Air Diffusion and Solid Contaminant Behaviour in Room Ventilation – a CFD Based Integrated Approach

Doctoral Thesis

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ABSTRACT

One of the most fundamental human needs is fresh air. It has been estimated that people spend comparatively much time in indoor premises. That creates an elevated need for high-quality ventilation systems in buildings. The ventilation airflow rate is recognised as the main parameter for measuring the indoor air quality. It has been shown that the ventilation airflow rates have effects on respiratory diseases, on “sick building syndrome” symptoms, on productivity and perceived air quality. Ventilation is necessary to remove indoor-generated pollutants by diluting these to an acceptable level. The choice of ventilation airflow rate is often based on norms or standards in which the airflow rate is determined based on epidemiological research and field or laboratory measurements. However, the determination of ventilation flow rate is far more complex. Indoor air quality in the occupied zone can be dependent of many factors such as outdoor air quality, airflow rate, indoor generation of pollutants, moisture content, thermal environment and how the air is supplied into the human occupied zone. One needs to acknowledge the importance of air distribution which clearly affects the comfort of occupants. To design a ventilation system which considers all aspects of room ventilation can only be achieved by computer modelling. The objective of this thesis is to investigate air diffusion, indoor air quality and comfort issues by CFD (computational fluid dynamics) modelling. The crucial part of the CFD modelling is to adopt BCs (boundary conditions) for a successful and accurate modelling procedure. Assessing the CFD simulations by validated BCs enabled constructing the ventilation system virtually and various system layouts were tested to meet given design criteria. In parallel, full-scale measurements were conducted to validate the diffuser models and the implemented simplified particle-settling model. Both the simulations and the measurements reveal the full complexity of air diffusion coupled with solid contaminants. The air supply method is an important factor for distribution of heat, air velocity and solid contaminants. The influence of air supply diffuser location, contaminant source location and air supply method was tested both numerically and by measurements to investigate the influence of different parameters on the efficiency of room ventilation. As example of this, the well-known displacement ventilation is not fully able to evacuate large 10 µm airborne particles from a room. Ventilation should control the conditions in the human breathing zone and therefore the ventilation efficiency is an important parameter. A properly designed ventilation system could use less fresh air to maintain an acceptable level of contaminant concentration in the human breathing zone. That is why complete mixing of air is not recommended as the ventilation efficiency is low and the necessary airflow rate is relatively high compared to other ventilation strategies. Especially buoyancy-driven airflows from heat sources are an important part of ventilation and should not be hampered by supply airflow from the diffusers. All the results revealed that CFD presently is the only reliable method for optimising a ventilation system considering the air diffusion and contaminant level in all locations of any kind of room. The last part of the thesis addresses the possibility to integrate the CFD modelling into a building design process where architectural space geometry, thermal simulations and diffuser BCs could be embedded into a normal building design project.

KEYWORDS: CFD modelling, airflow rate, ventilation efficiency, diffusers, solid contaminants, IAQ
PREFACE

This thesis is submitted in accordance with the conditions for attaining the PhD degree at KTH (The Royal Institute of Technology).

The work presented in the thesis has been carried out as a collaboration work between KTH South Department of Constructional Engineering and Design and KTH Department of Energy Technology as well as industry partners, i.e. former ABB Ventilation (now Fläkt Woods), Halton OY and Olof Granlund OY. The following work was funded by the industrial partners and started with a project “Improved Ventilation and Filtration”. The main focus of this project was on airborne particle control, thermal comfort, energy use and healthy indoor conditions.

The thesis has been completed with the help of many individuals and I wish to express my sincere gratitude to my supervisor Sture Holmberg and all collaboration partners who participated in this project. Above all I want to thank Reijo Hänninen who arranged a way to finance my studies during the years 2003-2004.

Special thanks goes to my many co-authors Hannu Koskela, Kim Hagström, Panu Mustakallio, Tuomas Laine for making this thesis a fruitful experience. My fellow doctoral students at KTH Syd need special recognition and I encourage them to go on with their research.

I also want to thank my colleagues at KTH South, R&D staff at Halton OY and Olof Granlund OY who have helped me morally and financially during my PhD studies.

The language of the summary and the appended papers in the thesis were mainly checked by Christina Hörnell at KTH who made my English more understandable and easier to read.

Finally I want to express my gratitude to my family and friends. My wife Silja and sister Irene have helped me very much during 3½ years of PhD studies. There have been some ups and downs during this time, when sometimes I did not believe myself to be able to finish. Nevertheless my 22 years of school time have come to an end and this thesis is a proof of what I have learned during that time. Most of the work done during the PhD studies is uploaded on my personal homepage at http://eplet.syd.kth.se/~gery.

Gery Einberg
April 2005
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ABBREVIATIONS

AC – air conditioning
ACH – air exchange rate
CAD – computer aided design
IAQ – indoor air quality
3D – three dimensional
ATD – air terminal device
BC – boundary conditions (plural BCs)
CFD – computational fluid dynamics
DNS – direct numerical simulation
HVAC – heating, ventilation and air conditioning
IFC – industry foundation classes
nd – non-dimensional
PC – personal computer
PM – particulate matter
PM$_{2.5}$ – particulate matter $< 2.5 \, \mu m$
PM$_{10}$ – particulate matter $< 10 \, \mu m$
PMV – predicted mean vote
PPD – predicted percentage of dissatisfied
RH – relative humidity
RSP – respirable suspended particles
UFP – ultra fine particles
TSP – total suspended particles
VOC – volatile organic compounds
NOMENCLATURE

\( a \) acceleration (m/s\(^2\))
\( A \) area (m\(^2\))
\( Ar \) Archimedes number (nd)
\( C \) concentration (kg/m\(^3\))
\( Cd \) dimensionless drag coefficient (nd)
\( d \) diameter (m)
\( DR \) draught rate (\%)
\( E \) energy (W)
\( F \) momentum (force) (N)
\( g \) acceleration due to gravity (m/s\(^2\))
\( Gr \) Grashof number (ratio of buoyancy forces to viscous forces, nd)
\( H \) height (m)
\( h \) enthalpy (kJ/kg)
\( h_j \) enthalpy of species \( j \) (kJ/kg)
\( J_j \) diffusion flux of species \( j \) (kg/m\(^2\)s)
\( K \) correction factor describing the particle growth in humid air (nd)
\( k \) turbulent kinetic energy (J/kg)
\( l \) turbulent length scale (m)
\( l_k \) Kolmogorov length scale (m)
\( m \) mass flow rate of contaminants (kg/s)
\( m \) mass of contaminants (kg)
\( N \) number (particles, cells etc., nd)
\( o \) coefficient for discretization equation (nd)
\( P \) heat transfer from heat sources (W)
\( p \) pressure (N/m\(^2\) or Pa)
\( Q \) airflow rate (m\(^3\)/s)
\( Q \) mass flow rate (kg/s)
\( R \) under-relaxation factor (nd)
\( R^\phi \) residual of scalar quantity (nd)
\( Re \) Reynolds number (nd)
\( S_c \) volumetric source value (N/m\(^3\))
\( S_0 \) source term for discretization equation (by variable)
\( S_h \) source term in energy equation (W/m\(^3\))
\( S_p \) relative particle-settling factor (nd)
\( T \) temperature (K)
\( t \) time (s)
\( Tu \) turbulence intensity (\%)
\( v \) velocity (m/s)
\( V \) volume (m\(^3\))
\( v^+ \) wall non-dimensional velocity (nd)
\( u, v, w \) three velocity components (also written as \( v_x, v_y, v_z \) m/s)
\( x, y, z \) coordinates \( (x=Y, y=Y, z=Z) \) also subscripts
\( y^+ \) non-dimensional length parameter for walls (nd)
Greek symbols

- \( \alpha \) angle (°)
- \( \alpha_c \) local convective heat transfer coefficient (W/m²K)
- \( \alpha_d \) deposition value (kg/s)
- \( \alpha_k \) volume fraction of phase \( k \) (nd)
- \( \beta \) volume expansion coefficient (1/K)
- \( \delta \) standard deviation (by variable, for velocity m/s)
- \( \Delta_s \) displacement vector (m/s)
- \( \varepsilon \) rate of dissipation of turbulent kinetic energy (J/kgs)
- \( \varepsilon_C \) contaminant removal efficiency (nd)
- \( \varepsilon_T \) heat removal efficiency (nd)
- \( \varepsilon_l \) local ventilation efficiency (nd)
- \( \varepsilon_v \) ventilation efficiency (nd)
- \( \phi \) scalar quantity (nd)
- \( \Gamma_c, \Gamma_\phi \) diffusion coefficients for \( C \) and \( \phi \) (m²/s)
- \( \lambda \) thermal conductivity (W/mK)
- \( \mu \) dynamic viscosity (kg/ms)
- \( \rho \) density (kg/m³)
- \( \tau \) time constant (s)
- \( \upsilon \) kinematic viscosity (m²/s)

**Empirical non-dimensional constants for \( k-\varepsilon \) turbulence model**

- \( C_{\mu} \) 0.09
- \( C_{1\varepsilon} \) depends on flow type
- \( C_{2\varepsilon} \) depends on flow type
- \( \sigma_k \) depends on flow type
- \( \sigma_\varepsilon \) depends on flow type

**Subscripts**

- 1,2,3 particle index
- a air value
- bz breathing zone value
- c convective
- cc cell centre value
- \( D \) drag value
- f face value
- g gravitation value
- hi highest allowed (harmful) value
- i free index
- in supply opening (inlet) value
- l local value
- m mixture value
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<tr>
<td>n</td>
<td>normal value</td>
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<tr>
<td>nb</td>
<td>neighbouring point value</td>
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<td>nd</td>
<td>non-dimensional value</td>
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<td>nw</td>
<td>normal grid wall value</td>
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<td>old</td>
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<td>R</td>
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<td>rad</td>
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<tr>
<td>t</td>
<td>time-dependent value</td>
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<tr>
<td>tot</td>
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<tr>
<td>turb</td>
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<td>w</td>
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<tr>
<td>v</td>
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<td>z</td>
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<td>ΔT</td>
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<tr>
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<td>τ</td>
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LIST OF PUBLICATIONS

The thesis comprises the following nine papers which are referred to by their Roman numerals:


VII. Einberg G, The Influence of Airflow Profile and Heat Source Location on Heat Removal Efficiency, Accepted for publication in Energy and Buildings


IX. Einberg G, Laine T, Holmberg S, CFD Modelling as a Part of Integrated Design Process for Optimized Indoor Environment, submitted to Automation in Construction

The author is the principal author of publications Papers I, III-IX. In Paper II the author was responsible for analysing the measurement results from the ABB Enköping laboratory and simulation results. The CFD simulations in Papers I & II were carried out by the co-author Sture Holmberg. The measurement results in Papers II & V-VII were performed as a collaboration work, which means that actual measurements on site were carried out by co-authors or collaborators.
1 INTRODUCTION

In this thesis the main focus is the influence of air diffusion on thermal conditions and airborne particle concentrations. The task is to systemise the many aspects of modelling involved in a building project. Computer modelling is a vital part of everyday design in a building project. CFD modelling gives an opportunity to assess the indoor climate by virtually constructing a room and testing different system layouts to meet the predetermined design criteria. A successful design of a ventilation system points out the need for a total system view concerning air diffusion, thermal conditions and solid contaminant behaviour. Until now these parts have been performed separately. Simulating only one part implies the risk that the designed system meets the requirements of, for instance, air velocity level in a human occupied zone, but fails to remove harmful pollutants. Typically the IAQ (indoor air quality) is assessed by means of total airflow supplied to the room, which should not be the only considered parameter in room ventilation because the air supply method and room internal configuration as well as heat sources have considerable effects on room air diffusion. Additionally air diffusion has effects on thermal conditions, moisture, draught and the concentration of solid contaminants in different parts of the room. That is why the design of ventilation systems and AC (air conditioning) should be integrated considering all aspects of IAQ problems.

