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Computational Fluid Dynamics and Room Air Movement

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Published in:
Indoor Air

Publication date:
2004

Document Version
Early version, also known as pre-print

[Link to publication from Aalborg University](#)

Citation for published version (APA):
Nielsen, P. V. (2004). Computational Fluid Dynamics and Room Air Movement. *Indoor Air*, 14(Supplement 7), 134-143.

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Computational fluid dynamics and room air movement

Abstract Computational Fluid Dynamics (CFD) and new developments of CFD in the indoor environment as well as quality considerations are important elements in the study of energy consumption, thermal comfort and indoor air quality in buildings. The paper discusses the quality level of Computational Fluid Dynamics and the involved schemes (first, second and third order schemes) by the use of the Smith and Hutton problem on the mass fraction transport equation. The importance of "false" or numerical diffusion is also addressed in connection with the simple description of a supply opening. The different aspects of boundary conditions in the indoor environment as, e.g., the simulation of Air Terminal Devices and the simulation of furnishings and occupants are discussed. The prediction of the flow in a room with a three-dimensional wall jet by the use of different turbulence models such as the $k-\epsilon$ model, the V^2-f model and the Reynolds Stress model is addressed in the last chapter of the paper.

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Key words: Computational fluid dynamics; Room air distribution; Turbulence models; Supply opening; Furnishing; Thermal manikin.

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Practical Implications

The use of computational Fluid Dynamics as a practical design method for room air distribution is widespread. It is important to consider the quality of the predictions in order to obtain a sufficient level of accuracy. It is also important to work with a practical description of supply openings as well as with the right level of details in the occupied zone and the right turbulence model. All these aspects are addressed in the article.

Introduction

The indoor environment community has adopted computational fluid dynamics (CFD) as a useful tool for the prediction of air movement in ventilated spaces. The method has been used for many years as a research tool, see, e.g., Nielsen (1973 and 1975) and Jones and Whittle (1992). Now it is used routinely in civil engineering when a large or complicated ventilation system is to be designed.

This paper describes developments which can be important for the use of CFD in the indoor environment, and it discusses quality considerations that are also important because of the large number of new CFD users.

The quality level of different schemes is discussed in the chapter on numerical background, and it considers different aspects of the boundary conditions of supply openings. Problems in connection with the simulation of people and the occupied zone are discussed, and prediction of wall jets by different turbulence models is addressed in the last chapter of the paper.

Numerical background and the accuracy of the numerical schemes

The prediction of flow is based on a solution of the fundamental flow equations. They consist of the equation of continuity, three momentum equations (one in each coordinate direction), the energy equation and perhaps a transport equation for contaminant distribution. All equations are time-averaged and the local turbulence is often expressed as a variable diffusion coefficient called the turbulent viscosity. This viscosity is often calculated from two additional transport equations, namely the equation for turbulent kinetic energy and the equation for dissipation of turbulent kinetic energy. The room is divided into grid points. The differential equations are transformed into discretization equations formulated around each grid point and an iterative procedure is used in the numerical method.

The number of grid points is an important aspect for the quality of the predictions. It is obvious that an increased number of grid points decreases the difference between the solution found by the discretization

equations and the solution represented by the differential equations. It is, on the other hand, expensive to use more grid points than "necessary", and different numerical schemes have been developed during the last 40 years to economize on the grid points.

The numerical schemes developed in the sixties were often based on a central difference description of terms in the flow equations. This type of scheme was unstable (gave oscillatory or wiggly solutions) when it was used for prediction of convective flow. The problem could only be solved by the use of a number of grid points that were far too high for computers of that time.

A large step forward was taken when Courant et al. (1952) suggested the upwind scheme with almost unconditional stability. The upwind scheme is called a first order scheme because the truncation error obtained by this scheme is proportional to the grid point distance Δx , see Ferziger and Peric (1999).

In the early seventies it seemed that the use of an upwind scheme had opened the way to make numerical simulations of flow phenomena at indefinitely high Reynolds numbers. However, before the end of the decade it had become clear that there could be large errors in the predictions, although a high stability was obtained. The error is connected with situations where the flow has an angle to the grid lines, and the error reaches its maximum when the angle is 45° (in a square grid). It causes a numerical error called "false diffusion" or "smearing" where this false diffusion is proportional to the velocity and to the distance between the grid points. Huang et al. (1985) conclude that many studies at the end of the seventies had a false diffusion, which was larger than diffusion of physical kind.

The QUICK scheme by Leonard (1979) is an improved scheme for the convection term which produces a low level of false diffusion, and it has a third order accuracy (second order accuracy in two and three-dimensional flow) in comparison with the first order accuracy of the upwind scheme. The third order of accuracy means that the truncation error is proportional to Δx^3 .

The second order upwind scheme and the van Leer scheme are two other schemes which take account of the fact that the upstream conditions have a greater influence on the variables than the downstream conditions. They both have a second order of accuracy.

It should be mentioned that the order of accuracy indicates how fast the error is reduced when the grid is refined; it does not indicate the absolute magnitude of the error.

