Chapter 6
Application of numerical simulation to ventilated airflow problems

This chapter describes the application of the numerical methods described and tested in the previous chapters, and a comparison to results obtained with the commercial computational fluid dynamics software CFX version 4.2 is made. In addition results from using the research code LESROOM developed by Mochida and Murakami, at the University of Tokyo are also included.

Special attention is given to recirculation of air flow in ventilated enclosures, which is related to flow problems in ventilated livestock buildings. All the cases are of the mixing type flows, where forced convection has been used. Several factors affecting the simulated results are investigated such as computational efficiency, resolution requirements, effects of different traditional turbulence models on the results e.g. the k-\(\varepsilon\) model, the low-Reynolds number k-\(\varepsilon\) model, the low-Reynolds number k-\(\omega\) (The Wilcox model), the renormalised group (RNG) k-\(\varepsilon\) model and finally the Reynolds Stress models which are all included in the CFX software. Afterwards, the results obtained with the two-equation turbulence models are compared to Large Eddy Simulation results with different subgrid scale models, and pros and cons for using LES is discussed. Finally, the feasibility of using LES and the computational costs of carrying out LES for air flow in ventilated enclosures is discussed.

Unfortunately some errors were found within the Solve4LES code late in the project, which has led to the extensive validation of both the Solve4k\(\varepsilon\) and Solve4LES code described the previous chapter. The effect of these errors was found to increase the total amount of kinetic energy in the computational domain, thereby increasing the velocity level. They were related to errors in the discretization scheme and the implementation of the boundary conditions at the inlet and outlet. After the discovery of these errors, all simulations were redone, although time was limited. Therefore the results provided in this chapter will only derive from the simulations which have been finished in time.
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6.1 Introduction

Airflow in ventilated enclosures can be divided into the following groups: mixing type where the flow is driven by forced convection, and natural convection where the main driving force is the buoyancy. A flow will be considered as forced convection if the driving force is pressure. The cases studied here are all related to the mixing type and forced convection. Although this is only a small part of the complete flow picture occurring in ventilated spaces (see Chapter 1), it is important to understand the basic features in the flow field. One of the important features in ventilated buildings is the recirculating flow phenomenon on which exists in almost all ventilated spaces where a mixture with supplied air is required. With a mixing ventilation system, new air will be supplied into the room through an inlet device close to the ceiling to produce an overall recirculating flow field, which will greatly affect the indoor air quality, the thermal comfort and the energy consumption. The awareness of the indoor air quality as an important factor for the overall health, welfare and comfort of both humans and animals is recognized. Therefore, to obtain accurate knowledge of the indoor airflow pattern it is necessary to investigate other components like thermal comfort and transport of pollutants. But the recirculating airflow will generates a shear layer between the inlet jet and the recirculating flow in the rest of the room. This will generate turbulence and hence enhance the mixing and the loss of kinetic energy.

In the beginning, the computer simulation of air flows by the computational fluid dynamic technique was restricted to simple laminar and turbulent flows in one or two dimensions under steady and isothermal conditions. The turbulence models were of the zero, one or two-equation k-ε model types. In the ‘seventies and the beginning of the ‘eighties, the computer models were extended to included the well-known two-equation k-ε models for three dimensional cases. Later in the ‘eighties the turbulence models were refined to different versions of the k-ε model and an extension to other two-equation turbulence models, like the low-Reynolds number version of the k-ε model and the k-ω model. In the ‘nineties further extensions to different Reynolds stress turbulence models were made. And finally, the development and application of the large eddy simulation model were made in the late nineties.

An extensive literature review on the application of CFD to building ventilation and indoor air quality problems was performed recently (Emmerich, 1997). Applications discussed in the literature include room airflow case studies involving calculation of airflow patterns, temperatures, ventilation system performance and thermal comfort for various ventilation systems. Furthermore, Chen (1995) studied the application of different k-ε turbulence models for various two-dimensional indoor air problems, both isothermal and non-isothermal. He recommended the use of the RNG k-ε turbulence model for indoor airflow problems. He also found that the different versions of the k-ε models had difficulties in providing accurate prediction of secondary recirculation in the airflow. Peng et al. (1996) studied the application and development of different types of the k-ω model. They referred to some of the same indoor air flow problems like Chen (1995) and found that the k-ω model was more suitable for prediction of velocity levels for both full turbulence and transitional air flow problems, although some discrepancies between the simulated and the experimental profiles of the kinetic energy still exist. They also said that the k-ω model had a better
convergence behaviour than the low Reynolds number k-ε models, since it has a severe restriction of the location at the first grid point from the wall. Chen (1996) applied different Reynolds Stress models to the same type of airflow problems as in Chen (1995). And he found that the performances of the different Reynolds Stress models were much alike and that the models were able to predict the secondary recirculations in the airflow, although not very satisfactorily. He finally noted that the use of two-dimensional simulations only may have suppressed some of the flow features that are related to three-dimensional flows. Chen (1997) made some further recommendations on the application of computational fluid dynamics to indoor airflow problems, with special attention to grid type, grid quality, and boundary conditions. Nielsen (1998) made some comments on the selection of different turbulence models for the prediction of indoor airflows, and he demonstrated that in some cases simple models such as the zero-equations turbulence model will be able to outdo the more advanced k-ε turbulence models. In addition, a discussion of the application of low-Reynolds number k-ε is made, and accurate results can be obtained from the Annex20 test case (Restivo (1997), Nielsen (1990)), which is also used in this project. Finally, large eddy simulation results on the same geometry were depicted. The velocity profile was of the same accuracy as the low-Reynolds number k-ε, although the recirculation velocity was underestimated in the first part of the room. Emmerich and McGrattan (1998) also used the large eddy simulation method to study the Annex20 test case with some success.