Given that each discipline has a different view and interpretation of its special part of the modelling, the author hopes to contribute with integrating these disciplines. The research on air diffuser BCs (boundary conditions) and particle research are classically done separately. Nevertheless, the particle or contaminant concentration is greatly dependent on air diffusion in the room. To model the interaction of air diffusion and solid contaminant behaviour one needs validated models from both calculation disciplines. Moreover, the modelling of indoor environment relies on many input parameters such as diffuser BCs, wall conditions and models of calculating the concentration of solid contaminants. All the input parameters used in CFD should be carefully determined and the choice of certain models or BCs should be well justified. To improve the CFD modelling the author has introduced a new concept on how the fluid and contaminant modelling can be coupled with a building’s design process to optimise the indoor environment. This is a fundamental way to improve the pre-design of various ventilation systems by using reliable numerical input parameters generated for CFD simulation in various stages of any kind of building project. In parallel many simplified models of different types of air diffusers and a drift-flux particle model with an Eulerian approach were further developed during the project.

The first goal for the project was to test an air diffuser which could control airborne particle concentration in the occupied zone in a normal office. The other goal for this research aimed at developing a new type of ventilation system or configuration where all contaminants (gases as well as different-sized particles) should be controlled and efficiently evacuated. It is a well-known fact that most ventilation and air conditioning systems are designed without too much concern about how solid contaminants behave in the ventilation airflow. For displacement ventilation systems designers normally assume all pollutants to be following the buoyant airflow into an upper zone where they are evacuated. This is, however, seldom the case. Studies show that settling RSP (respirable suspended particles) are found in increasing concentrations in the breathing zone where the exposure concentrations can be a health hazard to occupants (Mattsson,
The question on how ventilation systems should be designed to eliminate RSP from the breathing zone is here emphasised. The supply and exhaust conditions of the ventilation airflow are shown to play an important role in the air quality control. Other important parameters include air velocity, air temperature, heat load in the room and particle characteristics. It is also important to find out which kind of air distribution method should be used to reduce the particle concentration in a room. That is the main reason why this thesis consists of many known research topics such as particle modelling, simplified diffuser BCs for CFD modelling and the integrated approach for coupling building energy programs, diffuser selection programs for the CFD modelling to improve the overall simulation results. Current research practice lacks this kind of expertise. It is understandable that to perform a high-quality CFD particle simulation one needs to have broad knowledge associated to the diffuser BCs, wall BCs and other BCs in conjunction with operating a particle model within the CFD. The results from this thesis hopefully contribute to the improved knowledge concerning several aspects of CFD modelling. There is still no standardisation or fundamental way to perform CFD simulations concerning choice of diffusers from the manufacturer, although there is a strong effort to create guidelines on how to perform the simulations, how to verify, validate and report the CFD modelling results (Casey & Wintergerste, 2000, Chen & Srebric, 2001, www.ercoftac.org). At present clear instructions on how to insert the air diffuser into the CFD simulation case have not been presented. For instance grid layout and the choice of model treatment such as the prescribed velocity method on the boundary of the diffuser or the box method or something else is entirely an open issue for the CFD user. As CFD modelling has gained more popularity it is very necessary that the choice of sub-models in CFD should be well justified and based on reliable input data.

Another concern in the present work was to study ventilation configurations numerically by reference examples and hereafter modify system solutions for improved function by using CFD. The IAQ assessment included a minimised risk of high exposure levels in the breathing zone as well as a low risk of cross infection in the room. The simulations consisted of tasks such as space cooling with the ventilation air by testing various locations of ATDs (air terminal devices) as well the spatial relationships between the heat sources vs. diffuser location.
2 SUMMARY OF PAPER CONTRIBUTIONS

The main aim of the conducted research was to develop and link together many aspects of CFD modelling. A significant part of the work is devoted to the most important pollutant indoors, airborne particles Papers I-IV & VIII. Many recent studies have shown that increased concentration of environmental PM (particulate matter) is related to many respiratory diseases (Ormstad, 2000). To model this is a complicated task and needs many numerical input values. In the following objectives of and contributions from the included papers are highlighted.

The main task of Paper I was to find out how particles behave in a room with multiple heat sources. Particle concentration in a room was modelled by using simplified models of humans and low velocity diffusers. The modelling was achieved with a simple Eulerian-approach drift-flux particle model. Special topics investigated in this paper were particle spread pattern and source behaviour. Simulations revealed that the floor can be both particle sink and source. The modelled 10 µm particles followed the buoyant airflows created by the heat sources. This was based on modelling particle concentration in a classroom with multiple heat sources representing pupils. The paper used displacement ventilation and preliminary results showed that large particles, 10 µm, do not follow the air streams exactly. The paper revealed that particles tend to accumulate in the space and can be found in the corners of the room rather than following the main air stream to the exhaust outlet.

Both measurements and numerical simulations of particle behaviour in a reference room with displacement ventilation are evaluated in Paper II. A comparison between measured and CFD simulated results was performed. The results indicate that the wall function treatment in the numerical simulations is unable to fully deal with the convective heat transfer from solid boundaries. The experimental work suffered from limitations in generating low particle mass flows from the particle source. The experience from this investigation shows the importance of working with measurements and simulations in parallel. Guidelines on how to combine results are discussed in this paper. Accurate control and good understanding of different parameter variations are emphasised.

The behaviour of particles in airflow is important for identifying those in various locations in a ventilated space. The main aim of Paper III was to propose a new modelling concept and perform a literature review about particle research. The new proposed model includes different-sized particles, with realistic distribution. The particle diameter for the model is chosen by the specific behaviour in air. As most particle models suffer the limitation of non-existing distribution, the new model approach suggests that particles can be divided into three groups by their behaviour. This makes the particle model more systematic and covers all different sizes of particles found in ambient air. The proposed modelling approach is presented and used later in Paper VIII.

Paper IV reports on the differences in particle removal efficiency for various locations of supply and exhaust devices. Numerical simulations were carried out in a simple test room to illustrate the particle concentrations with different configurations of room ventilation. Several particle sizes were used and the influence of different flow patterns and air change rates were investigated. Particles were supplied to the room with the incoming air. Isothermal conditions
with varying air supply velocities were used in the paper. Preliminary results indicated that particle removal efficiency is not predominantly influenced by air exchange rate; the location of the supply or exhaust device had been underestimated as an indicator of the particle elimination process.

The main objective in air diffuser research is creating reliable BCs for CFD modelling. Paper V focused on studying simplified BCs for a new type of air diffuser. The model of the diffuser was validated by careful full-scale laboratory measurements. Preliminary results show that simplified BCs performed quite well in predicting velocity field and thermal behaviour in the near zone of the diffuser. Additionally Paper VI used similar methods for describing BCs for a high induction swirl diffuser. Turbulence was modelled in this paper by a \( k-\varepsilon \) RNG model for swirl-dominated flow. The paper confirmed that the simplified BCs provided by the manufacturer could model diffuser performance accurately enough not only very close to the diffuser, but also in other parts of the ventilated room.

Paper VII summarises the results of 10 simulation cases with the two types of air diffusers used in Papers V & VI. All the 10 simulation cases were confirmed by full-scale laboratory measurements. This paper focused on how the air distribution method influences the heat removal efficiency of the system. Parameters such as heat source location, heat source strength, airflow rate and type of air diffuser were studied in connection with the heat removal efficiency. The paper confirmed that if a designer can use reliable diffuser BCs for the CFD modelling it is possible to optimise the ventilation for removing excess heat and contaminants. The critical interaction between plume airflow and diffuser supply airflow can only be modelled in CFD programs. The paper revealed that the CFD simulation method is superior to analytical methods in designing cooling with the ventilation air.

Multi-zone methods are primarily used for evaluating the airflow behaviour between compartments or rooms in a building. Paper VIII uses a multi-zone method to evaluate the particle mass transport within one room. This new application improves the evaluation of the results from particle simulations. The particle model was adopted from Paper III. In this paper two different particle sizes were used to evaluate simulated mixing and displacement ventilation in a small office. The low velocity ATD (air terminal device) used in the modelling was similar to the one used in Paper II and high velocity diffuser model was adopted from the manufacturer’s database. Both diffusers were modelled by simplified means. Modelling the contaminant source from the floor level represented conditions similar to a dusty floor. The multi-zone model approach showed that similarly to the study in Paper I most of the particles follow the convective plumes generated by the heat sources. The method also revealed the exact locations (in rooms) where particle contamination is to be expected.

The last paper, Paper IX, deals with improving the CFD application to optimise the indoor environment through using an integrated design process. The integrated design process is a method to systemise a building project in such a way that earlier calculations and design processes may promote the quality of the CFD simulation. This paper summarises the research done in previous articles by an example calculation of an office.
3 OBJECTIVES

The primary goal of the conducted research was to develop and link together many aspects of indoor air modelling. A significant part of the work is devoted to the primary pollutant indoors, airborne particles. The main problem of this thesis was to pinpoint the importance of different variables within the modelling. Comparatively many of the articles in the thesis are devoted to the modelling of air diffusers as they are primary engines behind the airflow behaviour in a space. The air diffuser performance is evaluated by how it removes the excess heat and airborne particles from a ventilated room. All the diffuser articles contain full-scale laboratory measurements which confirmed the modelling accuracy. Airflow behaviour of various diffuser types was evaluated in the testing facility. This verified that the diffuser type clearly affects the indoor airflow field. It is a well-known fact that the indoor airflow pattern influences the concentration of harmful contaminants in a room. That is why the modelling of solid contaminants as primary pollutants is in focus in this thesis. Furthermore the airflow pattern evidently influences also the concentration of solid contaminants in the human breathing zone. A major part of the thesis is devoted to investigate how the air distribution design affects the concentration of solid contaminants in various locations of a ventilated room. Different positions of ATDs and many particle diameters were investigated to find the reasons why some parts of a room are more contaminated than others.

It is expected that the thesis will contribute to a better knowledge of ventilation system functions. The methods presented here may improve future system designs. The CFD simulation is the main method for assessing the IAQ problems through the entire room space. There are two main topics in this thesis, i.e. air distribution design and airborne particle control using ventilation air. This thesis introduces the idea that the CFD modelling should be integrated more with ordinary building design to improve the overall modelling results. This can only be achieved when all the modelling variables are well justified. For instance, if one considers performing a CFD simulation of particle concentration in a room it is necessary to have a high-quality model of air diffuser(s) as well as of particles. If the BCs given to the air diffuser contain errors the simulation can never produce usable results from the particle modelling. That is why feasible results in “real rooms” can be achieved only by integrating different modelling disciplines into one core as different models depend on each other, Fig. 1.
Fig. 1. Data flow in the CFD modelling process in connection with error possibility

The procedure from the user-defined problem towards later result evaluation contains many steps. All of the steps in Fig.1 should be performed carefully as incorrectly determined space geometry could affect the quality of airflow or contaminant simulations.

Defining the IAQ modelling problem contains typically many steps, and especially in 3D, problems should be based on architectural CAD design which should not be oversimplified as the geometry of the room and obstructions clearly affect the room airflow pattern (Hagström, 2002). The BCs associated with the air diffusers have the same effect on the airflow simulation as well as the particle simulation results.

The research is based on commercial CFD platforms and one need to recognize some limitations of these programs as there is very little possibility to change the methods and models used within the software. However there are very few investigations on how to improve the modelling considering gathering of the input parameters for the simulation. That is why the designer can model a diffuser with simplified means or construct the diffuser in a CFD pre-processor based on actual real geometry. As there exists many different methods of how to describe the BCs for an air diffuser, it can be very confusing to the CFD user. That is why the CFD modelling needs more systematisation considering BCs as well as modelling methods and models to improve the end result.