The selection of a numerical scheme with a high order of accuracy improves the results if it is difficult to obtain a grid-independent solution. Sørensen and Nielsen (2003) has shown the influence of false diffusion in a case called the Smith and Hutton problem (1982). Figure 1(A) shows the case. The air is defined

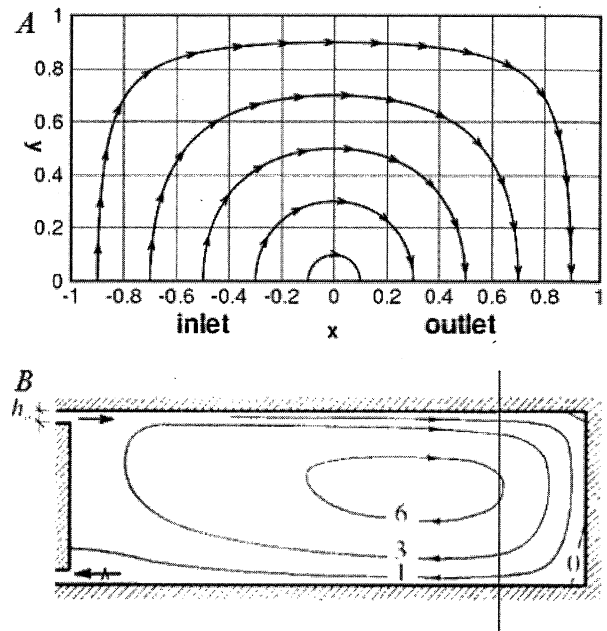


Fig. 1 The Smith and Hutton problem at the top (A), and typical flow in a room with mixing ventilation and slot inlet at the bottom (B).

as a two-dimensional flow in a "dead end channel" and the velocities are given by an analytical description. The situation is typical of room air movement (in certain areas) with mixing ventilation as indicated on the right side of Fig. 1(B).

A transport equation, e.g., the contaminant transport equation, is solved in the flow field in Fig. 1(A). This transport equation is *without physical diffusion* terms. The concentration will therefore be transported along with the flow, preserving the inlet values all the way to the outlet. Consequently, at the outlet any deviations between the exact and the computed concentration fields are due to inaccuracies in the numerical solution of the transport equation (false diffusion).

The computational grids are made with 80×40 cells in the x and y directions, respectively. The calculation of steady flow is made with three different discretization schemes. Figure 2 shows the concentration distributions for a first order upwind scheme (A), a second order scheme (B) and a third order QUICK scheme (C). Recalling that the distribution at the outlet should equal the distribution at the inlet, the false diffusion is evidenced by the large smearing of the distribution. The second order scheme transports the concentration with less smearing. Finally, the third order scheme transports the concentration almost without change. Thus, the example shows that higher order schemes perform significantly better than lower order schemes for a given grid size. The predictions in Fig. 2 are made by 3200 grid points which are a small number. An equivalent grid density in the whole room in

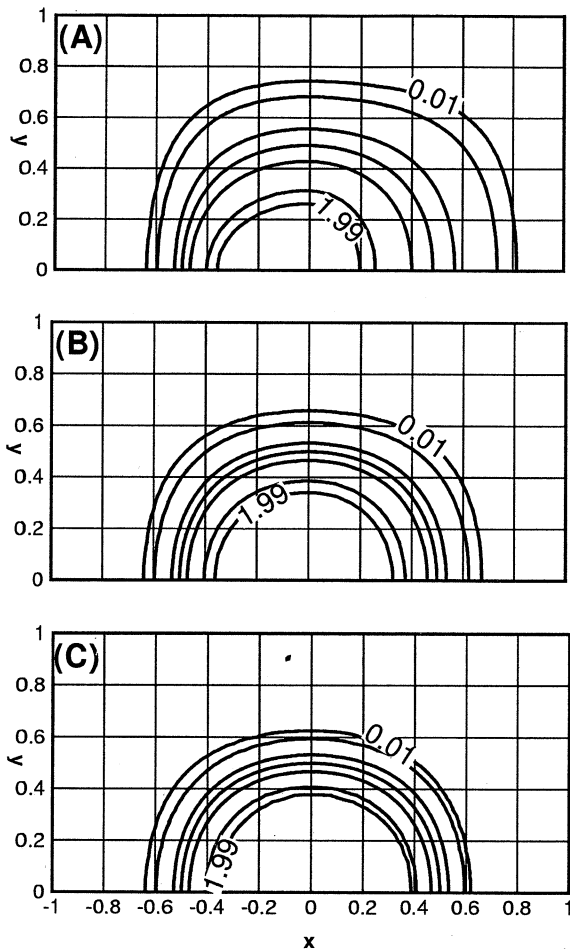


Fig. 2 Concentration distributions predicted by three different discretization schemes. (A): first order upwind scheme (B): second order scheme (C): third order QUICK scheme. Grid size is 80×40 cells. Contours are shown for concentration levels of 0.01, 0.05, 0.5, 1.0, 1.5, 1.95 and 1.99.

Fig. 1 (with three-dimensional flow) demands about one million grid points which in practice is typical of many predictions. Other predictions with a lower and a higher number of grid points are also given by Sørensen and Nielsen (2003). It is shown that an increased number of grid points improves the first and second order schemes.