In the following sections, the Annex 20 test case (Restivo (1997), Nielsen (1990)), a backward facing step geometry with high step size (Restivo (1979) and the SJVF room (Bjerg et al. (1999)) will be investigated by means of large eddy simulation with different subgrid scale models. Some of the results are compared with predictions by traditional turbulence models, like the k-ε model, the low Reynolds number k-ε, the low-Reynolds k-ω model, the ReNormalized Group k-ε model, the two-layer k-ε model, the Algebraic Reynolds Stress model and the Differential Stress model. To study the results and the computational efficiency and feasibility of the Large Eddy Simulation method, three different implementations were tested. The first three different subgrid scale models for LES were implemented into the commercial CFD code, CFX (See Appendix B for description), and later the research code LESROOM (See Appendix A for description, Murakami et al. (1987), Mochida et al. (1993)) was tested. This code only included the Smagorinsky subgrid scale model. Finally, the code described in Chapter 4 was tested with four different subgrid scale models.

6.2 The Annex 20 test case

The first ventilation test case considered is the Annex 20 test case. The room is almost similar to a section in a modern livestock building. Although the inlet and outlet geometries are quite simple, this test case contains several problems, e.g. wall and recirculating flow. Experimental data from Laser-Doppler measurements for this case are given in Restivo (1979) and in Nielsen (1990). This geometry has been extensively used by different authors for validation of many different CFD codes and different turbulence models, as already discussed. Furthermore, due to the simplicity of the geometry and the boundary conditions, the inlet height is for instance relatively large compared to the room height, as the main part
of the inlet flow will pass outside the boundary regions at the ceiling. This will lower the need for high grid density in the near-wall region, thus making the flow less sensitive to boundary conditions at the walls.

The geometry of the test case has the following specifications (Figure 6.1):

The inlet conditions for the velocities are given by: \( \text{Re} = \frac{h \times U_{in}}{v} \approx 5000 \). For the numerical simulation the following parameter was used: \( H = 3.0 \text{ m} \), at a kinematic viscosity of \( \nu = 1.5 \times 10^{-6} \text{ m}^2/\text{s} \) at an inlet temperature of 20°C. The Reynolds number is based on the inlet slot height, because the flow in the ceiling region and in the rest of the room will be strongly influenced by the inlet condition. At the inlet the following boundary condition for the turbulent kinetic energy \( k \) and the dissipation \( \varepsilon \) was used:

\[
\begin{align*}
\kappa_{in} &= 1.5 \left( 0.04 \, U_{in} \right)^2, \\
\varepsilon_{in} &= \left( \kappa_{in} \right)^{3/2} / l_0 \\
\end{align*}
\]

This inlet condition corresponds to a turbulent intensity of 4%.

The numerical simulation was conducted in both two and three dimensions and with different grid densities. Since strong flow gradients were expected near the walls, grid clustering was desired at these locations. The grid was therefore generated by using a hyperbolic tangent function for all three directions. The experimental data from Restivo (1979) have been extensively used for testing and validating other numerical simulations (Chen, 1995, Chen, 1996, Emvin, 1997 and Peng et al. (1996)) for both traditional turbulence modelling, like the \( k-\varepsilon \) model, and for Large Eddy Simulation (Davidson and Nielsen, 1996)) to name a few.
6.2.1 The CFX Simulation

The following simulation by use of the commercial CFD code CFX (see Appendix B for additional information) was performed with two different grid densities of 72×48 and 144×96 cells in two dimensions to ensure insensitivity of further grid refinement. The predictions were so much alike that only the results obtained by using the 144×96 grid points will be given in the following two-dimensional predictions. Different turbulence models supplied within the CFX code were applied. Despite the fact that we are mainly concentrating on three-dimensional flows, these simulations were performed anyway.

The following turbulence models were applied: the standard k-ε model, a low-Reynolds number k-ε model, a low-Reynolds k-ω model by Wilcox, an Algebraic Stress model, and a Differential Reynolds Stress model. The velocity profile from experiments at two vertical lines was available together with two horizontal lines. To reduce the order of numerical diffusion, the velocity equations were discretized by the QUICK scheme and the hybrid scheme was used for the equations of turbulence variables (k, ε or ω). This combination of QUICK and Hybrid schemes seems to give the best results. The SIMPLEC method was applied to handle the pressure and velocity coupling. When solving the equations, under-relaxation was applied for both the velocity equations and the equations for turbulence variables. When the two-equation turbulence models were used the under-relaxation parameter was set at 0.3 and 0.4 for the velocity and turbulence equations, respectively. When the Algebraic Reynolds Stress and Differential Stress models were used it was necessary to apply an under-relaxation of 0.1 for the velocity equations. As a rule-of-thumb, it was found that the number of iterations before convergence was achieved would be approximately equal to 16 times the square root of the number of grid points for two-dimensional simulation. The two different Reynolds Stress models required about 25-40% more iterations in order to achieve convergence. The criterion for convergence of the mass residual was be below $10^{-3}$. The law of the wall (CFX-Solver manual, 1997) was used at the walls, where a no-slip condition was applied. Besides the configuration, standard parameters were used in CFX, together with the prescription of the inlet boundary condition for velocities, kinetic energy and dissipation of energy as previously described.