The specific objectives for the research were:

- To develop and validate a particle-settling model including a realistic distribution of particles in atmospheric air
- To study the influence of air supply method on
  - Air diffusion
  - Thermal behaviour
  - Solid contaminant behaviour in different parts of the room
- To study the efficiency of different ventilation systems concerning
  - Solid contaminants
- Excess heat
- Spatial relationships
- Different types of air diffusers
- Various locations of air diffusers

- To develop and validate different air diffuser models for CFD modelling
  - Low velocity diffuser
  - High velocity diffuser – swirl diffuser
  - Industrial air diffuser

- To evaluate the room ventilation by different ventilation configurations
  - Mixing ventilation
  - Displacement ventilation
  - Zoning strategy

- To develop a new method for how to evaluate the particle simulation results – multi-zone approach.

- Conducted research hopes to answer questions as:
  - How improve various air diffuser models in CFD?
  - How does the air supply method influence room airflow velocity, thermal and contaminant behaviour?
  - How improve the particle modelling in CFD?
  - How improve the evaluation of particle modelling results?
  - Where do the particles reside in a ventilated room?
  - Which air supply method is the best for removal of particles of all sizes?
  - Is it possible to adopt BCs from other calculation disciplines?
  - Which spaces actually need CFD modelling?
  - Can CFD modelling be more integrated into the building design process?
4 THE IMPORTANCE OF MODELLING THE INDOOR CLIMATE

The indoor air is something that people are exposed to during the major part of their lives. Most people spend most of their time in artificial climates such as work/home environments and transport vehicles (Brohus, 1997, Luo, 2003, Matson, 2004). Clean air in a room is an essential component for a healthy indoor environment. Air is considered to be polluted when it contains certain substances in concentrations high enough and lasting long enough to cause harm or undesirable effects. In indoor environments, particles are the main cause of air pollution and of adverse effects on human health (Jones, 1999). It is a well-known fact that indoor pollution originates from indoor processes and from outdoors. This makes the IAQ problems very complex. The personal exposure to contaminants is primarily affected by the ventilation airflow and that is the function of total airflow rate in a closed compartment (room) as well as local airflow behaviour (Brohus, 1997). Essentially, a human is exposed to the contaminants which are found in the occupied zone. If one considers that the heat sources generate convective plumes, which are also part of the indoor airflow field then the modelling of indoor pollution without sophisticated computer software tools is almost impossible. Cold draughts from windows, convective plumes from radiators, plumes above human heads and airflow created by air diffusers are combined to the total indoor airflow field. Most of the contaminants such as CO₂, SO₂, CO, NOₓ etc. move in the same manner as the primary airflows and do not constitute an extra challenge for the modelling. But this is not the case with solid airborne particles, because they have a different behaviour than the primary airflows. Particles in indoor environments can contain inorganic and organic constituents such as PAH, VOC, foreign proteins, bacteria, different chemicals, parts of different materials etc. and they are also carriers of odours. All the particles found in ambient air have some distribution from small size ultra-fine particles to comparatively large particles (Kocifaj & Lukac, 1995). Comparatively large particles, 20 µm, have a strong settling behaviour which needs to be considered when calculating the indoor concentration. The concentration of different-sized particles indoors is a challenging task, because the concentration is determined by the kinetic properties of the fluid (air) and other external forces that act on the particles, including the settling velocity (Murakami et al., 1996). Another important property of particles is their deposition on internal wall surfaces. Solid contaminants tend to accumulate in a ventilated space with low level of supply air, and then they become the sources of later indoor contamination. Therefore it is extremely difficult to determine the particle sources for the modelling as they come from outdoor air, are generated indoors and sink/source behaviour is affected entirely by the indoor airflow field. It can be concluded that particle concentration in room air is an important measure of IAQ though environmental tobacco smoke has been the focus of researchers for decades (Hackshaw et al., 1997, Armitage et al., 1997).

4.1 Ventilation and air supply principles

Ventilation is the process of supplying fresh air to an enclosed space in order to refresh/remove/replace the existing atmosphere. Ventilation is commonly used to remove contaminants such as gases, dust occurring as particles or vapours and provide a healthy and safe working environment; in other words, it is an engineering control. It can be accomplished by natural means (e.g., opening a window or door) or mechanical means (e.g., fans or blowers).
Natural ventilation effects are uncertain, unreliable and difficult to control. The room airflow motion is entirely created by indoor and outdoor temperature and/or pressure differences through infiltration and ex-filtration (Einberg, 2001). It may be satisfactory in some cases, but mechanical ventilation has become an essential part of good ventilation. Ideally, ventilation provides constant temperature, humidity and air quality within the enclosed space. To be more specific it is necessary to control air quality in the human-occupied zone. This can be achieved by air diffusers of different kinds and with various ventilation methods. Usually devices controlling the room ventilation are called ATDs (air terminal devices), a general term used to describe supply, exhaust or transfer diffusers and grilles.

4.1.1 Mixing ventilation

In mixing ventilation, fresh air, $Q_{in}$, is supplied at a high momentum to induce overall recirculation of air and promote sufficient mixture of contaminants and fresh air, Fig. 2. It is thus aimed at diluting the contamination level, $C_R$, down to an acceptable level in all parts of the room. In mixing ventilation the air is typically supplied to the space at ceiling level with a high momentum in order to create a well-mixed flow field without any concentration gradients or temperature gradients in the ideal case. In mixing ventilation the supply conditions will mainly determine the velocity conditions, $v_R$, in the room (Djuanedy & Cheong, 2002, Zoe, 2001). In mixing ventilation air jets are primary factors affecting room air motion.

Mixing ventilation has its advantages and disadvantages. The ideal mixing ventilation uses comparatively high supply airflow rate, $Q_{in}$, which makes it an inefficient solution concerning the energy aspects. The high initial momentum from the air diffuser should be sufficient to mix the air in the room. This means that the diffuser has a high pressure loss, high noise pressure level and fans in such a system consume more electricity as the electrical energy used in the system is a function of the total pressure loss of the system. The significant advantage of mixing ventilation is the easier calculations of the system. The system can be calculated using a simple mass-balance model to assess the concentration level in the room. However, the mixing ventilation system seldom works ideally. The real working systems reveal local concentration gradients which can expose occupants to higher doses of contaminants, $m$, than calculated (Rodes et al., 1991, Brohus & Nielsen, 1995). This configuration was assessed by calculating the particle concentrations in Papers IV & VIII which also revealed local concentration gradients.
4.1.2 Displacement ventilation

In displacement ventilation, cooled fresh air, $Q_{in}$, is supplied at floor level with low momentum by low velocity diffuser(s), Fig. 3. Sometimes this configuration is called stratification ventilation, because the flow field is almost entirely created by density, $\rho_a$, differences. The ventilation air will naturally move from the human occupied zone to the upper zone of the room where the air is extracted by the exhaust diffuser(s). Upward buoyant convection created by indoor heat sources, $P$, carries contaminants and extra heat into the upper zones of the room where the air is extracted by exhaust terminals. The system is thus delivering the fresh sub-temperature, $T_{in}$, air, $Q_{in}$, typically 2-4 °C lower than ambient air to the occupied zone, where the indoor airflow field is mostly controlled by the heat sources, as presented in Papers I-II & VIII. The flow is thermally controlled and is dependent of Archimedes number, $Ar$. The airflow is dependent on both Reynolds number $Re$ and Grashof number $Gr$ (Brohus, 1997). The $Ar$ number in front of the diffuser can be calculated as in Paper V.

Displacement ventilation is difficult to calculate numerically (Peng, 1998) as upward thermal plumes from heat sources are creating instabilities in the CFD simulation process. Typically in displacement-ventilated rooms linear temperature and concentration gradients occur (Mundt, 1996). Displacement ventilation can be used in cooling conditions only. The airflow is characterised by stable thermal stratification with linear vertical temperature distribution in the room created by the heat sources. The most significant advantage of displacement ventilation is the use of smaller airflow rate compared to complete mixing ventilation. Displacement ventilation is significantly influenced by the heat sources of the room and they are actively displacing the contaminants and heat to the upper parts of the room (Skistad et al., 2002). The air supplied with a low velocity diffuser with sub-temperature air can cause some thermal discomfort if the temperature differences are too large along a vertical height axis (Mundt, 1995).
4.1.3 Piston ventilation

In the case of piston ventilation which is used only in clean-rooms, a low turbulence and relatively low velocity airflow is supplied across an entire cross-section of the room, pushing forward the entire air volume to an exhaust which is also cross-section-wide (Hagström, 2000, Luo, 2003). To remove the contaminants throughout the room this method is ultimately the best. Additionally the concentration of contaminants is easy to calculate with simple mass-balance models. However this strategy is inefficient as it uses a large volume of supply air and a lot of energy. This was the main reason why this configuration was not used at all during the simulation cases.

4.1.4 Zoning strategy

In the zoning strategy fresh air is supplied at a high momentum in a higher level to the occupied zone. This configuration uses special diffusers which should be characterised by high velocity and temperature decay, see Paper V. The goal for this type of ventilation is to control air conditions within the selected zone in the room by the supply air and allow stratification of heat and contaminants in other room areas (Hagström, 2000). It can control the airflow parameters of a vertical or horizontal zone in the room. In most cases the accumulation of heat and contaminants to the upper zone is desired and utilised as depicted in Fig. 4. This kind of ventilation is a good compromise between mixing and displacement ventilation. The efficiency of removing contaminants, extra heat and relative humidity from the controlled zone is very dependent on air distribution method and internal room configuration, Papers V & VII. Moreover, with a proper design the ventilation efficiency, $\varepsilon_v$, of this configuration can be comparatively high.
Air Diffusion and Solid Contaminant Behaviour in Room Ventilation – a CFD Based Integrated Approach

Figure 4. Zoning ventilation configuration with the diffusers and convective heat sources generating the plumes. It is important that the occupied zone and the upper contaminant zone are not mixed for efficient system solutions.

The occupied zone is characterised by constant temperature, $T_{oz}$, and contaminant level, $C_{oz}$. Room airflow pattern is controlled partly by supply air and partly by buoyancy. The results of testing the zoning strategy of removing the excess heat from the occupied zone with two different air diffusers are presented in Paper VII. In conclusion, room velocity conditions, $v_R$, are partly a function of supply air momentum. It is important how the ventilation air is delivered into the room, i.e. supply air direction and the momentum.

For instance, the airflow created by the heat sources is basically having an effect on thermal buoyancy. That is why the distribution of air should be minimised in the horizontal direction as it has dumping effects and the ventilation system’s efficiency of removing contaminants and extra heat will decrease, see Fig. 4 and Paper VII. Researchers have for a long time tried to establish the relationships between incoming air momentum and room velocities. However, room air movement is to a greater degree three dimensional without a specific direction, which makes it difficult to describe in a general case using momentum that is a vector quantity. Additionally, the room air velocities are significantly influenced by the internal heat sources, Paper VII. That is why it is highly important to design the air distribution because if the room air is controlled by the momentum from the heat sources, this could naturally ease the airflow upwards towards the exhaust outlets (Skistad et al., 2002).

4.2 The evaluation of IAQ

The evaluation of the performance of a ventilation system is carried through in many papers by estimating the IAQ in the breathing zone. The breathing zone is defined in this research as the zone where a human occupant is taking breathing air, $H = 1.5 – 1.8$ m above the floor level. Additionally, the occupied zone in this thesis is assessed as the whole volume of the room from $H = 0 – 1.8$ m. Occupied zone average values are primarily assessed for evaluating the thermal comfort which clearly affects the whole human body. That is the main reason why the
contaminant concentration is primarily assessed by evaluating the breathing zone value, but other parameters are calculated on the whole occupied zone.