Another example of the importance of false diffusion and of the order of accuracy of the transport equations is shown in Fig. 3. Figure 3 (A) shows the prediction of flow from a wall-mounted opening of the size 6.8 cm times 52 cm located in the wall 0.5 m below the ceiling. The flow is directed upward from the opening ($u, v = 3.1, 2.6$ m/s) and the predictions are made in a grid with 30000 cells. The grid is rectangular and the flow close to the opening has therefore an angle to the grid lines. Figure 3(B) shows the predicted profile below the ceiling 1 m from the wall. The two profiles show the large change which is obtained by the use of a second order upwind scheme instead of a first order scheme. Predictions made by a

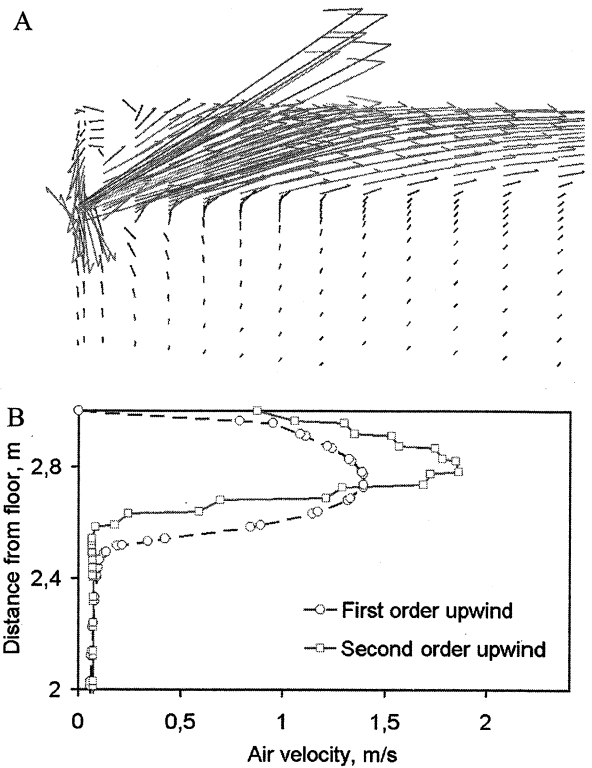


Fig. 3 Prediction of the isothermal flow close to an opening which is located in the wall 0.5 m below the ceiling. The lowest graph shows the velocity distribution below the ceiling 1 m from the wall. Svdt, 1999).

second order upwind scheme indicate non-physical wiggles which in this case are the result of an insufficient number of grid points. It is indicated that convergence problems may arise when the second order upwind scheme is used.

It is always recommended to use a scheme of second order accuracy if it is available and if convergence can be obtained, see Casey and Wintergerste (2000) and Sørensen and Nielsen (2003).

Boundary conditions at the supply opening

Together with the governing equations the boundary conditions are another important part of the physics. It is not easy to handle all the boundary conditions with a high level of accuracy, and especially the supply opening for the flow may cause problems. Usually the flow from a diffuser depends on small details in the design. This means that a numerical prediction method should be able to handle small details in dimensions of a fraction of a millimeter as well as dimensions of several meters. This wide range of the geometry necessitates a large number of cells in the numerical procedure which will increase the prediction cost and computation time to a high level. The very fine details in the flow profiles that are generated by a diffuser are also very difficult to measure and to specify.

Different simplifications are suggested. The most obvious method is to replace the actual diffuser with a less complicated geometry that supplies the same momentum flow to the room, called Simplified Boundary Conditions (SBC). This may be obtained by a single opening with an area equivalent to the total supply area of the diffuser. The flow from the opening is specified to be in the same direction as used in the actual diffuser.

An example of the use of simplified boundary conditions is shown by Topp et al. (2001). A diffuser which consists of 84 nozzles with a supply direction which is 40° to horizontal is simulated by two simplified openings, diffusers A and B. Diffuser A has the same width as the actual diffuser and diffuser B has a width which is 1.5 times the actual diffuser (Fig. 4).

The simulations show that both diffusers are able to predict the maximum velocity in the jet below the ceiling. None of the diffusers predict the width of the jet, although the predictions for diffuser B are improved compared to the predictions for diffuser A (Fig. 5). The predictions are made by a $k-\epsilon$ model and the last chapter "Turbulence models and predictions of a three-dimensional wall jet" discusses the effect of different turbulence models in this situation. This example, with two different suggestions for a diffuser, shows that SBC necessitate a number of CFD

predictions as well as measurements for comparison to select the right diffuser.

The Box Method is a method based on the wall jet flow generated close to the diffuser (Nielsen, 1973). Figure 6 shows the location of the boundary conditions around the diffuser. The details of the flow in the immediate vicinity of the supply opening are ignored, and the supplied jet is described by values along the surfaces a and b . Two advantages are obtained by using these boundary conditions. First, it is not required to use a grid as fine as is the case with a fully numerical prediction of the wall jet development close to the diffuser. Secondly, it is possible to make two-dimensional predictions for supply openings that are three-dimensional, provided that the jets develop into a two-dimensional wall jet or free jet at a certain distance from the openings.

The Prescribed Velocity Method has also been successfully used in the numerical prediction of room air movement. Figure 7 shows the details of the method. The inlet profiles are given as boundary conditions at the diffuser in the usual way (simplified boundary conditions), although they are represented only by a few grid points. All the variables, except the velocities u and w , are predicted in a volume close to the diffuser (x_a, y_b) as well as in the rest of the room. The velocities u and w are prescribed in the volume in front of the diffuser as the analytical values obtained

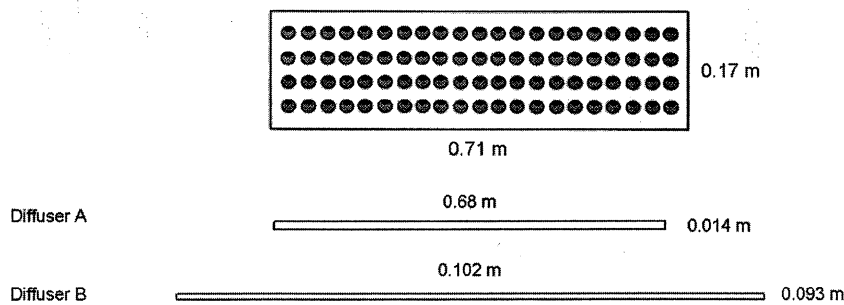


Fig. 4 The IEA Annex 20 diffuser and outline of two different geometric specifications of CFD boundary conditions.