In the following two figures the predicted velocity profiles at two different vertical cross sections, x/H = 1 and x/H = 2, for the two-dimensional simulation and five different turbulence models are depicted.
Figure 6.2: Comparison between the predicted mean velocity at $x/H = 1$ and the experimental data (Restivo (1979)) for different turbulence models within CFX. Two-dimensional simulations.

Figure 6.3: Comparison between the predicted mean velocity at $x/H = 2$ and the experimental data (Restivo (1979)) for different turbulence models within CFX. Two-dimensional simulation.
The simulated velocity profile is in good agreement with the experimental data of Restivo, but small variations are seen. For \( x/H = 1 \), the \( k-\varepsilon \), the low Reynolds \( k-\omega \) and the Algebraic Stress models somewhat underestimate the core jet, as well as they over-predict the velocities in the return flow at the floor. The Differential Stress model gives a slightly higher velocity in the core jet and also a closer agreement with the return flow at the floor. The low-Reynolds number \( k-\varepsilon \) model and the Differential Stress model have a more narrow core jets than the experiments seem to indicate. At the vertical cross section, \( x/H=2 \) there was a very good agreement between simulated velocity profiles and experiments on the return flow at the floor. Some difference were observed in the core jet at the ceiling. Again, the low-Reynolds number \( k-\varepsilon \) and the Differential Stress model predict a narrow core jet. The following three figures (6.4-6.6) depict the vector field of the three different two-equation turbulence models. The three models are all able to predict secondary recirculation in the upper right and the bottom-left corners of the room. But there is a clear difference in the size of the secondary recirculation. These secondary motions are driven by pressure gradients. It is well-known that the two-equation models assume that the flow is isotropic, and they will therefore have problems predicting separation due to pressure gradients and consequently they will have problems in generating secondary recirculation zones. But the two-equation model does not seem to have problems predicting the secondary recirculation zones in the upper-right and the bottom-left corners. The reason for this may lie within the implementation in the CFX code. Others have reported similar problems with the same two-equations turbulence models (Peng (1994), Chen (1995), Chen (1996), Peng et al. (1997)), although some have used fewer grid points.

In Figure 6.7 the velocity in the return flow at \( y=h/2 \) is compared with the experiments. The prediction by the low-Reynolds \( k-\omega \) gives the largest recirculation zone in the corners, but also the highest velocity in the return airflow at the floor. The standard \( k-\varepsilon \) and the low Reynolds number \( k-\varepsilon \) model have difficulties in predicting the right size and magnitude of the recirculation in the bottom left corner. Even so, the velocity level as far as the recirculation zone corresponded very well with the experiments.

![Figure 6.4: Vector plot of the velocities \( U/U_\infty \) from a simulation obtained by using the \( k-\varepsilon \) turbulence model in CFX](image)
Figure 6.5: Vector plot of the velocities $U/U_{in}$ from a simulation obtained by using the low Reynolds number $k$-$\varepsilon$ turbulence model in CFX.

Figure 6.6: Vector plot of the velocities $U/U_{in}$ from a simulation obtained by using the low Reynolds number $k$-$\omega$ turbulence model in CFX.
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Next, the three-dimensional model of the Annex 20 test case was simulated within the CFX code, and different turbulence models provided in it were applied. Again, different grid densities were used to check and ensure that the solution was grid independent. The number of grid points used in the x-, y-, and z-directions were 64x48x32, 64x64x32, 96x64x32, respectively. The prediction velocity profile was virtually unchanged so therefore only the results obtained from using the 96x64x32 grid points will be given in the following three-dimensional predictions. The number of grids point used was somewhat higher than the number used by other authors. Furthermore, three two-equations model, namely the k-ε, the low-Reynolds k-ε and the ReNormalized Group k-ε models were tested on a very fine grid; 84x72x72 in the x-,y- and z-directions, respectively. The following turbulence models were applied: the standard k-ε model, a low-Reynolds number k-ε model, a low-Reynolds k-ω model by Wilcox, a renormalised Group k-ε model, an Algebraic Stress model and a Differential Reynolds Stress model. In the following, the models will be represented by the following abbreviations: the k-ε, the low-Re k-ε, the low-Re k-ω, the RNG k-ε, the ASM and finally the DSM. The computer prediction was again compared with the experimental data by Restivo (1979) at two vertical and two horizontal lines for velocity and kinetic energy. The velocity equations were discretized by the QUICK scheme and the hybrid scheme was used for the equations of turbulence variables (k, ε or ω). The SIMPLEC method was applied to handle the pressure and velocity coupling. When solving the equations under-relaxation was applied for both the velocity equations and the equations for the turbulence variables. When using the two-equations turbulence models, the under-relaxations parameter was set at 0.25 and 0.4 velocity and turbulence equations, respectively. When using the Algebraic Reynolds Stress and Differential Stress models it was necessary

![Figure 6.7: Velocity profile at y = h/2 for three different two-equations turbulence models. Two dimensional prediction by the CFX code.](image-url)
to apply an under-relaxation of 0.1 for the velocity equations.