4.2.1 Determination of the necessary airflow rate

Determination of ventilation airflow rate should be based on generation of pollutant, \( m \), and the efficiency, \( \varepsilon_v \), of the ventilation system. Sometimes ventilation airflow rate is given as ACH (air exchange rate), it shows how much air is exchanged in a room in one hour. If the system is efficient then the necessary airflow rate could be reduced by a factor of \( 1/\varepsilon_v \). Another important aspect with solid contaminants is the fallout or deposition on internal wall surfaces. Additionally it is important to consider a pollutant which is transported by the ventilation air into the room in the form of supply air concentration \( C_{in} \). The necessary airflow rate needed considering all the parameters then becomes, according to Seppänen & Fisk (2004),

\[
Q_{in} = \frac{m - \alpha_d}{C_{bc} - C_{in}} \cdot \frac{1}{\varepsilon_v}
\]

\( Q_{in} \) - contaminant production rate (kg/s)
\( C_{bc} \) - limiting (acceptable) contaminant concentration value in the human breathing zone (kg/m³)
\( C_{in} \) - the contaminant concentration supplied to the room, Figs. 2-3 (kg/m³)
\( \alpha_d \) - total rate of the removal of contaminant, i.e. deposition or fallout of contaminants, filtration, chemical reactions (kg/s)
\( \varepsilon_v \) - ventilation efficiency (nd, maximum 2 for ideal piston flow)

From Eq. (1) it is possible to observe the complexity of determination of necessary airflow rate. Because of this complex relationship typical epidemiological studies have failed to determine the necessary airflow rate for different types of buildings and rooms. Often such factors as outdoor concentration and local ventilation efficiency are neglected. Increased incoming concentration, \( C_{in} \), could be caused by improperly maintained ventilation systems, where particles could originate from duct surfaces or dumped air filters. This is the main reason why the necessary airflow should be calculated based on allowed concentration in the human breathing zone \( C_{bc} \). It is understandable that in Eq. (1) the concentration, \( C_{bc} \), is the only fixed variable representing the maximum limiting value of contaminant in the human breathing zone (should be taken from norms or regulations), when other variables may change depending on building type, location and ventilation configuration. Basically, satisfactory ventilation should the fulfil requirements in Eq (4) where \( m \rightarrow 0, C_{in} \rightarrow 0 \) and \( \varepsilon_v \rightarrow \text{max} \) (for ideal piston flow 2).

4.2.2 Ventilation efficiency of contaminant removal

One of the most important measures of ventilation system performance is its ability remove contaminants. To describe the efficiency of a ventilation system many different quantities are
used to evaluate the system performance. The mean ventilation efficiency, $\varepsilon_C$, in the room is defined as

$$\varepsilon_C = \frac{C_{\text{out}} - C_{\text{in}}}{\overline{C}_R - C_{\text{in}}}$$

(2)

where

- $C_{\text{out}}$ – concentration at exhaust opening (kg/m$^3$)
- $\overline{C}_R$ – mean concentration in the room, see Figs. 2-3 (kg/m$^3$)
- $C_{\text{in}}$ – concentration at supply opening (kg/m$^3$)

The ventilation efficiency of contaminant removal was mainly used for different-sized particles. Mainly, contaminant removal efficiency is expressed for three types of particles simulated in this thesis, see Figs. 6-7. The relative air quality in the breathing zone can be expressed by the particle removal efficiency, $\varepsilon_{bz}$. This efficiency gives a relative comparison between particle concentrations at the exhaust outlet and in the breathing zone, Paper III. The ventilation efficiency in the breathing zone for different particles is given by

$$\left(\varepsilon_{bz}\right)_{1-3} = \frac{C_{\text{out}} - C_{\text{in}}}{C_{bz} - C_{\text{in}}}$$

(3)

$C_{bz}$ – concentration in the breathing zone (kg/m$^3$)

1-3 – particle size index used in this thesis, see Papers I, III, VIII.

If the supply air is uncontaminated then Eq. (3) is transformed to

$$\left(\varepsilon_{bz}\right)_{1-3} = \frac{C_{\text{out}}}{C_{bz}}$$

(4)

The equation can be used for gases as well to evaluate the removal of some harmful contaminant from the human breathing zone. Particle removal efficiency for an ideal mixing system is unity (1.0). Higher values (>1.0) indicate improved indoor air quality conditions in the breathing zone. This may be arranged by properly designed ventilation in combination with CFD and some results are presented in Papers I & VIII. The local ventilation efficiency, $\varepsilon_l$, at any point $l$ can be given as

$$\varepsilon_l = \frac{C_{\text{out}}}{C_{l}}$$

(5)

Here, $C_l$ (kg/m$^3$), could represent the concentration a person in a given location is exposed to. With this parameter it is possible to assess the ventilation efficiency actually experienced by a human occupant.
4.2.3 Concentration

The concentration in the room, $C_R$, or given volume, corresponds to the amount of air which is contaminated by particles or harmful gases. The concentration is highest close to the source. Concentration can be expressed in two ways, the first option is to use the contaminant source, $m$, or it can be expressed by using a room volume and the amount of harmful contaminant in the same volume.

$$C_R = \frac{\rho_p \pi d^3}{6}N = \frac{m/\dot{V}}{V/\dot{Q}_{out}} = \frac{m}{Q_{out}}$$ (6)

$\rho_p$ – particle density (kg/m$^3$)
$d$ – particle aerodynamic diameter (m)
$N$ – number of particles in the room (nd)
$m/\dot{V}$ – mass of particles produced in a room, later replaced by $m$ (kg/s)
$V/\dot{Q}_{out}$ – volumetric flow rate in a room (m$^3$/s)

The concentration is assessed in this thesis at steady-state conditions where the average concentration in a given time range, $t \to 0$, is

$$C_i = \frac{1}{t} \int_0^t C dt$$ (7)

$C_i$ – average concentration in a given time range (kg/m$^3$)
$C$ – concentration (kg/m$^3$)
t – time (s) here $t = 0$

Usually, ventilated rooms contain more than one type of contaminant. Basically, the effects of different types of harmful contaminants $i$ can be summed, as the allowed concentration of a single substance should fulfill the condition $C < C_{hi}$. The sum of $i$ number of contaminants which is compared to highest allowed value, $C_{hi}$, should be less than 1 according to Eq. (8)

$$\sum_i \frac{C_i}{C_{hi}} \leq 1$$ (8)

$C_i$ – measured or known concentration in a certain location (kg/m$^3$)
$C_{hi}$ – harmful concentration of pollutant (kg/m$^3$)

The breathing zone concentration is the most important value for human exposure. Human exposure can also be modelled by methods presented in some recent studies (Brohus, 1997, Hayashi et al., 2002, Murakami et al., 1996). In this thesis human exposure is assessed by simplified means by average concentration over the whole occupied zone volume,
\[ C_{bz} = \frac{1}{V} \sum_{i=1}^{n} C_{bz|V_{bz}} = \frac{\int C_{bz} dV_{bz}}{V_{bz}} = \frac{1}{V_{bz}} \int C_{bz} dV_{bz} \]  

(9)

where \( V_{bz} (m^3) \) is the breathing zone volume and \( C_{bz} (kg/m^3) \) stands for concentration in the breathing zone. Here \( i \) stand for a given spot in a volume and the concentration in this spot, respectively. The integral is taken for having a volume-weighted average concentration value. Therefore, the volume-weighted average concentration is computed by dividing the sum of the concentration and sub-volume by the total volume of the breathing zone (breathing zone \( h = 1.5 \sim 1.8 \) m). Similarly Eq. (9) can be used for the occupied zone as well, then all the variables will be altered to occupied zone values.

The relative concentration concept is introduced here for presenting non-dimensionalised results. The non-dimensionalised values are usually presented by comparing the concentration values to the room average value. Particle settling in certain zones or in breathing zone was evaluated by introducing the dimensionless concentration, \( C_{nd} \) concept, Papers I, IV, VIII. Basically, the concentration, \( C_i (kg/m^3) \), of particles in a given spot or zone, \( V_i (m^3) \), is compared to the average concentration, \( C_R (kg/m^3) \), in a room (volume \( V_R, m^3 \)).

\[ C_{nd} = \frac{\int C_i dV_i}{\int C_R dV_R} \]  

(10)

### 4.2.4 Heat removal efficiency

The heat removal efficiency, \( \varepsilon_T \), equation is defined by measuring or modelling the average temperature in the occupied zone, \( T_{oz} (K) \), as well as in supply, \( T_{in} (K) \), and exhaust air, \( T_{out} (K) \), Paper VII.

\[ \varepsilon_T = \frac{T_{out} - T_{in}}{T_{oz} - T_{in}} \]  

(11)

The average temperature in the occupied zone, \( \bar{T}_{oz} (K) \), is very similar to Eq. (9), as it can be written as follows

\[ \bar{T}_{oz} = \frac{1}{V_{oz}} \int T_{oz} dV_{oz} \]  

(12)

In Eq. (12), \( T_{oz} (K) \), is the occupied zone temperature (\( H = 0 \sim 1.8 \) m above the floor) and \( V_{oz} (m^3) \) is the volume of the occupied zone. Generally this equation shows how large the portion of heat is in a lower zone of the room compared to the whole volume of the room. It is evident that the temperature in the occupied zone in Eq. (11) is an important input parameter for designing an efficient ventilation system and this is recognised in some studies of air distribution (Awbi, 1998,
Behne, 1999, Mundt, 1995). In the calculations of heat removal efficiency the occupied zone temperature is mainly used as the human occupant senses thermal variations with the whole body. The effective system solutions focusing on heat removal efficiency were tested in Paper VII.

4.2.5 Draught

If one considers thermal comfort and people’s well-being in a ventilated room the effect of draught, $DR \, (%)$, should be taken into account. Another good feature of Eq. (13) is the coupling of temperature, velocity and turbulence values into one equation. Fanger (1988) has suggested $DR$ for calculating the draught rate, i.e. PPD (percentage of people dissatisfied) due to draught as follows,

$$DR = (3.143 + 0.37v_{oz}Tu_{oz})^{0.62}$$

In Eq. (13), $T_{oz}$ is the air temperature, $v_{oz}$ (m/s) is the air velocity ($\geq 0.05$ m/s) and $Tu_{oz}$ (%) is the turbulence intensity in the occupied zone, respectively. Turbulence intensity is defined as ($\delta_{v_{oz}}$) x 100%, where $\delta$ is the standard deviation of the air velocity. Draught rate is introduced here for parameter analysis to evaluate how closely the draught rating is associated to the heat and contaminant removal efficiency in Paper VII.

4.2.6 Other comfort evaluation equations

The occupant appreciates the indoor climate by its air quality and thermal conditions. The prediction of thermal sensation of indoor climate can be achieved by an index called predicted mean vote, PMV, developed by Fanger (1970). Even if the index is not used in this thesis it reveals the importance of considering many parameters in calculation of comfort of human beings indoors. Such variables as activity level, clothing, air temperature, mean radiant temperature, air velocity and RH (relative humidity) should be considered. The thesis mainly focuses on air velocity and thermal performance of ventilation systems coupled to particle concentration in various room locations.

4.3 IAQ assessment – particles in indoor air

Often in air pollution control, one can be interested in separating out particles from the indoor air in which they are suspended. TSP (total suspended particles) in the airflow constitutes an important component of air pollution (Ormstad, 2000). In this thesis we are especially interested in particles 0.1 – 20 µm. There are several terms for the different size fractions; UFPs is used for very small particles less than 0.1 µm (Matson, 2004). In this thesis UFPs are not modelled as they have been assumed to move in the same manner as the primary airflows (settling velocity is very small) and do not constitute an extra challenge for modelling. Additionally, PM$_{2.5}$ and PM$_{10}$ are commonly used for particle sizes less than 2.5 µm and 10 µm, respectively (Diociaiuti et al.,...
The origin and composition of airborne particles found in indoor air is quite complex (Owen, 1992). The distribution of particles in the air is the most problematic issue in the modelling. This problem was assessed already in 1955 by Junge who investigated the particle distribution in atmospheric air (Junge, 1955). Particle characteristics and distribution in atmospheric air is a constant research topic for aerosol scientists (Carfora et al., 1998, Esposito et al., 1995, Frishman et al., 1999, Harris & Marieq, 2001, Horvath et al., 1996, Kocifaj & Lukac, 1995, Lyubovtseva, 1995, Mathiesen, 2000, Mirme et al., 1995, Voutilainen & Kaipio, 2001).