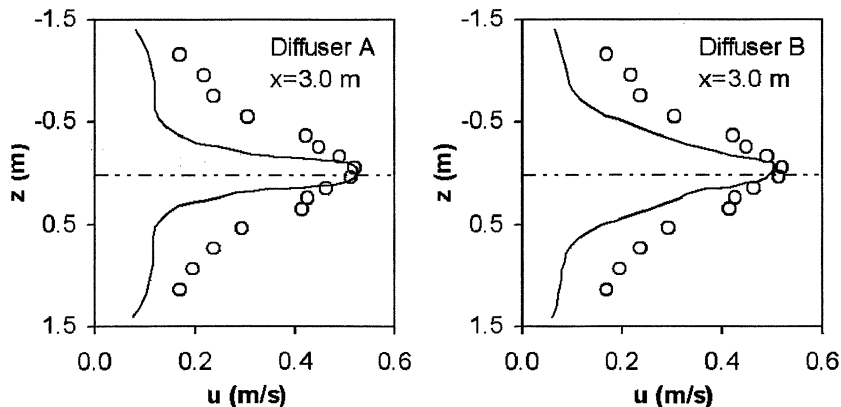


Fig. 5 Horizontal velocity profiles for diffuser models A and B compared to experiments at a distance of 3 m from the diffuser.

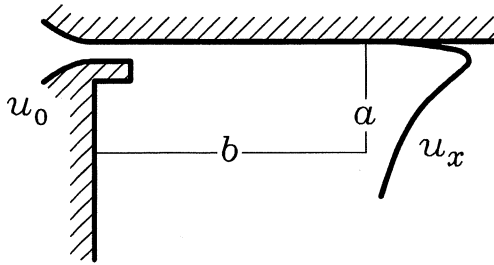


Fig. 6 Location of boundary conditions around the diffuser as used in the box method.

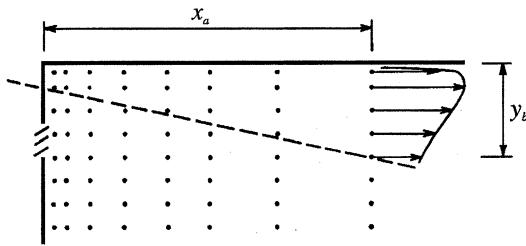


Fig. 7 Prescribed velocity field close to the supply opening.

for a wall jet from the diffuser, or they are given as measured values in front of the diffuser (Goman et al., 1980; Nielsen, 1992).

The necessary data for velocity distribution in a wall jet (or a free jet) generated by different commercial diffusers can be obtained from diffuser catalogues or design guide books such as ASHRAE Handbook of Fundamentals (1997) and from textbooks, e.g., by Awbi (1991) and Rajaratnam (1976).

Figure 8 shows predictions and measurements of the maximum velocity in the occupied zone made in IEA Annex 20. Both the prescribed velocity method and the simplified boundary condition method are used. The simplified boundary condition can be applied without knowing many details of the actual diffuser, but comparisons with measurements show that the maximum velocity in the occupied zone obtained by the predictions is overestimated by 40%.

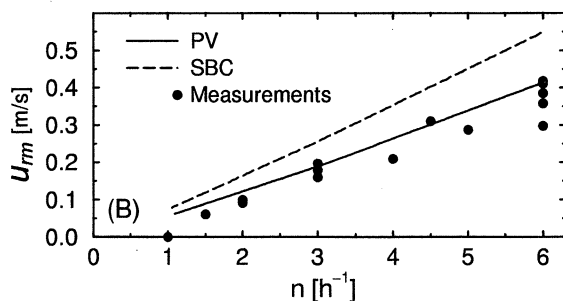


Fig. 8 IEA Annex 20 work, isothermal flow. Maximum velocity in the occupied zone vs. rate of air change. PV: Prescribed Velocity boundary conditions, SBC: Simplified Boundary Conditions.

The work, ASHRAE RP-1009, Chen and Srebric (2001), gives a very detailed discussion of simplified diffuser boundary conditions for numerical room air flow models. They recommend to use the box method or the momentum method. The momentum method is a method where the momentum and mass flow are decoupled in the CFD simulation of the diffuser, and the initial momentum and mass flow rate from the diffuser are used as the boundary conditions. The momentum method is recommended for square, round and vortex ceiling diffusers and for diffusers in displacement ventilation. The box method is recommended for nozzles, linear slots and valves.

Continuous development of the computer capacity and speed will undoubtedly make the direct methods with local grid refinements possible. Promising results are shown by Bjerg et al. (2002) for diffusers in livestock buildings. Figure 9 shows a typical diffuser and the grid distribution for the diffuser and the room. 86,000 cells are used in the predictions. As seen in Fig. 9 it is necessary to have some indication of the flow field close to the diffuser before the first set of predictions is made.

The occupied zone

The occupied zone of a large room or an atrium can have a very complicated geometry due to furnishings and people and the geometry will even change from time to time. Most measurements and predictions are made in empty rooms, but it is of course important to be able to make CFD predictions of the velocity level in occupied areas.

One possibility is to model all the obstacles in the flow field but it will be very grid point demanding. Figure 10 A shows both small and large elements in the occupied zone, and it will be difficult to select the right simplification.