As a rule-of-thumb, it was found that the number of iterations before convergence was achieved would be approximately equal to 10-12 times the square root of the number of grid points used for the three-dimensional prediction. The two different Reynolds Stress model nearly required a 30-45% higher iteration in order to achieve convergence. Therefore, the rule-of-thumb mostly counts for the two-equation turbulence models within the CFX code. The criterion for convergence was for the mass residual to be below $10^{-3}$. The law of the wall (CFX-Solver manual, 1997) is to be used at the walls, where a no-slip condition is applied. Besides the described configuration, standard parameters were used in CFX, together with the prescription of the inlet boundary condition for velocities, kinetic energy and the previously described dissipation of energy.

The velocity profile at the two vertical cross section $x/H = 1$ and $x/H = 2$ as depicted in Figures 6.8 and 6.9, and the horizontal line were $y = H-h/2$ and $y = h/2$ as depicted in Figures 6.10 and 6.11. For $x/H = 1$, the low-Re $k-\omega$, the RNG $k-\varepsilon$, and the DSM models predict a narrow core jet at the ceiling. In the return flow at the floor, the low-Re $k-\omega$, the RNG $k-\varepsilon$ and the DSM over-predict the velocities. In the middle of the room there is good agreement between the prediction and the experiments. For $x/H = 2$, the return flow is well predicted by most turbulence models, except the ASM, which tends to decline too early. At the ceiling the low-Re $k-\omega$ and the DSM predicts a very narrow core jet compared to the experiments and the other turbulence models.

For the horizontal line at $y = H-h/2$, all models seem to decline too early, and a large variation in the size of the recirculation zone will be observed. All turbulence models are able to predict the secondary motion in the upper right corner of the room.

![Figure 6.8](image_url)  
**Figure 6.8:** Velocity profile $U$ at vertical cross section $x/H = 1$ from computer prediction within the CFX code and using different turbulence models. The grid was 96×64×32.
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Figure 6.9: Velocity profile \( U \) at vertical cross section \( x/H = 2 \) from computer prediction within the CFX code and by use of different turbulence models. The grid was 96x64x32.

This is in contrast with the results obtained by Chen (1995), Chen (1996) and Peng et al. (1997). But their results only refer to two-dimensional simulations, and they would probably be different for three-dimensional predictions.

Figure 6.10: Velocity profile \( U \) at horizontal line \( y=H-h/2 \) from computer prediction with the CFX code and by use of different turbulence models. The grid was 96x64x32.
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Figure 6.11: Velocity profile $U$ at horizontal line $y=h/2$ from computer prediction with the CFX code and by use of different turbulence models. The grid was $96\times64\times32$.

For $y = h/2$ close to the floor, a large variation in the size of the recirculation zone in the lower left corner is seen. The low-Re $k$-$\omega$ model greatly over-predicts the size and the velocity level. Also, the DSM model

Figure 6.12: Profiles of turbulent intensity normalized by inlet velocity $U_{in}$ for the different turbulence models in the CFX code at the vertical line: $x/H = 1$. The grid used was $96\times64\times32$. 

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predicts an earlier separation of the flow from the floor than it was seen at the experiments. Generally, the computed profile along the floor shows a significant difference from that found at the experiments.

**Figure 6.13:** Profiles of turbulent intensity normalized by inlet velocity $U_{in}$ for the different turbulence models in the CFX code at the vertical line: $x/H = 2$. The grid used was 96×64×32.
Figure 6.14: Profiles of turbulent intensity normalized by inlet velocity $U_{in}$ for the different turbulence models in the CFX code at the horizontal line: $y = H-h/2$. The grid used was 96x64x32.

Figure 6.15: Profiles of turbulent intensity normalized by inlet velocity $U_{in}$ for the different turbulence models in the CFX code at the horizontal line: $y = h/2$. The grid used was 96x64x32.
The profiles of turbulent intensity predicted by the different turbulence models are compared to the experimental data in Figures 6.12-6.15. A significant difference between the experimental data and the computer prediction can be observed. The computer prediction especially underestimates the turbulent intensity when the horizontal lines are compared. These somewhat concur with the findings of Chen (1995) and Chen (1996), although their prediction was only for a two-dimensional simulation. The deviation seen in Figure 6.14 indicates a much faster decline of the velocity in the core jet. And it furthermore indicates that the highest level of turbulent intensity measured in the room is located at the recirculation zone in the right upper corner, which none of the turbulence models were able to predict. Close to the floor at y= h/2 the deviations from the experiments are also depicted in Figure 6.15, thus indicating that the velocity decline in the return flow should be larger.

Next, the vector plot from the prediction by the six different turbulence models in z/H = 0.5 plane is depicted. The overall flow features are captured by all the turbulence models, and besides the variations in size and magnitude of the recirculation zone in the corner are the same.

![Figure 6.16: Vector plot of the airflow pattern from simulation with the k-ε turbulence model. At z/H = 0.5.](image)

![Figure 6.17: Vector plot of airflow pattern of from simulation with the low Reynolds k-ω turbulence model at z/H = 0.5.](image)
Figure 6.18: Vector plot of the airflow pattern from simulation with the low Reynolds k-\( \epsilon \) turbulence model at \( z/H = 0.5 \).

Figure 6.19: Vector plot of airflow pattern from the simulation with the RNG k-\( \epsilon \) turbulence model at \( z/H = 0.5 \).

