mesh refinement. Each one of the codes gave more emphasis to the mathematical models of specific physical phenomena. Thus, depending on the physical phenomena that it is intended to simulate should be given higher superiority to one of the codes. In the personal opinion of the authors, due to the deepest knowledge of code FLUENT<sup>®</sup> and as the experience in the code CFX<sup>®</sup> is reduced in function of its recent acquisition, the first code has greater capabilities in the modelation of more common physical phenomena and for these cases the variety of mathematical models and numerical procedures are superior. They can't be compared since each one contains distinct mathematical models, discretisation schemes and other functionalities. Relatively to the solvers, the codes can be considered at an equality situation because some of the possibilities

are identical. During the iterative procedure both present the evolution of the normalized residuals. The two codes incorporate in the source program the post-processor functionalities. These functionalities concern the profiles predictions visualisation capacities and have a friendly GUI and local values achievement due to the innumerable available options. For each code, it can be found in respective user manual details concerning all the specification issues.

## 5 Numerical predictions evaluation

The convergence of the numerical solution is accomplished when the residual error of the several dependent variables goes under 0.5%. The difference between the convergences of the solutions wasn't significant and could be associated to the numerical method of solution. 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 are presented several velocities profiles for different planes intersections.

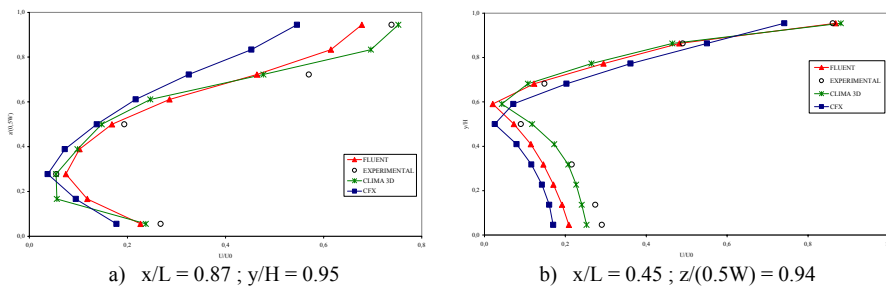


Figure 2. Adimensional velocity magnitude profile.

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 code FLUENT<sup>®</sup> 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 code FLUENT<sup>®</sup> predicts with greater precision the phenomenon than the code CFX<sup>®</sup>, which sub-predict the velocity for all the domain points compared. With the same representation as before, in Figure 3 are presented several temperature profiles for different planes intersections.



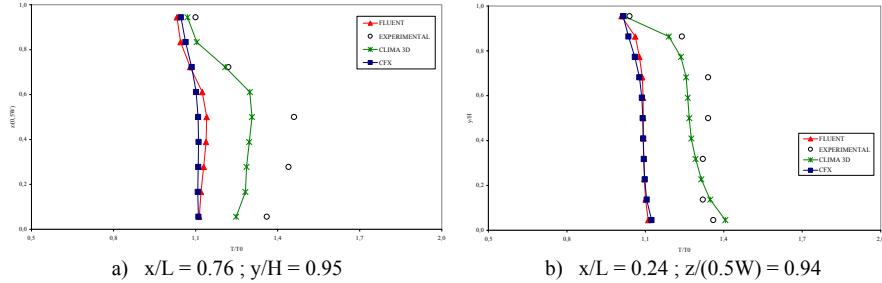


Figure 3. Adimensional temperature profile.

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 comparison between experiment measurements and the numerical results of temperature obtained with the two commercial codes shows some qualitative agreement, but not for the quantitative values. This difference is attributed to the different boundary conditions imposed at the walls. In Table 4 the mean absolute and relative errors for the velocities and temperature predictions are presented.

Table 4: Mean absolute and relative errors.

Errors	CLIMA 3D	FLUENT <sup>®</sup>	CFX <sup>®</sup>
$ U_{num} - U_{exp}  /  U_{exp} $	0.09	0.13	0.28
$ U_{num} - U_{exp} $ [m/s]	0.03	0.04	0.09
$ T_{num} - T_{exp}  /  T_{exp} $	0.06	0.32	0.31
$ T_{num} - T_{exp} $ [K]	17.54	87.98	87.99

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, especially for the temperature. 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 code CLIMA 3D. The comparison between only the two commercial codes shows that the code FLUENT<sup>®</sup> code predicts better the physical properties distributions than does the code CFX<sup>®</sup>.

## 6 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 large due to the different method of modelling the heat transfer. 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 has by default several different mathematical models of physical phenomena, numerical techniques and validation cases. Relative to these items, the code FLUENT<sup>®</sup> includes a greater amount of mathematical models and numerical techniques for a wider range of physical phenomena. 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 code CFX<sup>®</sup> hold greater capabilities, most due to the geometry and mesh generator. This last one has a higher speed convergence of the solution as the complexity of the phenomena increases and an easier user interface. Both commercial codes present some difficulties on the construction of structured computational meshes. Evaluating the commercial codes by the numerical results for the tested practical case, the mean errors of the numerical predictions in relation to the experimental values are lower on the simulation performed with the code FLUENT<sup>®</sup>, 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, are much closer to the experimental data. 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 was to research the difference in modelling physical phenomena with academic self-programmed and commercial codes despite the errors of the experimental measurements. These commercial codes, by its easiness, simplicity and versatility of use, are a powerful tool for the simulation of the most distinct engineering physical phenomena but it is still fundamental and determinative the user experience in CFD to guarantee the realism of the numerical predictions.

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