A promising method is to consider the furniture and other obstacles as one volume with an additional pressure drop in the momentum equations, representing the flow resistance from the obstacles (Fig. 10B).

Experiments and predictions show that furniture and obstacles redistribute the velocity field in the occupied zone. The velocity increases in some areas and decreases in other areas. Figure 11 shows that the maximum velocity u_{rm} is reduced compared to the value in an empty room $u_{rm,o}$ in the case of isothermal flow. Office furniture as, e.g., desk, computer and chair typically covers the length of 2 m. The figure shows that the maximum velocity is reduced to 80% of the value in the empty room. The predictions in Fig. 11 are confirmed by measurements.

Figure 12 shows the effect of obstacles in the occupied zone of a room with two-dimensional and isothermal recirculating flow. Obstacles in the lower part of the room have only a small influence on the

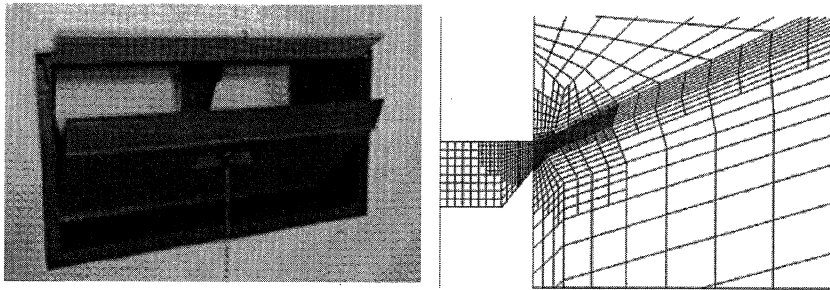


Fig. 9 Diffuser for a livestock building and typical grid point distribution both in the diffuser and in the room.

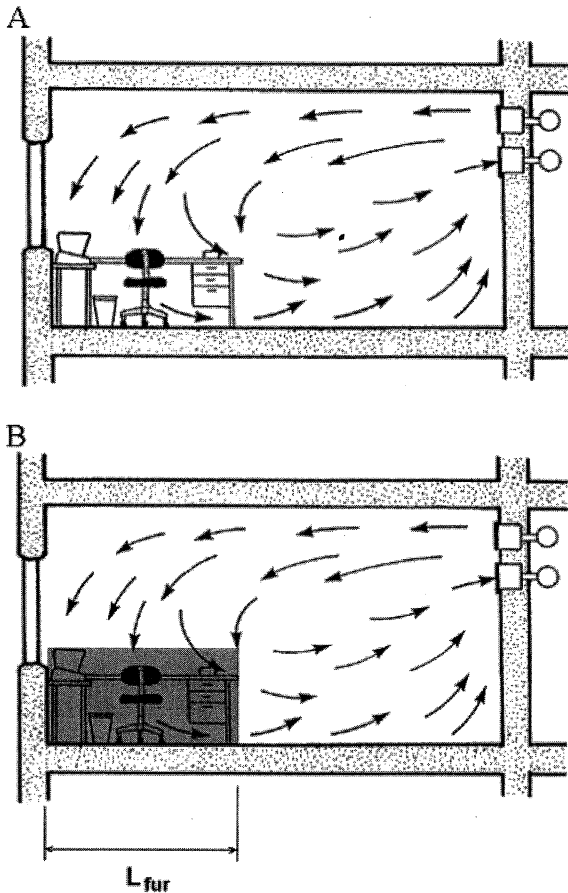


Fig. 10 A: Room with mixing ventilation, isothermal flow and obstacles in the occupied zone. B: The obstacles are replaced by a volume with an additional pressure drop. The length of the furnishings is L_{fur} .

maximum velocity in the two-dimensional wall jet below the ceiling. The obstacles reduce the momentum flow in the wall jet due to a reduction in the forward flow in the low velocity regime of the air movement. It is also typical that the obstacles decrease the vertical gradient of the velocity in the occupied zone but they do not necessarily decrease the volume flow through this area.

It should be stressed that non-isothermal conditions change the results shown in Figs 11 and 12, and they

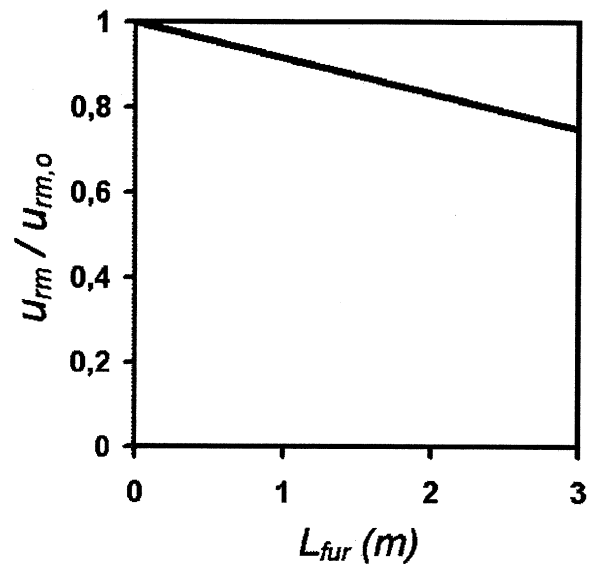


Fig. 11 The ratio between maximum velocity in the occupied zone and the same velocity in an empty room $u_{rm,o}$ vs. the length of the zone with furnishings L_{fur} . Mixing ventilation and isothermal flow (Nielsen et al., 1997).