Figure 6.20: Vector plot of the airflow pattern from the simulation with the Algebraic Stress model at \( z/H = 0.5 \).
Finally, an attempt to use further grid refinement was investigated, where the number of grid points in the stationary simulation was increased to $84 \times 72 \times 72$. The same discretization schemes and the same method to solve the pressure-velocity coupling were used.

Although this high grid density was used in the simulation, the standard k-$\epsilon$ model did not show any larger improvement compared to the results depicted previously where the number of grid point was $96 \times 64 \times 32$ (Figure 6.22). Some small variations are seen in the upper right corner where the secondary recirculation has changed in size and shape. The separation point from the floor has moved closer to the left wall. For the low-Re k-$\epsilon$ turbulence, the vector plot is almost identical to the standard k-$\epsilon$ model. Hardly any change due the further grid refinement occurred previously. In the lower left corner, the secondary flow is better defined than in Figure 6.17. The point of detachment from the floor remains virtually unchanged.
Figure 6.23: Vector plot of velocities at z/H = 0.5 for the low Reynolds k-€ turbulence model in CFX code using 84×72×72 grid points.

In Figures 6.24 and 6.25, the corresponding vector field for the RNG k-€ and the low-Re k-ω turbulence models are depicted. For the RNG k-€, the secondary motion in the upper right corner is the same, and the point of separation from the floor also remains the same although more details are visible in the lower left corner. The low-Re k-ω model shows the same point of detachment from the ceiling, but some changes in the lower left corner are observed.

Figure 6.24: Vector plot of velocities at z/H = 0.5 for the RNG k-€ turbulence model in CFX code using 84×72×72 grid points.
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Figure 6.25: Vector plot of velocities at z/H = 0.5 for the low-Re $k$-$\omega$ turbulence model in CFX code using $84 \times 72 \times 72$ grid points.

The result obtained from using the ASM and DSM has been omitted, because these had problems obtaining a converged solution, although heavy under-relaxation was used. It is very likely that additional tuning of the models would provide a converged solution. But due to time limits, the results were not included. Line plots of the velocities profiles at four different cross sections are depicted in the next four figures, all for the middle plane: $z/H = 0.5$.

Figure 6.26: Velocity profile $U$ at vertical cross section $x/H = 1$ from computer prediction within the CFX code and where different turbulence models were used. The grid was $84 \times 72 \times 72$. 
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Figure 6.27: Velocity profile $U$ at vertical cross section $x/H = 2$ from computer prediction within the CFX code and when different turbulence models were used. The grid was $84\times72\times72$.

Figure 6.28: Velocity profile $U$ at horizontal line $y = H - h/2$ from computer prediction within the CFX code and when different turbulence models were used. The grid was $84\times72\times72$. 
Although the number of grid points were increased by more than 2.2 time, the predictions by the different two-equation turbulence models does not become marginally better. Especially the two Reynolds Stress models included in the CFX code become dramatically more numerically unstable. Generally speaking the turbulence model included in the CFX code predicted the velocity profile well for the Annex 20 test case.

But there were problems in computing the right level of turbulence intensity. Although not displayed here, this tendency does not get better, when large numbers of grid points are used, as in the case discussed above.
The computational efficiency of the commercial CFD code CFX is depicted below:

<table>
<thead>
<tr>
<th>Turbulence Model</th>
<th>SGI Indy</th>
<th>PC[Pentium II Xeon]</th>
<th>SGI Origin 200</th>
</tr>
</thead>
<tbody>
<tr>
<td>k-ε</td>
<td>$4.427 \times 10^{-4}$</td>
<td>$1.003 \times 10^{-4}$</td>
<td>$0.849 \times 10^{-4}$</td>
</tr>
<tr>
<td>Low-Re k-ε</td>
<td>$5.235 \times 10^{-4}$</td>
<td>$1.392 \times 10^{-4}$</td>
<td>$1.107 \times 10^{-4}$</td>
</tr>
<tr>
<td>Low-Re k-ω</td>
<td>$4.166 \times 10^{-4}$</td>
<td>$1.604 \times 10^{-4}$</td>
<td>$1.498 \times 10^{-4}$</td>
</tr>
<tr>
<td>RNG k-ε</td>
<td>$4.356 \times 10^{-4}$</td>
<td>$1.112 \times 10^{-4}$</td>
<td>$0.956 \times 10^{-4}$</td>
</tr>
<tr>
<td>ASM</td>
<td>-</td>
<td>$2.734 \times 10^{-4}$</td>
<td>-</td>
</tr>
<tr>
<td>DSM</td>
<td>-</td>
<td>$3.722 \times 10^{-4}$</td>
<td>-</td>
</tr>
</tbody>
</table>

Table 6.1: Comparison of cpu time per grid point and iterations for the different turbulence models within the CFD code, CFX. The second column represents the Silicon Graphics Indy Workstation with a R4600 @ 133 Mhz. The third column represents a PC with a Pentium II Xeon processor @ 450 Mhz and Windows NT 4.0. The fourth column is a small Unix server from Silicon Graphics, The Origin 200 with a R10000 processor @ 180 Mhz.