4.3.1 Characteristics of particles

Real particles are not spherical in form, but have different shapes as given in Fig. 5. That is why the aerodynamic particle diameter is introduced for simulations. The aerodynamic diameter used in the simulations, $d_p$, is the diameter of the unit density ($\rho_p = 1 \text{ g/cm}^3$) sphere that has the same settling velocity as the particle. Particles can appear as human hair, parts of human skin and parts of different building or other materials (Hinds, 1999).

In Fig. 5 one can observe the fine fraction of particles, often referred to as PM$_{2.5}$. If ultrafine particles less than 0.1 $\mu$m are not considered then particles from 0.1 – 2.5 $\mu$m dominate both by number and mass concentration in atmospheric air. This can be observed in Fig. 6 and Paper III. Additionally, in Fig. 6 the main behaviour of particles is presented. The behaviour is associated with the aerodynamic diameter of the particles, necessary to know for the modelling, Papers I-IV & VIII. Furthermore, the particles in Fig. 5 have a distribution in the air by the mass and number as indicated in Fig. 6.
Fig. 6. The main characteristics of particles – mass, size number distribution, settling velocity, aerodynamic diameter and behaviour in air

To take into account all sizes of particles in the air for modelling is troublesome; therefore only three particle sizes are used in the simulations. These three particle sizes represent all the particles found in atmospheric air. The three sub-models of particles are solved simultaneously and the total mass of monodisperse particles will be the real mass of the particles found in atmospheric air, Eqs.(14-17) and Fig. 7. For instance particles (0.1 – 1 \( \mu m \)) in the first group are modelled with the diameter 0.5 \( \mu m \). It represents the mean particle diameter which covers a certain range of particles. The number \( N_{1r} \) and mass \( m_{1r} \) of particles here (0.1 – 1 \( \mu m \)) is the highest, therefore the particle aerodynamic diameter, \( d_{1r} \), selected for the modelling should be carefully selected, as in Paper VIII.

Fig. 7. Change of particle size distribution with relative humidity and new modelling concept
Once the aerodynamic diameter, \(d_{1r}, d_{2r}, d_{3r}\) (m), of the particle is chosen for calculations it is possible to assess the particles with three sub-models as in Paper VIII and Eqs. (14-17).

\[
m_{1r} = \rho_p \frac{\pi d_{1r}^3}{6} \Sigma N_{1r} \quad (14)
\]
\[
m_{2r} = \rho_p \frac{\pi d_{2r}^3}{6} \Sigma N_{2r} \quad (15)
\]
\[
m_{3r} = \rho_p \frac{\pi d_{3r}^3}{6} \Sigma N_{3r} \quad (16)
\]

\[
\sum m_p = \rho_p \frac{\pi}{6} (d_{1r}^3 N_{1r} + d_{2r}^3 N_{2r} + d_{3r}^3 N_{3r}) \quad (17)
\]

Here the total mass of the particles, \(m_p\) (kg), is equal in Eq. (17) to the whole mass of particles found in ambient air. In Eq. (17), \(\rho_p\) is the particle density (kg/m\(^3\)), \(d_{1r}, d_{2r}, d_{3r}\), is the particle diameter (m) and \(N_{1r}, N_{2r}, N_{3r}\) is the number of particles in a certain group.

However there are several limitations of the used particle model: 1) heat and mass transfer between air and particles is neglected, the air turbulence influences the particles but the particles do not influence air turbulence back (one-way coupling) 2) no particle coagulation 3) no particle re-suspension when it has reached a wall 4) all particles are solid spheres 5) the chemical composition of the particles is ignored (the particle is chemically neutral).

All additional particle mechanics are ignored, such as Brownian diffusion and nucleation. Particle deposition on wall surfaces is assessed by simplified means, see Section 4.3.3. The present model only accounts for the gravitational settling of particles at steady-state.

### 4.3.2 Gravitational settling

The terminal settling velocity of an airborne particle is an important quantity for characterizing the settling behaviour of the particle. The aerodynamic diameter of a particle, a key property for characterizing particle deposition, is dependent upon the settling velocity. A particle will reach its settling velocity when the drag force and buoyancy force balance with the gravitational force on the particle. In calculations the consideration of fluid physics is important. Particle motion with a moving fluid is described by Newton’s second law, which states that the sum of external forces exerted on a particle is equal to the rate of its linear momentum, in this case,

\[
\rho_p \frac{\pi d_r^3}{6} \frac{dv}{dt} = F_D + F_g \quad (18)
\]
where $\rho_p$ (kg/m$^3$), $d_p$ (m) and $d\vec{v}/dt$ (m/s$^2$) represent particle density, aerodynamic diameter and acceleration, respectively, and $\vec{F}_D$ (N) and $\vec{F}_g$ (N) are the drag and gravitational forces on the particle. The air velocity field and gravitational settling force primarily affect the motion of small particles suspended in a ventilation flow. Once the particle settles due to the force of gravity, $F_g = \rho_p(\pi d_p^3/6)g$, a drag force is created due to viscous friction. In the gravitational force equation $g$ stands for acceleration due to gravity. The total resisting force (air resistance) on a spherical particle moving through the air with a velocity, $v_p$ (m/s), is called drag force $F_D$. In the laminar case $Re \leq 0.5$ the air resistance (drag) can also be obtained by integrating the normal force $F_n = \pi \mu v_p d_p$ and the tangential force, $F_t = 2\pi \mu v_p d_p$, over the particle. These two components are combined to give the drag force, $F_D$, Eq. (19).

$$F_D = 3\pi \mu v_p d_p \Rightarrow C_d = \frac{3 \pi}{8} \rho_p v_p^3 d_p^2$$

(19)

where $\mu$ (kg/ms) and $C_d$ (nd) represent the dynamic viscosity of the air and the dimensionless drag coefficient, respectively. Drag is the force of resistance on an object (in our case a particle) due to a fluid. The drag coefficient, $C_d$, is a value that describes all of the complex dependencies of shape, inclination, and some flow conditions on drag. The coefficient is a function of Reynolds number and it is determined experimentally. It is a coefficient, which describes the shape of the particle (Hinds, 1999) and can be expressed for the Stokes region airflows, where $Re \leq 0.5$ by $C_d = 24/Re$, Fig. 8. Stokes’ law is a solution of the Navier – Stokes equations for low Reynolds number fluid motion.

![Fig. 8. Drag coefficient for different Reynolds numbers](image)

Free settling of the particles in ventilation air seldom happens, because particle behaviour is disturbed by primary airflows caused by air diffusers and secondary airflow movements. Secondary airflow is caused by heat and cold sources which play an important part in room ventilation, Paper VII. Forces influencing particles in a ventilation system are far more complex, because of buoyancy, the term created by temperature, $T$ (K), density differences in the air, $\rho_a = f(T)$. Usually, the buoyancy, $\rho_a(\pi d_p^3/6)g$, due to differences in air densities, will affect the particle
movements. The settling velocity in air is calculated by Eq. (20). Balancing the drag, the gravitational force and the buoyancy, results in the particle terminal settling velocity \( v_p \), Fig. 9.

\[
\frac{(\rho_p - \rho_a)}{6} g = \frac{3\pi \mu v_p d}{18 \mu} \Rightarrow v_p = \frac{g (\rho_p - \rho_a) d^2}{18 \mu} = \frac{g \rho_p d^2 c}{18 \mu}
\]

(Eq. 20)

The slip correction factor, \( c \), denotes that the air surrounding the particle is not fully homogeneous, but a mixture of moving individual molecules. This is significant for very small particles with an aerodynamic diameter less than 0.06 \( \mu \)m at normal pressure and temperature.

One can observe that the behaviour of big particles (\( p \) replaced by group) in group “3” or small particles, group “1”, is totally different as the particle aerodynamic diameter is an important variable.

\[
v_p = \frac{g \rho_p d^2 c}{18 \mu} > \frac{g \rho_p d^2 c}{18 \mu}
\]

(Eq. 21)

One can assume that \( (g \rho_p c)/18 \mu \) is constant and the particle aerodynamic diameter is the most important parameter for the settling. The constant thus can be replaced by \( S_p \).
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\[ v_p = S_p (d_{0.1 \mu m}^2) < S_p (d_{20 \mu m}^2) \]  \hspace{1cm} (22)

\[ v_p = S_p (d_{1.0}^2) < S_p (d_{2.0}^2) \]  \hspace{1cm} (23)

The constant, \( S_p \) (nd), in Eq. (22) is introduced as a particle-flow factor, which shows how many much particles are settled from one location to the other location. If we consider that \( H_z \) (m) is the height of the sub-domain in the room and \( A_z \) (m\(^2\)) is the area of the cubical sub-domain then the time constant, \( \tau_z \) (s), in the sub-domain is,

\[ \tau_z = \frac{A_z H_z}{Q_z} \]  \hspace{1cm} (24)

where \( Q_z \) (m\(^3\)/s) is the flow rate in the sub-domain. Particle-settling from one part of the room to the modelled part of the room (for instance the occupied zone) can be somewhat characterised by the distance \( \tau_{vp} \). A relative expression for particle-flow factor, \( S_p \), from zone to zone could be given by the particle-settling distance divided by the sub-domain height, \( H_z \) (m), in the uni-directional flow field in Eq. (27).

\[ S_p = \frac{\tau_z v_p}{H_z} = \frac{A_z v_p}{Q_z} \]  \hspace{1cm} (25)

The settling of particles only occurs when \( v_a < v_p \). This proves that the particle-settling factor is a function of velocity conditions and particle aerodynamic diameter \( S_p = f(Q_z, d_p) \). The areas which are contaminated with particles probably have very low velocity as results indicate in Papers I – IV & VIII.

**4.3.3 Deposition**

Deposition of particles was assessed by simplified means in all papers. Particle deposition on the walls and internal wall surfaces is a research field were all the problems concerning particle deposition on solid surfaces are not solved (Anand & McFarland, 1989, Lange, 1995). When particles are dispersed into the air, the random movement will always result in a net transport towards areas of lower concentration, and the slip (drift) velocity, \( v_{pa} \), is proportional to the gradient of the pollutant concentration (Lange, 1995). Deposition to solid surfaces can thus, in a simplified approach, be controlled by giving different BCs for the particle concentration at the wall \( C_w \) (kg/m\(^3\)). In the present thesis it is assumed that particles deposit by diffusion (Holmberg & Li, 1998).

\[ C_w = \alpha_d C_{nw} \]  \hspace{1cm} (26)

\( C_{nw} \) (kg/m\(^3\)) is the first normal grid point concentration. This is an empirical approach where appropriate deposition, \( \alpha_d \), values could be found from measurements or literature. Unfortunately, this value is grid-dependent. The present thesis assumes that \( \alpha_d \) is equal to 0. It
should be noted here that the particle deposition on wall surfaces was modelled as a perfect deposition situation, i.e. once a particle goes to a wall it becomes a part of the wall. This was achieved by putting a no-slip condition at the physical boundary of the wall as zero concentration at the wall $C_w = 0$ (Holmberg & Li, 1998). The deposition is also important for dimensioning of necessary flow rate to maintain acceptable breathing zone concentration, as in Eq. (1).
5 METHODS

5.1 Numerical simulation of IAQ parameters by CFD

Numerical methods by means of CFD modelling are used throughout the thesis. It has been used for calculating the indoor airflow field concerning research on air diffusers and investigating the particle concentration in different parts of ventilated rooms. CFD calculation represents a superior method to calculate the indoor airflow, because semi-empirical and purely analytical methods fail for different room layout conditions. The temperature or contaminant gradients and convection flows from heat sources could be calculated by models developed by Mundt (1996) and Krühne (1995), but these models are not applicable in all room layout situations. Basically because of these restrictions, the use of CFD as a universal tool to predict indoor airflows has grown dramatically. Another significant advantage of CFD is the possibility to test different system configurations virtually without constructing the real systems. In this way it is possible to optimise the ventilation system to remove pollutants by numerical methods. That option is widely used in this thesis by validated models of diffusers. The main limitation to the widespread use of CFD is the many model-specific values which depend on the behaviour of the flow in the turbulence model and so on (Casey & Wintergerste, 2000, Chen & Srebric, 2001, Davidson, 2003, Versteeg & Malalasekera, 1995).