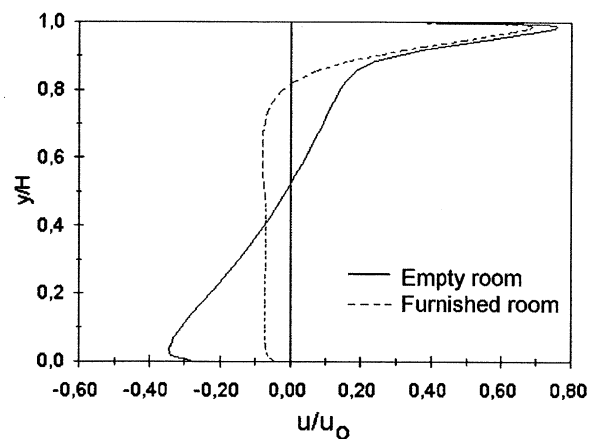


Fig. 12 Velocity profiles in a room with two-dimensional isothermal recirculating flow. The profiles are located outside the length L_{fur} of the occupied part of the flow. The pressure drop in the momentum equations is retained at a value which in this case is high for a furnished room.

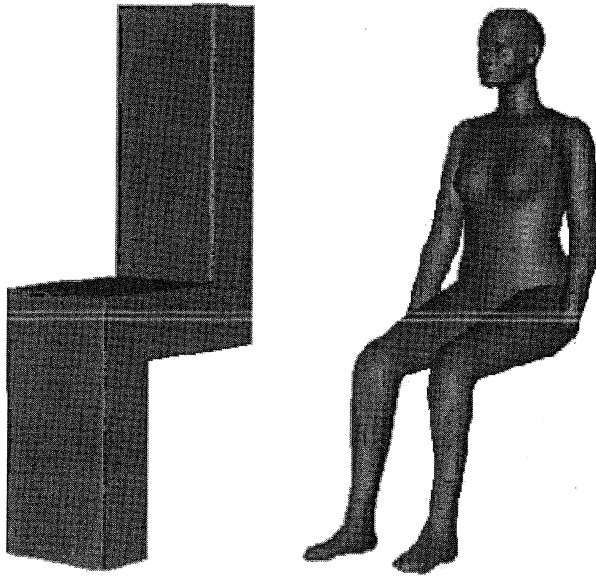


Fig. 13 Two different sets of boundary conditions for a computer simulated person. CSP1 has a height of 1.3 m and an area of 1.61 m², while CSP2 has a height of 1.36 m and an area of 1.52 m².

will often increase the maximum velocity u_{rm} in the occupied zone.

It is in some situations necessary to work with a detailed description of the occupied zone. This is for example the case if problems such as cross infection or passive smoking are considered. Those problems involve prediction of mass flow and concentration distribution in connection with exhalation and inhalation between persons.

How detailed should a detailed description be? This question has been studied by the use of two different grid distributions for a computer simulated person (CSP) (Fig. 13). The simplified geometry is

rectangular (CSP1) and therefore easy to handle in a CFD flow domain, while the other geometry is very detailed (CSP2) and established by an unstructured grid.

The two different models are located in an area with horizontal flow (0.05 m/s) and local as well as global velocities are compared (Topp et al., 2002).

Figure 14 shows the velocity distribution around the computer simulated persons when they are located in a horizontal flow field. It is seen that CSP1 generates a high vertical velocity behind the back compared with the same location at CSP2. The reason is probably the large vertical area and the sharp edges of CSP1. The lack of two separate legs will also influence the flow around CSP1. At some distance from the mannequin the flow is in practice similar.

The concentration distributions in the predictions in Fig. 15 are obtained from a source distributed along the floor in the section where the mannequins are located. The figure shows that there is a large difference in the predicted concentration distribution for the two mannequins. CSP1 shows a very large concentration close to the face, probably due to the upward movement of contaminant from the floor region because of the absence of the separated legs of this model and also because there is some reverse flow above the CSP1.

The predictions in Figs 14 and 15 are a part of a general benchmark test for computer simulated persons (Nielsen et al., 2003).

It is a general conclusion that it is necessary to work with a detailed model in cases such as cross infection, passive smoking and other local air quality problems, while more simplified models can be used when the mannequins act as boundary conditions for a global velocity temperature or concentration distribution in the room.

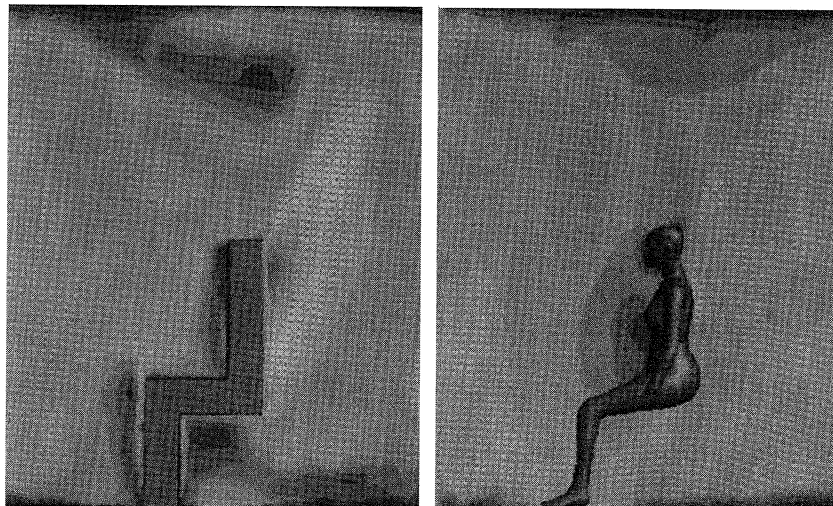


Fig. 14 Velocity distribution around CSP1 and CSP2 in a horizontal flow field of 0.05 m s⁻¹.

