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Validation of external BES-CFD coupling by inter-model comparison

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ABSTRACT
Conflation of computational fluid dynamics (CFD) and building energy simulation (BES) has been used in recent years in order to improve the estimation of surface coefficients for studies on thermal comfort, mold growth and other performance aspects of a building. BES can provide more realistic boundary conditions for CFD, while CFD can provide higher resolution modelling of flow patterns within air volumes and convective heat transfer coefficients (CHTC) for BES. BES and CFD can be internally or externally coupled. Internal coupling is the traditional way of expanding software by which the code is expanded by adding new modules and it entails a lot of effort in terms of debugging, maintenance etc. On the other hand, developing and maintaining one single package to include all geometrical and physical domains is expensive and includes: the background research, development of a pilot program, improvement of the software etc. (Maver and Ellis, 1982).

A solution which has been adopted recently is run-time external coupling of distributed applications. By this approach the existing numerical packages for specific geometrical or physical domains work together and exchange data at predefined or calculated time steps. It has been recognized and justified that the final distributed simulation environment is more flexible, practical and powerful than the sum of the individual software programs (Hensen, 2002).

In the past, there were some attempts to validate external coupling between ESP-r (BES) and FLUENT (CFD) by using experimental data and inter-model comparisons for room air temperature and surface coefficients (Djunaedy, 2005). Because of uncertainties associated with experimental data and the discrepancies observed in the other validation technique for CHTC, a new inter-model comparison procedure is proposed. In this inter-model comparison, a CFD conjugate heat transfer simulation is used to assess the performance of external BES-CFD coupling, focusing on the validation of the external coupling for average air temperature, surface temperature and CHTC. The conjugate heat transfer model performs the coupled simulation of solid and fluid domain completely within CFD. In BES-CFD coupling,
CFD is only applied for the fluid domain and then the transfer coefficients are passed to BES which is mainly responsible for the solid domain.

This paper is structured as follows. First the methodology and the model description are explained. Then the different steps necessary for the conjugate heat transfer simulations for a cubic cavity in CFD are described. Next, an external BES-CFD coupling for the same case is presented. After, the response of the BES-CFD model and of the conjugate heat transfer model to a 20 K step change in surface temperature are compared to each other. Finally, a discussion and the conclusions of the work are presented.

2. METHODOLOGY

Figure 1 shows a schematic view of the inter-model comparison procedure. At the left hand side the external BES-CFD coupling prototype is shown. As it can be seen in this figure, the loose coupling strategy has been applied. In this strategy, two or more sets of equations are solved separately and exchange data at each predefined or calculated time step. The internal surface temperatures which are calculated by BES are passed to CFD at each time step. Then the calculated convective heat transfer coefficients (CHTC) from the converged CFD solution is passed to BES for the next time step calculation. There is no iteration process between the two programs to get an agreement on the values at each time step.

At the right hand side of Figure 1, the fluid and solid domain which are solved separately in the prototype, are both modeled and solved within CFD including the radiation model to form what is called the conjugate heat transfer model or the CFD stand-alone model in this paper. In other words, the boundary condition of the CFD model in the prototype is moved from the inside to the outside of the walls, and thus forming a single set of equations to be solved at each time step (i.e. strong coupling).

In order to perform the inter-model comparison, an effort has been put into making all the CFD settings the same in the prototype and in the CFD stand-alone simulations. They both use also the same model and boundary conditions which are explained in the following sections.

As indicated in Figure 1, there are two sets of results from the prototype and one set of result from the CFD stand-alone which will be compared in the last section of the paper.

3. DESCRIPTION OF THE MODEL

The geometry of the model is inspired from (Tian and Karayiannis, 2000) in which experimental data for natural convection flow in an air filled cavity has been presented. These experimental data are used to validate one of the steps in developing the CFD stand-alone model which will be explained in the next section. For reducing the computational time, the length of the cavity was chosen 75 cm. Therefore the volume of the cavity is half of that of the cavity used in the mentioned paper.

![Figure 2: Geometry of the cavity. Wall thickness = 8 (cm).](image)

The boundary conditions are applied at the exterior wall surfaces. As indicated in Figure 2, the south wall is kept at 30°C and a 20°C step change at the surface temperature of the north wall is applied. The rest of the walls are
adiabatic. The construction used for all walls is 8 (cm) concrete with the thermo-physical properties stated in Table 1.

Table 1: Thermal properties of concrete

<table>
<thead>
<tr>
<th>Property</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>Thermal conductivity [W m⁻¹°C⁻¹]</td>
<td>1.4</td>
</tr>
<tr>
<td>Specific heat capacity [kJ/kg °C⁻¹]</td>
<td>653</td>
</tr>
<tr>
<td>Density [kg m⁻³]</td>
<td>2100</td>
</tr>
</tbody>
</table>

4. CFD SIMULATIONS

The CFD commercial software FLUENT 6.3.26 was selected to be used for all the simulations throughout this study.

In order to obtain an optimum 3D grid for the CFD stand-alone simulation, three major steps had to be done:

First, a set of 2D simulations of just the cavity with zero wall thickness were performed and validated by experimental data provided by (Tian and Karayiannis, 2000). They measured the temperature and velocity field in an air filled cavity with the width and height of 75 (cm) and a depth of 150 (cm). Grid sensitivity analysis on the 2D simulations was performed before moving to 3D simulation.

Second, based on the optimum 2D grid and its validation, the maximum time step and the minimum number of iteration per time step required for the transient simulation was obtained through sensitivity analysis.

Finally, based on the settings obtained in the previous steps, the 3D grid including the walls was build for the final conjugate heat transfer simulation.