Table 6.1 shows a comparison between the cpu-time for each grid point and the iterations for three different computers running the same version of CFX software. The small Unix server SGI Origin 200 is about 16% - 18% faster than the PC computer. It should, however, be mentioned that the unix server is a multiuser system compared with the PC which will mostly be a single user system. This will sometimes be reflected in the overall computational time in favour of the PC system. The times displayed in table 6.1 will only be valid if the CFX is the only program running besides the operating system. The CFX contains a wide range of different linear equations solvers, like the line-Gauss solver, the Strongly Implicit Procedure (SIP), the Block-Strongly Implicit Procedure (B-SIP), the Conjugate Gradient with Incomplete Choleski preconditioning (ICCG), and finally a version of the Algebraic MultiGrid (AMG) solver. Different combinations of the linear equations solvers were tried, and for the kind of problem studied here, the fastest combination was to use the SIP method for the velocity equations and the Conjugate Gradient with the Incomplete Choleski preconditioning. Although numerically more efficient, the algebraic multigrid did not show any improvement compared to the ICCG method. The Line-Gauss solver and the Block-SIP method were within 5% of the SIP method used when comparing time consumption to solve a given set of linear equations.
6.2.2 CFX and Large Eddy Simulation

We will now move on to using the Large Eddy Simulation method implemented into the CFX code. By using the user fortran interface in the CFX it became possible to implement three different subgrid scale models, namely the Smagorinsky model, the mixed scale model and the dynamic model with planearranging in the spanwise direction. The last mentioned subgrid scale model was introduced in the previous chapter and its implementation was discussed. The CFX was set to do an unsteady laminar simulation and to apply the user Fortran interface to compute the subgrid scale viscosity from the subgrid scale model, and by adding it to the laminar viscosity, a CFX in Large Eddy Simulation was obtained.

To reduce the introduction of artificial viscosity when applying discretization, the central scheme was used for all variables. Although only second order accurate, it has been tested in many different implementations for LES. A QUICK scheme could be an alternative but this particular scheme belonging to the category of upwinding discretization schemes has in several numerical simulations turned out to introduce a too large dissipation (Breuer (1998), Rodi et al. (1996)). This will change the small scale structure and introduce damping of the fluctuations. Naturally this is an undesirable feature in a Large Eddy Simulation. The investigation of the effect of different discretization schemes on the Large Eddy Simulation would have been easy with the CFX code. However, it was not examined within the present simulations. To handle the time dependent terms, a Crank-Nicolson scheme was used, since it will allow a larger size of time steps than the explicit schemes. The pressure velocity coupling was again treated by the SIMPLEC (SIMPLE-Consistent) (Van Doormal and Raithby, 1984) method. The CFX also has the possibility to use the SIMPLE (Semi-implicit Method for Pressure-Linked Equations) (Patankar and Spalding, 1972) or the PISO (Pressure Implicit with Splitting of Operators) (Issa, 1986) method for the coupling. Initial tests were carried out, but no improvement in convergence or reduction in the need for computational time was observed. The boundary condition at the inlet was specified as a uniform velocity profile and then superimposed with random fluctuations to allow the turbulent fluctuation to develop more rapidly. The outlet was treated as a Neuman condition. At the wall a no-slip condition and a quadratic law of the wall were applied, which is the default setting in the CFX when the laminar simulation mode is used. The LES in CFX was started from a previous k-ε simulation in order not to waste time on reaching a fully developed flow. To estimate the number of time-steps needed in the averaging, the large eddy turn-over time (LETOT) which refers to the time the largest eddy inside the computational domain be needed in order to do one rotation. One LETOT ≈ 2L/Uin ≈ 40 seconds was used. When running CFX on the same PC as described in the previous section, a maximum number of 10 LETOT was performed for the averaging of first order statistics, like the time averaged velocity profiles. Two different grids were tested; one 64×32×32 and 64×64×32. Only results from the finest grid density will be reported since it presented superior prediction.
The Smagorinsky constant was set at 0.18 in the first computation and later raised to 0.21, which gave the best results compared to the experiments. The mixed scale model $\alpha$ and $C_{\text{mix}}$ were set at 0.5 and 1, respectively. The Crank-Nicolson scheme was used for time integration allowing the CFL-number to exceed 1. The time step was computed by using the restriction that $\text{CFL} \leq 1$ at any point in the domain. Within this limit the turbulent fluctuations could not be suppressed in any way, thereby forcing laminarized solution of the flow (Chol and Moin, 1994).

The costs in terms of cpu-time per time step for the Smagorinsky model, the mixed scale model and the dynamic model were equal to 20.1 sec., 23.4 sec and 68.8 sec, respectively, on the PC computer with the Pentium II Xeon processor at 450 MHz. Clearly, LES with the dynamic subgrid scale model is much more expensive than the Smagorinsky and the Mixed Scale models. In the next figures the mean velocity profile for the LES computations on the Annex 20 case with the CFX code is depicted.