5.2 General boundary conditions of the thesis

The CFD simulations throughout the thesis were performed in a similar way to ease the comparison of different modelling results. All the simulations performed in the thesis were done in 3D space with steady-state conditions using the commercial code FLUENT, except in last paper where CFX code was used. Turbulence was modelled in all cases with the standard \( k-\varepsilon \) model or its modifications. The RNG (mathematical technique called “Renormalisation group” theory) \( k-\varepsilon \) turbulence model (Versteeg & Malalasekera, 1995) and the same model with swirl modification suggested by the software manual were used as well (Fluent. Inc., 2003). The standard \( k-\varepsilon \) model was chosen to model turbulence because it represents the best known model utilized and validated for air diffuser performance. Wall treatment was achieved by standard wall functions provided by the software. Heat transfer in all simulations was enabled except in Paper IV. The radiation was not included in the simulations because of computer capacity restrictions. The computer used in this thesis was a Pentium III 850 MHz with 512 MB central memory which restricted utilising all possibilities in the software. For instance, the grids in the simulations were restricted to structured hexahedral mesh layout and a maximum cell number of 500 000 because of memory limitation. All the cases used segregated solver, except the last paper, to obtain results for flow, turbulence and energy throughout the computational domain. In the last paper the coupled solver was utilised. Discretisation of pressure was always second order accuracy and the pressure-velocity coupling was achieved by SIMPLE or SIMPLEC algorithms. The momentum and energy were always discretised in a second order upwind scheme (Versteeg & Malalasekera, 1995). Turbulent kinetic energy, \( k \), and turbulence dissipation rate, \( \varepsilon \), were in most cases solved by first order upwind accuracy. Specific under-relaxation factors for the segregated solver were modified to obtain converged results. All the BCs for walls, diffusers and other elements within the modelling are given in all papers.
5.3 Validations – using experiments and literature

To confirm the accuracy of the simulations a full-scale test room was used. The full-scale room had 4.0 m x 10 m floor area and 6.0 m height, Papers V- VII. It was thermally insulated from the surroundings by 50 mm ($\lambda = 0.03 \text{ Wm/K}$) thick polystyrene elements to minimize the heat flux through the wall boundaries. Air velocity was measured using Kaijo Denki WA – 390 ultrasonic sensors, which have an accuracy of 0.00 – 1.00 ($\pm 0.02$) m/s. The sensors sample the air velocity vector components with three pairs of ultrasonic transducers based on the flight time of the ultrasonic pulse. The air temperatures were measured by Fenwal thermistors with an accuracy of $\pm 0.1$ K. Measurements of air velocity and temperature were time averaged over 60-180 s (Paper V and Paper VI, respectively) and the values were recorded with a data logger. The sensors were attached to a computer-controlled traversing system moving them from point to point to scan the two predetermined measurement planes. The influence of airflow profile from air diffusers and heat source location on heat removal efficiency was measured in the same room. Totally 10 different ventilation configurations were validated by the measurements and part of the results are presented in APPENDIX D. In the test room only three components of velocity $v_x$, $v_y$, $v_z$ and air temperature were measured. In Paper II in addition to velocity and temperature also solid particles were measured.

It is extremely difficult and expensive to make controlled experimental investigations of particle movements in ventilated rooms. Real full-scale measurements of solid contaminants were performed in Paper II and mostly failed because of problems with generating constant concentration of 0.26, 1.0 and 10 $\mu$m particles, Fig. 10. For that reason the particle model was later validated based on results in the literature (Holmberg & Li, 1998, Mattsson, 2002, Murakami et al., 1996) in Paper VIII.

![Fig. 10. The variation of aerosol concentration (particles 0.26 $\mu$m) in the test room in Paper II. The average concentration in the room was 10 $\mu$g/m$^3$.](image-url)
5.4 Numerical simulation of ventilation airflows coupled with particles

For airflows, the CFD program solves conservation equations for mass and momentum. For flows involving heat transfer or compressibility, an additional equation for energy conservation is solved. Two additional transport equations are solved when the flow is turbulent, i.e. the turbulent transport quantities $k$ and $\varepsilon$ in the $k-\varepsilon$ model.

5.4.1 Mass conservation equation

The equation for conservation of mass, or continuity equation at steady state, can be written as follows:

$$\nabla \cdot (\bar{v} \rho) = 0 \quad (27)$$

Eq. (27) is the general form of the mass conservation equation and is valid for incompressible as well as compressible flows, where $\bar{v}$ is the velocity vector and $\rho$ is the fluid density.

5.4.2 Momentum conservation equation

The momentum equation can be expressed by Navier-Stokes equations by describing Newton’s second law of fluid flow. The momentum equation can be expressed in vector form as

$$\nabla \cdot (\rho \bar{v} \otimes \bar{v}) = \nabla \cdot (\mu_{\text{tot}} \nabla \bar{v}) - \nabla p + \bar{F}_g + \bar{F}_{\Delta T} \quad (28)$$

where $\bar{v}$, $\rho$, $p$ (Pa), $F_{\Delta T}$ (N) are the velocity vector, density, pressure and thermal differences in the buoyancy term, respectively. It is worth mentioning that in turbulent flow the viscosity, $\mu_{\text{tot}}$ (kg/ms), is the sum of molecular and turbulent viscosity. Natural convection is modelled by the Boussinesq approximation. As we can see from Eq. (28) it resembles the typical momentum equation with the addition of the gravitational settling force and buoyancy terms being included in the source term. The external body forces, $F_g + F_{\Delta T}$, contain parameters such as thermal differences, which give the extra momentum to the flow. The buoyancy term, $\bar{F}_{\Delta T}$, was modelled by Boussinesq approximation in the momentum Eq. (28) and is given as:

$$(\rho - \rho_{\text{ref}})g \approx -\rho_{\text{ref}} \beta (T - T_{\text{ref}})g \quad (29)$$

where $\rho_{\text{ref}}$ is the reference density of the flow (kg/m$^3$), $T$ (K) the temperature of the air, $T_{\text{ref}}$ (K) is the reference temperature and $\beta$ (1/K) is the thermal expansion coefficient. This approximation is accurate as long as changes in actual density are small in the simulated space. Reference values can be, for instance, room average values. Naturally, gravitational acceleration acts in the direction of the height coordinate and affects the buoyancy forces in all directions of Cartesian coordinates and the $Ar$ number in the momentum equations.
5.4.3 Energy conservation equation

To obtain a description of the temperature distribution throughout the non-isothermal flow domain the energy equation is used. Energy, $E$, in the air is defined as the sum of internal thermal energy, kinetic energy of velocity components and the gravitational potential energy typical in buoyancy-driven flows. Conservation of energy at steady state is described by

$$\nabla \cdot (\rho E + p) = \nabla \cdot \left( \sum_{j} h_{j} J_{j} \right) + S_{h}$$  \hspace{1cm} (30)

where $J_{j}$ is the diffusion flux of species $j$ (kg/m$^{2}$/s), $h_{j}$ is the enthalpy (kJ/kg) of species $j$ and $S_{h}$ (W/m$^{3}$) includes the heat or any other volumetric heat sources defined in the simulation process.

5.4.4 Particle concentration equation

The general concentration equation for particles in the particle-settling model used in most of the papers is presented below,

$$\rho C + \nabla \cdot (\rho \left( \bar{v}_{a} + \bar{v}_{p} \right)) = \nabla \cdot (\Gamma_{c} \nabla C) + S_{c}$$ \hspace{1cm} (31)

where $C$ is the volume concentration of particles, usually very small ($10^{-8}$ volume fraction). The dimensionless number, $\Gamma_{c}$ (m$^{2}$/s), stands for the diffusion coefficient. The term $S_{c}$ includes any other volumetric sources meant for concentration, for instance relative humidity dependence which will be discussed more closely later.

Particle concentration in the control volume influenced by convective diffusion in a field with an external force can be described by the following general concentration Eqs. (32-34) (Jin, 1993).

$$C_{1} - \Delta C + \nabla \cdot \left( C_{1} \left( \bar{v}_{a} + \bar{v}_{p} K \right) \right) = \nabla \cdot (\Gamma_{c} \nabla C_{1}) + S_{c1}$$ \hspace{1cm} (32)

$$C_{2} - \Delta C + \nabla \cdot \left( C_{2} \left( \bar{v}_{a} + \bar{v}_{p} K \right) \right) = \nabla \cdot (\Gamma_{c} \nabla C_{2}) + S_{c2}$$ \hspace{1cm} (33)

$$C_{3} - \Delta C + \nabla \cdot \left( C_{3} \left( \bar{v}_{a} + \bar{v}_{p} K \right) \right) = \nabla \cdot (\Gamma_{c} \nabla C_{3}) + S_{c3}$$ \hspace{1cm} (34)

where indices 1-3 represent the particle group, Figs. 6-7. In this case we assume that $C_{1}$ is the number concentration of particles 0.1–1 $\mu$m with similar behaviour. Eqs. (32-35) use coagulation and growth to determine the concentration modification, $\Delta C$, which is the change of particle mass concentration in the control volume. The settling velocity correction factor, $K$ (nd), describes the growth of the aerodynamic diameter. It is especially significant from RH 70% onwards (Busch et al., 1995). In the third group “3” (5-50 $\mu$m) the settling force is significant, but the coagulation and growth are relatively insignificant. In the first group “1” the situation is the opposite. One of the trickiest things is to determine the particle diameter $d$, $\Delta C$, and the settling velocity correction factor, $K$, when using transient calculations. Transient calculations are neglected in this thesis and can be the base of future studies, see Paper III.
If we replace the particle group number by \( N \) and neglect all the modification terms the concentration equation at steady-state condition is similar to Eq. (31)

\[
\rho C_N + \nabla \cdot (\rho C_N (v_a + v_p)) = \nabla \cdot (\Gamma_c \nabla C_N) + S_{CN} \tag{35}
\]

5.4.5 Turbulence modelling with the k-\( \varepsilon \) model

Air movements in a room are usually turbulent and need be modelled in CFD. In turbulent flow we can divide the variables into one time-averaged part of the velocity \( \bar{v} \) (when the mean flow is steady) and one fluctuating part \( v \), so that \( \bar{v} + v \). In the standard \( k-\varepsilon \) model the modelled transport equations for turbulent kinetic energy, \( k \), and its dissipation rate, \( \varepsilon \), are solved. The present model assumes that the flow is fully turbulent and the effects of molecular viscosity are small compared to the turbulent viscosity, \( \mu_{tot} = \mu + \mu_{turb} \). That is why this model is very suitable for fully turbulent flows and it calculates the turbulence isotropically. That is why the anisotropic flows such as wall jets should be calculated with other turbulence models. Turbulent viscosity in this model is computed as

\[
\mu_{turb} = C \mu \frac{k}{\varepsilon} \tag{36}
\]

In transport equations of \( k \) and \( \varepsilon \) one need values for 5 unknown constants (Davidson, 2003). Unfortunately these constants are not universal for all types of flows. The present thesis used default values, \( C_{1k} = 1.44; C_{2k} = 1.92; C_{\mu} = 0.09; \sigma_k = 1.0; \sigma_\varepsilon = 1.3 \). When using \( k-\varepsilon \) model modifications the default values provided by Fluent Inc. (2003) were used as well. More information about the standard \( k-\varepsilon \) turbulence model can be found in numerous publications (Davidson, 2003, Launder & Spalding, 1974, Versteeg & Malalasekera, 1995). Other turbulence models are not discussed in this thesis, but quite broad knowledge about different turbulent models within CFD is given by Davidson (2003).