4.1. 2D simulations

2D CFD simulations were performed on a non-uniform rectangular grid. Four different grid sizes of 30 × 30, 50 × 50, 100 × 100 and 150 × 150 were tested. The residuals, variables and $y^+$ value were monitored and checked. The k-ω model was chosen for modelling the turbulence and enhanced wall treatment was applied. Boussinesq approximation was considered while solving the momentum equation. To account for the radiation exchange between surfaces in the cavity, the S2S radiation model available in FLUENT was chosen. The corresponding Rayleigh number in the experiment was equal to $1.58 \times 10^9$ which is the indication of a turbulent natural convection flow.

Figure 3 shows a typical result obtained from the finest mesh which is in good agreement with experimental data (Figure 4). In these figures, X and Y are dimensionless coordinates and L is the width of the cavity. The same results were obtained from 30 × 30 (coarsest) grid which conforms with the work done by (Omri and Galanis, 2007). Therefore the computational domain with the grid size of 30 × 30 was chosen for the next step. Note that the $y^+$ value was less than unity for this case.

Figure 3: Temperature distribution at different heights obtained from 2D simulations.

Figure 4: Temperature distribution measured by (Tian and Karayiannis, 2000).
4.2. Best settings for 2D transient simulation

Having the grid ready from the previous step, a set of transient CFD simulations were performed in order to investigate the sensitivity of the residuals and the variables to the size of time step and the number of iterations required per time step. The boundary conditions are the same as described in section 3. Time steps larger than 2 seconds caused some oscillation in the prediction of temperature distribution and also in convergence. In Figure 5, the difference between the predicted average CHTC on the south wall and that of the reference case can be observed. The reference case is the one with 100 iterations per time step which leads to residuals lower than $10^{-6}$.

As it can be seen from the Figure 5, the difference between the reference and the case with 10 iterations per time step is not remarkable. Furthermore, since the primary focus of this study is the validation of the coupling, the accuracy of the case with 10 iterations per time steps lies within an acceptable range for this purpose.

4.3. 3D simulation

The 3D grid including the walls (solid domain) was made based on the previous steps (Figure 6). In ESP-r, the 1D heat conduction equation is solved by the control volume method while the heat transfer mechanism in the solid domain in the present CFD model is 3D. In order to make this 3D effect less important, the corners of the cube were eliminated. The CFD simulation was run with the boundary conditions and the settings described in sections 2 and 3, respectively. The average cavity temperature, surface temperatures and convective heat transfer coefficients were extracted. These results are compared to those of BES-CFD coupling in section 6.

5. BES-CFD COUPLING

A loose coupling strategy was implemented between an open source building performance simulation software (ESP-r) and the commercial CFD package FLUENT. The 3D grid obtained in CFD stand-alone section excluding the walls was used to calculate the fluid domain (Figure 7).

![Figure 6: 3D computational grid for the CFD stand-alone model.](image)

![Figure 7: 3D computational grid for BES-CFD coupling.](image)

In Figure 8, the variation of Rayleigh number versus time in the cavity has been plotted after the temperature jump at the exterior north surface. Due to the presence of turbulence in the cavity, the coupling mechanism shown in Figure 9 was considered. In this coupling, at each time step the internal surface temperatures are extracted from BES and passed to FLUENT. In FLUENT, we first perform a steady state simulation with a one-order-lower Rayleigh
number and then a transient simulation with the real Rayleigh number. Then the CHTCs calculated by FLUENT are passed to ESP-r for the next time step.

The coupling was performed for one hour with the time step equal to 1 minute. Running the coupling with the same time step as CFD stand-alone would increase the computational time dramatically to 600 days which is not efficient. Then the coupling was terminated and ESP-r was run for more 2 hours in a stand-alone mode. The results are compared and presented in the next section.

6. RESULTS AND DISCUSSION

In order to evaluate the performance of the external coupling, the results from section 4 and 5 are presented and compared to each other. The average cavity temperature from the BES-CFD coupling is compared with that of CFD stand-alone and BES stand-alone in Figure 10. During the first hour of simulation the inter-model comparison of average temperature are in good agreement. At the end of the first hour, CFD is switched off and BES is used to predict the average temperature. While using BES-stand-alone, the empirical correlation equation for internal CHTC (Alamdari and Hammond, 1982) is applied. As it can be observed from Figure 10, there is 1°C difference between the results for this simple geometry while using empirical correlation.

![Figure 8: Rayleigh number variation in the co-simulation.](image)

![Figure 9: Coupling mechanism for the BES-CFD prototype.](image)

![Figure 10: Evolution of average temperature in different cases.](image)

![Figure 11: Comparison of average surface temperature for the north wall.](image)

Figure 11 shows the average surface temperature for the north wall. In CFD stand-alone, the 3D heat transfer in the solid which leads to a temperature distribution at the surface of the wall may contribute to the sooner jump before 0.2 (s) in the average surface temperature. The temperature contours are plotted for a typical time step in Figure 12. In contrast, in BES-CFD coupling there is no temperature distribution at the surfaces since the surface temperature is calculated from a 1D conduction equation in BES and passed to CFD as a uniform boundary condition at each time step. Figure 13 illustrates the comparison of CHTC for the north wall. The difference between the two curves originates from the difference between the time step chosen and
also 1D and 3D heat transfer in the solid domain in BES-CFD coupling and CFD stand-alone, respectively. Surface discretization in BES can enhance the conformity of curves in Figure 11 and Figure 13 and play an important role when studying mold growth and condensation.

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9. REFERENCES