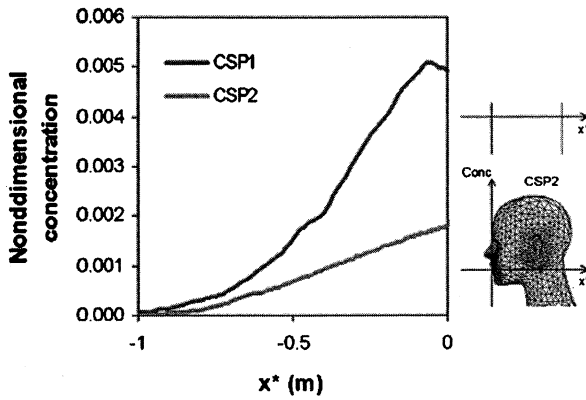


Fig. 15 Concentration distribution in front of the CSP1 and CSP2

Turbulence models and prediction of a three-dimensional wall jet

The quality level of a CFD prediction is not only a question of the applied numerical scheme and number of grid points, it is also a question of the fundamental equations used for description of the problem considered. This chapter discusses this aspect and shows predictions made by both the $k-\epsilon$ model and the Reynolds Stress Model (RSM) in the case of isothermal three-dimensional mixing ventilation (Schälin and Nielsen, 2004), as well as by the v^2-f model (Davidson et al., 2003).

The $k-\epsilon$ turbulence model is based on two transport equations, one for turbulent kinetic energy and one for dissipation of turbulent kinetic energy, and the model is most widely used in all engineering applications including room ventilation. This model was developed for fully turbulent channel flow and is well known to give good predictions in many situations, but also known to show deficiencies in some types of flow, which limits the accuracy for general applications.

An important limitation of the $k-\epsilon$ model is the assumption of turbulence isotropy. This model solves the turbulent kinetic energy k , which is an expression based on the fluctuating velocity components, and it solves the dissipation rate ϵ of the turbulent kinetic energy. The three fluctuating velocity components are treated equally in the expression for k . Individual influences of the fluctuating quantities on the flow are, however, quite important for some types of flow. Such effects are taken into account in anisotropic turbulence models as the RSM.

The following text deals with wall jets that are found frequently in mixing ventilated rooms with high velocity air terminal devices. It is known that the growth rate parallel to surfaces in a three-dimensional wall jet is too small when the $k-\epsilon$ model is used in the predictions (Craft & Launder, 2001). The reason for failure of the $k-\epsilon$ model in the wall jet predictions can

be ascribed to the fact that the damping of the turbulent velocity fluctuations perpendicular to the wall (an anisotropy effect) is inherently absent in the $k-\epsilon$ model. In the following text it is shown that the improvement can be obtained by the use of a RSM.

The CFD simulations have been made by the use of a commercial code. The turbulence models applied are the standard $k-\epsilon$ model and the RSM with the so-called wall reflection terms following the standard RSM approach described by Launder (1989). The wall reflection terms are responsible for the redistribution of normal stresses near the wall. They damp the turbulent fluctuations perpendicular to the wall and convert the energy to the fluctuations parallel to the wall. The calculated jet width perpendicular to the wall will be smaller, and the calculated jet width parallel to the wall will be wider, which is identical to the behavior in a real wall jet. The RSM without the wall reflection terms as well as other turbulence models is not able to take this effect into account.

The predictions are made in a room with the dimensions, $h/H = 0.025$, $W/H = 4.7$, $w/W = 0.2$ and $t/H = 0.16$ (Fig. 16). The Reynolds number is equal to $Re = 4700$ based on the inlet height h . Two sets of geometric set-ups are studied, first a deep room with the length $L/H = 12.0$, and then a room with a conventional length of $L/H = 3.0$.

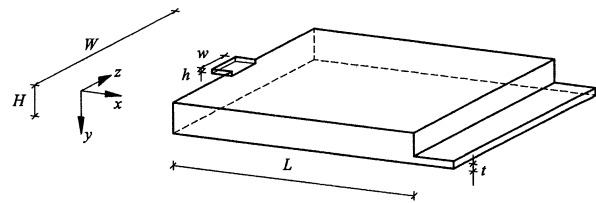


Fig. 16 A wide room with a single ventilation opening located below the ceiling. The room has two different lengths with L/H equal to 12.0 and 3.0, respectively.

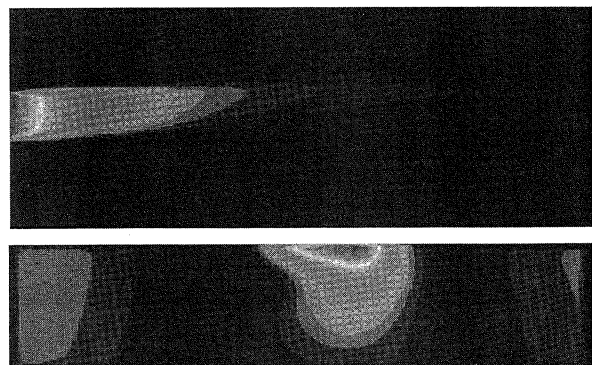


Fig. 17 Predicted flow in a deep room with a $k-\epsilon$ turbulence model. The upper illustration shows air flow in a horizontal top plane close to the ceiling ($y = 0.016 H$). The lowest illustration shows the air flow perpendicular to the wall jet in a vertical plane ($x = 4 H$).