If the Navier-Stokes equations are solved without using any approximations in turbulence modelling, the approach is called DNS (direct numerical simulation). Successful prediction with DNS needs a very fine mesh to capture all the smallest eddies in the flow. The smallest eddy size in the turbulent flow is of the order of the Kolmogorov length scale \( l_k \) (m).

\[
l_k = \left( \frac{\nu}{\varepsilon} \right)^{0.25} \tag{37}
\]

where \( \nu \) is the kinematic viscosity of air. For most of indoor airflow the Kolmogorov length scale is around 0.01 to 0.001 m. To use the DNS method the grid number for the simulation is very high and not feasible in today’s PC. Another important aspect of the Kolmogorov length scale is the solving of particles. As the current thesis uses Eulerian approach for the particle model it is necessary that the particle size should be significantly smaller than the Kolmogorov micro-scale (Holmberg & Li, 1998).
6 DIFFERENT COMPONENTS WITHIN THE MODELLING AND BOUNDARY CONDITIONS

It is a well-known fact that the accuracy of the CFD simulation or any kind of modelling greatly depends on its given numerical methods, the chosen models and input values. The CFD modelling is a very powerful method to solve indoor airflows, but it is very sensitive to its given numerical methods and BCs.

6.1 3D space model

The starting point of a room airflow analysis is to create a geometry model. By modelling geometry, spatial relationships and objects such as walls and windows should be created in a way that these should be relatively simple but at the same time representing realistic conditions so as not to compromise the modelling accuracy. Over-simplification of internal obstructions will lead to errors and altered airflow profile within the space. This will lead afterwards to erroneous predictions of solid contaminants within the modelled space. Therefore it is recommended to construct the room geometry based on the architect model and model even the furniture based on the manufacturer’s geometry model, Paper IX. A typical arrangement of a room with different modelling variables is given in Fig. 11.

![Fig. 11. Basic CFD modelling set-up variables](image-url)
In Fig. 11 one can recognise the complexity of the CFD simulations. That is why the CFD modelling needs more systematisation to use it as a reliable tool for optimising indoor climate parameters, Paper IX.

6.2 Products within the modelling

The modelling of indoor airflow could include many products from real manufacturers. For instance furniture, lamps, radiators and diffusers are produced by some real producer, Papers V, VI & IX. Usually the dimensions of these products and BCs are very specific and sometimes only known by the manufacturer. Furniture layout is already utilised in the selection programs, which can be used in the simulations. For instance over-simplification of furniture could lead to the wrong room volume in a small space, which as a result in CFD predicts higher/lower indoor air velocities compared to the actual values.

6.3 Internal heat and cold sources

Internal heat sources such as radiators, humans and windows generate airflows which are created by thermal buoyancy and are a crucial part of indoor airflow behaviour. This is especially true when one deals with displacement ventilation. In this case internal heat/cold sources dominate the airflow behaviour. The internal spatial relationships of heat sources are important for the efficiency of the ventilation system. This was tested in Papers VII-VIII. A crucial part of indoor airflow analysis is the human occupants. The mathematical models and measurements have clearly shown that the plumes above the human body can generate relatively high velocities, up to 0.26 m/s (Popiolek, 1981). That is why it is important to use a reliable mathematical model of the human body (Bjørn, 2001, Nilsson, 2004). Mathematical models of human bodies are important for modelling personal exposure to contaminants or climate (Brohus, 1997) and are important for affecting the flow field and thermal conditions in the room as the human body generates heat to the surroundings.

6.4 Numerical modelling of supply openings

The airflow from a diffuser greatly affects the airflow pattern in a room. Additionally, the diffuser type and the air supply parameters dominate the air diffusion in the room. In this thesis different kinds of diffusers were tested to find out how the air distribution affects the airflow behaviour, temperature distribution and particle concentration in different parts of a ventilated room. The primary goal of this research was to verify that air distribution in a room is a crucial part of efficient ventilation. The air supply from diffuser(s) partially determines the efficiency of the ventilation system. It is sometimes much more important to ask how the air is distributed into the space than to know the total ventilation flow rate (Awbi, 1998). In complex room situations the only solution for designing effective ventilation is to use calculation programs such as CFD. Still, the limitation of using CFD efficiently is the lack of air diffuser models within the program. The research in the field of CFD diffuser models has gained more attention recently as it directly determines the accuracy of the simulation (Djuanedy, 2000, Djuanedy, 2002, Fan, 1995,
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Fontaine, 2002, Hu, 2003, Huo et al., 2000, Luo, 2003, Nielsen, 2000, Koskela, 2004). In this thesis, four types of diffusers were studied: low velocity diffuser, multi-cone diffuser, swirl diffuser and industrial air diffuser. All the diffusers in this thesis were assessed by simplified means.

All the diffusers are possible to model by creating an exact real geometry. This method is very time consuming, but possible to test a single diffuser (Hu, 2003). In this method the BCs are given to the connection duct where for instance the velocity is a known value. The main challenge in the modelling of air diffusers is to account the grid layout for a small-scale opening compared to the scale of room layout, Papers V & VI. However, creating an exact geometry is not feasible in normal calculation cases because the number of grid points in a computational domain can increase dramatically.

Two other well-known methods for modelling air diffusers with simplified BCs (Chen & Srebric, 2000) are the momentum method and the box method. The momentum method assumes that the airflow from a particular diffuser can be predicted using the isothermal axisymmetric jet formula (Zoe, 2001). The box method was developed by Nielsen (1992) to decrease the number of grid points near the diffuser, where the airflow profile of the diffuser is specified inside a virtual box (Nagasawa & Kondo, 2002). The box method is not directly used in this thesis. Basically, velocity specification on the boundary of the model surfaces of the diffuser was used for high velocity diffusers, Paper VI, and the momentum method for low velocity diffusers, Papers I & II. A combination of these methods was used in Paper V.

The momentum source specification is a useful method if the diffuser outer area is not totally free for air to pass; it means that the diffuser effective area is much smaller than the free opening area. This is the typical case with low velocity diffusers, Fig. 12.

![Fig. 12. Low velocity diffuser, used in Papers I & VIII](image)

The momentum source is also used for nozzle duct diffusers (Koskela, 2004) and grilles (Huo et al., 2000) and other wall-mounted diffusers (Fan, 1995).

The low velocity diffuser depicted in Fig. 12 was used for modelling of the air diffuser in Paper I by using a momentum source to overcome the problem of giving the right flow rate in front of the perforated surface of the diffuser. The flow from the low velocity diffuser is either given by the volumetric flow rate, $Q_v (m^3/s)$, or by the face velocity, $v_{in} (m/s)$. In this case one assumes that the velocity is uniform all over the working surface of the diffuser.
\[
\nu_{in} = \frac{Q_{in}}{A_{in}}
\]

(38)

where \(A_{in}\) (m\(^2\)) is the total surface area of the perforated part of the diffuser. The geometry of the perforated surface (in percent, 10 \%=0.1) and the free nominal opening area, \(0.1A_{in}\), is much less than the whole area of the diffuser. We should note that \(A_{in}\) (m\(^2\)) is the same as the effective area of the diffuser. It is important that velocity or mass flow is not calculated from diffuser face area. To overcome the problem with correct flow rate, an extra momentum source is given in a sub-domain for accelerating the air velocity at horizontal \(x, z\) directions. The momentum source should be directed normal to the inlet boundary to avoid creating a complex perforated surface of the diffuser as a method for modelling ventilation devices, Papers I, II & V. The same BCs were used for the low velocity diffuser in CFD simulations. The momentum source in front of the low velocity diffuser in a sub-domain can be defined generally as

\[
F_{in} = \int \rho_a v_{in}^2 d\tilde{A}_n
\]

(39)

where \(\rho_a\) (kg/m\(^3\)) is the air density and \(v_{in}\) (m/s) is the air speed in a perforation hole.

If the right mass flow is maintained and non-isothermal conditions are used then the cold flow from the diffuser is influenced by vertical acceleration due to gravity. This is given by the Archimedes number, \(Ar\), for a flow from the diffuser, Paper V and Nielsen (2000). Paper V solved the BC specification by providing mixed BCs for two different parts of the industrial air diffuser in Fig. 13.

\[\text{Fig. 13. Industrial air diffuser geometry (A.) and CFD representation (B.), Paper V}\]

An extra momentum source in front of the cylindrical air diffuser was given in a small sub-domain, which generated a radial airflow with constant velocity at the supply covering. The determination of sub-domain size should be found in such a way that it is wide enough to accelerate the velocity in front of the diffuser to a correct velocity, as the given value in the
selection programs. The thickness of the sub-domain in Papers I, V & VIII in all cases was
taken to be 0.05 m.

The BCs for the circular multi-cone ceiling diffuser were generated without adding any source
terms in front of the diffuser. The air diffuser was simply modelled by supplementing the well-
specified boundary profile to the supply opening, similar to the prescribed velocity method where
velocity values typically are given in a closed domain (virtual box) in front of the diffuser. In this
way, it is possible to avoid giving only a supply airflow rate, \( \dot{Q}_m \) (kg/s), which generates a
uniform velocity profile on the boundary of the diffuser and underestimates the maximum
velocity values in the near zone. The area of a diffuser surface, \( A_m \), is divided by the facets that
contain specified velocity values from the profile \( v_m = f(H_m) \). \( H \) (m) here represents height of the
diffuser, but there are also other possibilities to give a profile which is a function of some
geometrical parameter. Then the mass flow rate, \( \dot{Q}_m \), can generally be given as

\[
\dot{Q}_m = \int \rho \vec{v}_m d\vec{A}_m
\]

With this kind specification it is also possible to direct velocity vectors downwards or upwards as
depicted in Fig. 14 and at the same time the profile is a function of height co-ordinate.

![Air velocity profile on the boundary of a multi-cone diffuser](image)

**Fig. 14. Air velocity profile on the boundary of a multi-cone diffuser**

The pre-described velocity on the boundary of the modelled diffuser was a successful method
also with a swirl diffuser, Paper VI and Fig. 15.
The initial air velocity was calculated from the diffuser volumetric flow rate, $Q_{in}$ (m$^3$/s), and the angle $\alpha$ of the velocity vectors, see also Paper VI.

$$v_{in} = \frac{Q_{in}}{\cos \alpha \pi H d}$$ (41)

The height of the diffuser, $H$ (m), and the diameter, $d$ (m), of the diffuser model make it possible to calculate the initial air velocity at the diffuser opening. In this way the airflow rate will be correct, but if the model is much smaller than the real diffuser then probably the velocity in the near zone will be over-predicted. Nevertheless, the results from simulations of various air diffusers reveal that the simplified methods described here can be used for most of the diffusers found on the market.

To conclude, almost any air diffuser can be modelled with a simple rectangular opening representing the air diffuser, but this kind of modelling procedure has some limitations as described in the literature (Heikkinen, 1990, Huo et al., 2000).

A cooled beam was used in Paper IX. This model used exactly same techniques as the diffuser models described before. The numerical parameters were described on the boundaries of the cooled beam CFD model.