<table>
<thead>
<tr>
<th>Code</th>
<th>CFX in LES</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\Delta x_{\text{min}} / H$</td>
<td>0.0026</td>
</tr>
<tr>
<td>$\Delta y_{\text{min}} / H$</td>
<td>0.0008</td>
</tr>
<tr>
<td>$\Delta z_{\text{min}} / H$</td>
<td>0.0036</td>
</tr>
<tr>
<td>$\Delta x_{\text{max}} / H$</td>
<td>0.1979</td>
</tr>
<tr>
<td>$\Delta y_{\text{max}} / H$</td>
<td>0.0368</td>
</tr>
<tr>
<td>$\Delta z_{\text{max}} / H$</td>
<td>0.1029</td>
</tr>
<tr>
<td>Grid</td>
<td>64x64x32</td>
</tr>
</tbody>
</table>

Table 6.2: Geometrical information of the grid used. Min. denotes the minimal distance from the solid wall to the first grid point. Max. denotes the maximal distance between two adjacent grid points.
 Generally speaking, the Smagorinsky will model underestimate the velocity profile in the inlet jet. The dynamic model seems to overcome the difficulties and will give better results. Also, the core jet profile at the ceiling is more narrow than the other subgrid scale models. This corresponds to the fact that the Smagorinsky model is known to be too dissipative and in lack of adjustment of the model constant, $C_s$. The Mixed Scale model is able to account for this by using the double filtering approach, and thereby it will account better for the energy transfer from the larger energy containing scale to the smaller and more homogenous scale. The return flows at the floor are underestimated at the vertical line: $x/H = 1$.

In Figures 6.22 and 6.23 the two iso-surfaces are compared. One instantaneous iso-surface of the $v$-velocity from a Large Eddy Simulation by means of the mixed scale sgs model is compared to a steady solution using the standard $k-\varepsilon$ turbulence model on the grid. The difference between simulation with the Reynolds Averaged Navier-Stokes equations using a two-equations turbulence model and simulation with the spatial filtered Navier-Stokes equations using a subgrid scale model is clearly visible. Early separation from the ceiling can be observed, together with an irregular iso surface in the spanwise direction indicating that although this problem can be predicted well by using only two-dimensional simulations, the flow is will act in all three dimensions. The second order statistical, rms-value of the velocity fluctuations was not collected, since the total averaging time was only 5 LETOT, which was not sufficient to collect accurate data.
CHAPTER 6 APPLICATION OF NUMERICAL SIMULATION TO VENTILATED FLOW PROBLEMS

1 Gflops: (GigaFlops): A computational rate of one billion floating-point operations per second.

Figure 6.31: Mean velocity profiles at the vertical cross section: $x/H = 2$ for three different subgrid scale models within CFX. The grid was 64×64×32.

The initial implementation and test of the LES method within the CFX was started on a Silicon Graphics workstation, Indy with the R4600 processor (@ 133Mhz). This computer was typically 3-5 times slower than the currently used PC (Table 6.3)). Jacobsen (1997) tested the CFX implementation by using two different subgrid scale models on a vector supercomputer, the Cray C92, which was available at UNI-C, located at the Technical University of Denmark, Copenhagen. Although faster than the present version used on the computer mentioned in Table 6.1, it could not compete with a special purpose code written for the Cray supercomputer. Actually, the computational speed of the CFX code was 15-20 times lower than the peak speed of approximately 1 Gflops\(^1\). A large amount of computer time will be necessary to obtain details about second statistics, and therefore further grid refinement is needed in order to test and validate LES for ventilation airflows. Therefore, it was decided to use a special purpose code for doing Large Eddy Simulation.

One of the options was the LESROOM code.

6.2.3 The LESROOM Simulation

The second code used was the LESROOM code which is a finite difference code based on a staggered grid configuration (see Appendix A). A second-order centred difference scheme was used for all spatial derivatives. For the time advancement, the Adams-Bashforth scheme was used for the convective terms,

\(^1\) Gflops: (GigaFlops): A computational rate of one billion floating-point operations per second.
and the Crank-Nicolson scheme was used for the diffusion terms. This is also known as a semi-implicit method for time advancement. For the numerical integration a version of the Simplified Marker And Cell (SMAC) method (Hirt and Cook, 1972) has been used, which employs simultaneous iterations for both pressure and velocities. Only the Smagorinsky subgrid scale model was implemented in the LESROOM code. For the treatment of solid walls the two-layer model based on the linear-power law expression proposed by Werner and Wengle (1991) was adopted. In order to account for near wall effects, a van Driest type wall damping function was introduced.

The LESROOM code is written in Fortran 77 and was supplied with virtually no documentation at all. Furthermore, the code only contained very few comments within the program. After some difficulties, the initial test run on the Cray vector supercomputer showed only an averaged speed of 13 Mflops\(^2\), which was quite disappointing.

\(^2\)Mflops: (MegaFlops): A computational rate of one million floating-point operations per second.
An analysis of the program structure and the way the program performed the memory access reveals some serious problems. By rearranging all the loops within the program which could improve the memory access pattern dramatically, the performance was increased to 360 Mflops. Further improvement was reached by loop unrolling (creation of fat loop), and reduction of procedure and function calls within loops (by inlining of function and procedure calls), reduction of branches (conditional statements (if-then)) within loops; the performance increased to 420 Mflops if 200,000 grid points or more were used, and up to 500-560 Mflops for grids exceeding 500,000 grid points. One very important factor to be considered when vector-supercomputers are used is to align the dimension, which has the most grid points within the inner-loop.

In the present case, the dimension which has the most grid points should be used in the x-direction. For additional information about optimization in scientific computer programmes, see Dowed (1993).

In the following, a laminar solution to the problem was first obtained, and the LES was then restarted from there. To overcome the adaption to fully turbulent flow from the laminar solution, 20 LETOT were performed, where the tolerance was lowered to $0.009 \times (U_{in} / H)$. The CFL-numbers for these simulation were limited to 0.15-0.2.
Only with these limits on the CFL-number, was LESROOM able to perform at the speed mentioned previously. The number of iterations for the solution of the pressure-velocity coupling was highly dependent on what limits were chosen. Doubling the CFL-number would more than triple the necessary number of iterations for solving the pressure-velocity coupling. And since the Highly Simplified Marker And Cell was the part of LESROOM which had the lowest performance, it would mean a substantial increase in cpu-time. The HSMAC method only performed 360 Mflops for grids exceeding 500,000 grid points. The result obtained by using a grid with 96x84x64 points is reported in the following.