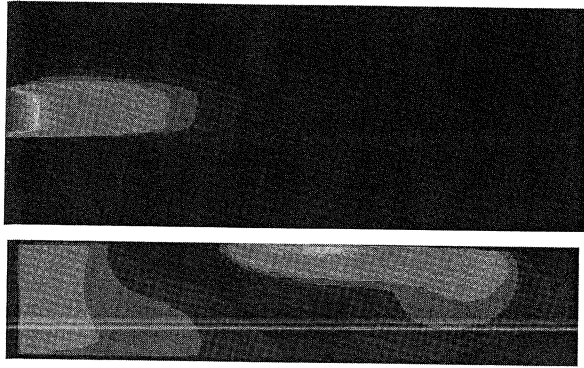


Fig. 18 Predicted flow in a deep room with a Reynolds stress turbulence model. The upper illustration shows air flow in a horizontal top plane close to the ceiling ($y = 0.016 H$). The lowest illustration shows the air flow perpendicular to the wall jet in a vertical plane ($x = 4 H$).

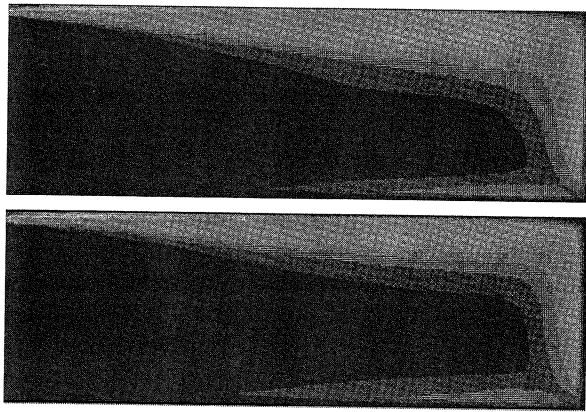


Fig. 19 Air flow in vertical mid-plane ($z = 0.5 W$). The upper illustration shows predictions based on the $k-\epsilon$ model and the lowest illustration shows predictions based on the Reynolds Stress Model.

Figures 17 and 18 show the predictions for a deep room made by a $k-\epsilon$ model and a Reynolds Stress Model with wall reflection terms, respectively (Schälin, 1999). The flow in the wall jet is different in the two cases. The growth rate of the wall jet perpendicular to the ceiling has the same level as in the direction parallel to the ceiling in the case where the $k-\epsilon$ model is used as a turbulence model. The RSM predictions with wall reflection terms show a growth rate parallel to the ceiling which is much higher than the growth rate perpendicular to the ceiling. This is in agreement with measurements.

The two predictions show that the flow in the occupied zone is also influenced by the turbulence model. The jet penetrates the lower part of the room with return flow on both sides of the jet when the $k-\epsilon$ model is used. The Reynolds stress model predicts a flow where the jet is attracted by one of the side walls in the room with return flow at the opposite side. This is in agreement with earlier measurements (Nielsen, 1974; Schälin & Nielsen, 2004).

The $k-\epsilon$ model is widely used in CFD predictions of room air distribution. The problem with incorrect prediction of the growth rate in a three-dimensional wall jet seems not to be a large problem in rooms of more conventional geometry. Figure 19 shows two predictions in a room with the length $L/H = 3.0$ (Schälin, 1999). The vertical growth rate of the jet in the two predictions based on the $k-\epsilon$ model and the Reynolds Stress Model has different values, but this has only a small influence on the flow in the jet. The flow in the occupied zone is rather similar in the two cases because the room has a short length compared to the penetration length of the jet in a deep room with the same cross-section.

The v^2-f model is a model where the wall-normal stress $\overline{v^2}$ is solved by a separate transport equation. A low Reynolds $k-\epsilon$ turbulence model with a v^2-f extension is not able to predict the growth rate δ_z parallel with the ceiling with a result which is better than the predictions found by the $k-\epsilon$ model alone (Davidson et al., 2003).

Conclusions

Computational fluid dynamics has been used for many years as a research tool for room air movement. It is important to consider the quality of CFD predictions because of the widespread use of the method.

It is concluded that numerical schemes with a second or third order of accuracy should be used whenever it is possible instead of schemes with first order of accuracy, but in some situations it can be difficult to obtain converged solutions by the last mentioned schemes.

Simulation of air terminal devices is an important part of a CFD prediction. The flow in a room is often controlled by the momentum flow from the supply openings and the quality of those boundary conditions therefore influences the total results of the predictions. The simplified boundary conditions, the box method and the prescribed velocity method have been discussed. Simplified boundary conditions are easy to describe but it is necessary to make several sets of predictions to obtain a certain level of quality. The box method and the prescribed velocity method work well when a wall-jet description of the flow from the diffuser is present. Increased computer capacity makes a direct description of the diffuser possible in practice.

It can be necessary to make predictions of the flow in an occupied zone with furniture and other obstacles. A promising method is to predict the flow in a global situation where the occupied zone is considered as a uniform volume with an additional pressure drop (in the momentum equations). A more detailed method is to take account of the details of the obstacles, which is necessary when predictions are made for problems

such as cross infection and other predictions involving local concentration distribution.

The $k-\epsilon$ turbulence model is an acceptable model in many situations in room air movement, but it is shown that the three-dimensional wall jet behavior can be

predicted with a higher accuracy by the use of wall reflection terms included in the RSM. A v^2-f model does not improve the prediction of a three-dimensional wall jet.

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