Figure 6.34: Number of iterations versus residuals to solve the pressure-velocity coupling by using the Highly Simplified Marker And Cell method in LESROOM. The Residual-Iterations are plotted for five succeeding time-steps.

Figure 6.35 depicts the number of iterations to obtain a solution in the HSMAC method when the flow was fully turbulent are depicted. As depicted, the number of iterations fluctuate very much. A basic element of LES is the appropriate formulation of the boundary conditions, where all boundaries in principle cause problems. Inhomogeneous flows will require better inflow and outflow boundary conditions. At the inlet section the three velocity components have to be prescribed. In contrast to laminar or Reynolds averaged flow computations for LES it is usually not sufficient to specify mean values at the inlet. Instead, a real time dependent velocity field has to be specified. This can be obtained from either numerical simulation (previously LES) or experimental results. For the LESROOM code it was attempted to apply a fluctuating boundary condition at the inlet in the same way as for the LES implementation in the CFX code.

The effect of this was that the number of iterations in the velocity-pressure solution obtained by using the SMAC method increased dramatically (see Figure 6.36).
Figure 6.35: LESROOM: Number of iterations in the velocity-pressure solution, HSMAC, obtained when the threshold was set to 0.009 \( (U_{in}/H) \) by using a stationary uniform inlet velocity profile.

Figure 6.36: Number of iterations in the velocity-pressure solution obtained by using the Highly Simplified Marker And Cell method in LESROOM. LES with a dynamic inlet boundary by using superimposed random fluctuations and an inlet boundary condition with no fluctuation are compared. The threshold in HSMAC was set to 0.009 \( (U_{in}/H) \).
The reason for the dramatic increase in the required number of iterations has not been located or explained.

In Figures 6.37 and 6.38, the mean velocity profile for two different Smagorinsky constants at the vertical cross section: \( x/H = 1 \) and \( x/H = 2 \) are depicted. The results are very similar to those obtained by the CFX code with LES implementations. The core jet profile will become more and more narrow as the Smagorinsky constant is increased. Also, the return flow at the floor will change as the Smagorinsky constant changes, thus indicating that the solution is quite dependent on the chosen value of the constant.

**Figure 6.37:** Mean velocity profile at \( x/H = 1 \) for the LESROOM with the Smagorinsky sgs model and two different Smagorinsky constants. 

**Figure 6.38:** Mean velocity profile at \( x/H = 2 \) for the LESROOM with the Smagorinsky sgs model and two different Smagorinsky constants.
It becomes clear that the return flow separates too early from the floor, compared to the experiments.

Figure 6.39: Time history of one point \((x/H, y/H, z/H) = (3/2H, h/H, 1/2H)\) for LESROOM, Smagorinsky model, \(C_s = 0.18\). Mesh: 96×84×64

Figure 6.39: The velocities in the x-, y- and z-directions are depicted and compared to the computed mean velocity at a given instant in the time. As shown, the monitor point was in the return flow in the room; a good mean representation was quickly achieved. Since it was not possible to superimpose random fluctuation at the inlet, because of limited computing resources, it was not possible to compare the solution with and without superimposed fluctuations at the inlet. If Figure 6.39 was compared to a result obtained by Davidson & Nielsen (1996), the predicted velocity fluctuation by LESROOM was not as fluctuating and rapid. This could stem from the lack of velocity fluctuation at the inlet.

In the next three figures, vector plots of instantaneous velocities of three different planes are depicted: \(z/H = 0.1, 0.5, \text{ and } 0.9\). These results were computed by using LESROOM and a Smagorinsky constant of 0.20, which gave the best overall results when comparing the mean vertical velocity profiles at \(x/H = 1.0 \text{ and } 2.0\). The variations in width of the core inlet jet is clearly seen, due to the mixing with the air outside the core jet. Also, the variation of the separation point from the ceiling over the width of the room is depicted. Close to the wall early separation occurs, compared to in the middle of the room. In the return flow at the floor a much earlier detachment can be seen compared to the vector plot of the velocity vector, by use of the traditional two-equation turbulence model as previously discussed. In Figure 6.43, the instantaneous iso-surface for the velocity \(\langle \vec{u} \rangle_t / U_{in} = 0.38\) is depicted. The non-uniformity of the inlet jet is seen, and the variation of the point of separation from the ceiling is also depicted. The locations of the inlet and outlet boundary conditions are depicted with the velocity vectors.
**Figure 6.40:** LESROOM: $C_s = 0.20$. Instantaneous velocity field at $z/H = 0.1$. Earlier separation from the ceiling.

**Figure 6.41:** LESROOM: $C_s = 0.20$. Instantaneous velocity field at $z/H = 0.5$
Figure 6.42: LESROOM: $C_s = 0.20$. Instantaneous velocity field at $z/H = 0.9$.

Figure 6.43: LESROOM: Annex 20: Iso-surface of instantaneous velocity: $\langle \vec{u} \rangle / U_{in} = 0.38$. 

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