### 6.4.1 Turbulence quantities for $k$ and $\varepsilon$ at supply openings

In the $k$–$\varepsilon$ turbulence model the modelled transport equations $k$ and $\varepsilon$ are solved. More detailed descriptions of the model can be found in the literature (Davidson, 2003, Versteeg & Malalasekera, 1995). As the explicit values of $k$ and $\varepsilon$ are not measured, the turbulent kinetic energy can be calculated by using the turbulence intensity at the inlet. The relationship between the turbulent kinetic energy at the supply inlet, $k_{in}$ (J/kg), and turbulence intensity, $Tu_{in}$ (%), is

$$k_{in} = \frac{3}{2} (v_{in} Tu_{in})^2$$ (42)

The turbulent dissipation rate is obtained from a length scale. If the turbulent length scale, $l_{in}$ (m), is known, $\varepsilon_{in}$ (m$^2$/s$^3$) can be determined from the relationship:
\[ \varepsilon_{in} = C_\mu^{3/4} \frac{k_{in}^{3/2}}{l_{in}} \]  

(43)

where \( C_\mu \) (nd) is an empirical constant specified in the turbulence model (approximately 0.09). The length scale, \( l_{in} = 0.07H \), can be approximated by the relevant dimension of the diffuser \( H \). The factor 0.07 is based on the maximum value of the mixing length in fully developed turbulent pipe flow.

### 6.5 Computational grid

Using a finite volume method the calculation domain in Fig. 16 is divided into a finite number of control volumes and grid points. Each grid point found in the computational domain is surrounded by one volume. All the variables chosen for the calculations are solved in these points. The calculation results by differential equations in these locations are replaced by discrete values. The current research used only the structured hexahedral mesh depicted in Fig. 16, except in the last paper where unstructured mesh was used, Paper IX. Since CFD computes partial differential equations into discrete form it necessary that the grid layout near the simulated air diffuser be sufficient to avoid unwanted numerical diffusion “false diffusion” near the supply opening. The proposed grid layout near an industrial air diffuser is given in Fig. 16.

![Fig. 16. Grid layout near an industrial air diffuser](image)

All the numerical variables are discretized in the computational domain and if the grid is not sufficient enough truncation of equations causes errors similar to real diffusion. Numerical diffusion is most noticeable when the real diffusion is small, that is, when the situation is convection-dominated. That is why it is highly important to perform the grid-independence tests by doubling the grid size. If doubling the grid produces the same result then the mesh layout used previously can be used, Paper V. It is rather important also to generate high-quality grid layout near the solid boundaries and the heat sources (Casey & Wintergerste, 2000, Chen & Srebric, 2001, Versteeg & Malalasekera, 1995).
6.6 Exhaust opening

There is very little impact on boundary conditions of an exhaust opening to room airflow. However it is a rather important parameter for influencing the numerical stability. The last component for complete ventilation is the specification of the exhaust condition. Zero gradients for all flow parameters were used as a BC for the exhaust opening in a normal direction. The airflow rate is distributed with a predetermined ratio through the outlets.

6.7 Modelling of solid contaminants and their source(s)

The modelling of solid contaminants, i.e. particles in indoor environments, is a demanding task. The particles originate from indoor sources and outdoor sources as well. Probably surface airflow movements will affect the material as well as particle emissions (Zhang & Haghighat, 1997). In this thesis modelling of solid contaminants is assessed by simplified means. Particles were supplied by ATDs into the room or some separate particle source was implemented in the simulation. Papers I-II, IV, VIII. The particle source was typically modelled usually as a tiny inlet with small inlet velocity and turbulence. Particles in the air were modelled as a virtual secondary phase within the primary phase air using the drift-flux model. Sometimes this modelling approach is called the single-fluid approach. Particle velocity, \( v_{pa} \) (m/s), is defined as the velocity of the particle phase, \( v_p \) (m/s), compared to the velocity of primary (air) phase \( v_a \) (m/s):

\[
\vec{v}_{pa} = \vec{v}_p - \vec{v}_a
\]  

(44)

The concentration of particles is solved calculating the slip velocity, i.e. particle relative velocity in the air, \( v_{pa} \) (m/s). The mixture model makes use of an algebraic slip formulation. The basic assumption of the algebraic slip mixture model is to prescribe an algebraic relation for the relative velocity, a local equilibrium between the phases should be reached over a short spatial length scale. Following Manninen et al., (1996) the form of the relative velocity is given similarly to Eq. (20) for particle settling velocity

\[
\vec{v}_{pa} = \frac{(\rho_p - \rho_m)d_p^2}{18\mu_{m,ph}F_D} \tilde{a}
\]  

(45)

here \( \rho_m \) (kg/m\(^3\)) is the mixture density and \( \tilde{a} = \frac{d\sigma}{dt} \) (m/s\(^2\)) is the secondary-phase particles’ acceleration. The mixture density in the drift-flux model can be expressed by

\[
\rho_m = \sum_{k=1}^{n} \alpha_k \rho_k
\]  

(46)
where \( \alpha_k \) (nd) is the volume fraction of phase \( k \), similar to concentration. One should still keep in mind that the mixture model uses the so-called single fluid approach (Fluent Inc, 2003). The mixture model in the program solves the continuity equation for the mixture, the momentum equation for the mixture, the energy equation for the mixture and the volume fraction equation for the secondary phases, as well as algebraic expressions for the relative velocities (if the phases are moving at different velocities). The mixture model allows accommodating \( k \) different particle sizes within in a single primary air phase, in our case 3 different sub-models.

### 6.7.1 Modelling of particle behaviour – sources & sinks

The modelling of particle sources is troublesome, because particles originate from many different places, from indoors and outdoor sources. In mathematical modelling, one question always arises, where to put the source. In this thesis the point source is neglected and particles are modelled through air inlets. As mentioned before, the current model uses Eulerian approach to treat particles evenly distributed in the control volume. The continuum criterion is valid when there are enough particles in the computational element (one finite volume) so that statistically average properties can be assumed, see Eq. (37). In this sense the model is very different compared to Langrangian discrete phase modelling as the Langrangian model solves particle equations for each particle individually.

If one assumes that outdoor air contains a certain amount of particles, \( C_{in} \) (kg/m\(^3\)), then the particle source could be given at the supply opening with an airflow profile. Particles are assumed to be fully mixed with the ambient air when certain average properties are assumed for the control volume.

\[
m_{in} = C_{in}Q_{in} = \rho_p \frac{\pi d_p^3}{6} \int v_{in} dA_{in}
\]

if the velocity is constant over the supply opening boundary, \( dA_{in} \), then integration is not necessary. In general particle sources were modelled by tiny inlets as in Paper VIII. Particles were supplied into the room together with incoming air from two small rectangular slots, 0.05 m x 0.05 m, near the floor. Simulations in Paper VIII showed that such a source simulates well a floor-type particle source such as a carpet or a dusty floor. This source could be also combined with a source originating from the ATD. In CFD software often the volume fraction, \( \alpha_k \), of contaminant is used when inserting the source. The particle source, \( m_{in} \) (kg/s), with supply opening, \( A_{in} \) (m\(^2\)), and with an uniform velocity, \( v_{in} \) (m/s), can be calculated as follows,

\[
m_{in} = \rho_p \alpha_k v_{in} A_{in}
\]

The contaminant in the air will be calculated by its momentum flow rate, \( F_{pu} \) (N), created by the mass generation, \( \dot{m} \) (kg/s), and relative velocity, \( v_{pu} \) (m/s), of contaminant mixture. If the velocity conditions are not favourable then settling will occur,
\[ \dot{F}_{pa} = \dot{m} \dot{v}_{pa} \]  

In Eq. (49) it is possible to observe that the gravitational settling only occurs when the relative velocity, \( \dot{v}_{pa} \) (m/s), is higher than the air velocity, \( \dot{v}_a \) (m/s). Additionally particle mass transport in different parts of the room is very much dependent on velocity conditions in the room. The particle loss through deposition is dependent on wall grid, because when the particle reaches the first grid point in the wall, deposition will occur. Therefore, the velocity conditions near walls are very important as they influence the particle re-suspension into the ambient air. For instance, convective heat sources can bring particles back to the airflow, this means that the floor in Fig. 17 can be considered to be either a particle sink or source, Paper I. Because of this dynamic behaviour it is sometimes very hard to determine where the particle sources and sinks are. Additionally particle behaviour is generally influenced by the airflow conditions in the indoor environment, Paper III.

![Fig. 17. Settling particles re-entering convective air plumes](image)

That is why the modelling of particles in three sub-models is justified, as the behaviour of particles clearly is a function of their mass. The particles are behaving in the general airflows in a similar way as was tested in Paper IV for an isothermal case. Some expected particle dispersion patterns near humans are shown in Fig. 18. Large particles, group “3”, have a strong settling behaviour. Measurements demonstrate that super micron particles, group “2”, will settle in low velocity airflows and, at the same time, they may be brought up to higher elevations with local convective heat sources. Small, sub micron particles, group “1”, follow the airflow almost exactly as depicted in Fig. 18.
6.8 Finite volume method and discretization

Discretization in a room (computational space) requires the flow field to be divided into small control volumes. As mentioned before the current thesis used mainly one type of grid topology: hexahedral mesh. The software used a control volume-based technique to convert the governing equations to algebraic equations that were solved numerically. This control volume technique consists of integrating the governing equations about each control volume, yielding discrete equations that conserve each quantity on a control-volume basis. Discretization of the governing equations can be illustrated most easily by considering the steady-state conservation equation for transport of a scalar quantity \( \phi \) (nd). This is demonstrated by the following equation written in integral form for an arbitrary control volume, \( V \) (m\(^3\)), as follows:

\[
\int_S \rho \phi v \cdot dA + \int \int \int S_\phi \rho \phi \cdot d\Gamma = \int S_\phi dV
\]

Here the scalar quantity represents discretization of each of the three velocity components \( u, v, w \) (m/s), the kinetic energy of turbulence, \( k \) (J/kg), the dissipation rate, \( \varepsilon \) (m\(^2\)/s\(^3\)), and air enthalpy, \( h_a \) (kJ/kg). \( \nabla \phi \) is the gradient of scalar quantity in all three dimensions, \( \rho \) (kg/m\(^3\)) is the fluid element density, \( \Gamma_\phi \) (m\(^2\)/s) is the diffusion coefficient for \( \phi \) and \( S_\phi \) (nd) source of \( \phi \) per unit of volume.

A first-order scheme according to the Taylor expansion series is used in computing the turbulence quantities \( k \) and \( \varepsilon \). All quantities at cell faces are determined by assuming that the cell-center values of any field variable represent a cell-average value and hold throughout the entire cell; the face quantities are identical to the cell quantities (Versteeg & Malalasekera, 1995). Thus when the first-order upwind scheme is selected, the face value, \( \phi_f \), is set equal to the cell-center value of \( \phi \) in the upstream cell. However, most of the variables calculated in CFD were discretized with second-order accuracy (convection + diffusion terms) and quantities at cell faces
were computed using a multidimensional linear reconstruction approach (Pantakar, 1980). In this approach, higher-order accuracy is achieved at cell faces through a Taylor series expansion of the cell-centred solution about the cell centroid. Thus, when a second-order upwind scheme is selected, the face value, \( \phi_f \), is computed using the following expression,

\[
\phi_f = \phi + \nabla \phi \cdot \Delta s
\]

where \( \phi \) and \( \nabla \phi \) are the cell-centred value and its gradient in the upstream cell, and \( \Delta s \) is the displacement vector from the upstream cell centroid to the face centroid. This formulation requires the determination of the gradient \( \nabla \phi \) in each cell. This gradient is computed using the divergence theorem, which in discrete form is written as

\[
\nabla \phi = \frac{1}{V} \sum_f \tilde{\phi}_f \tilde{A}
\]

Here the face values, \( \tilde{\phi}_f \), are computed by averaging \( \phi \) from the two cells adjacent to the face.

Discretization of pressure was typically performed using a body-force weighted scheme provided by the software and pressure-velocity coupling was achieved by SIMPLE or SIMPLEC algorithms (Pantakar, 1980, Versteeg & Malalasekera, 1995).

A linearised form of the discretization equation of particle concentration is obtained from Pantakar’s SIMPLE approach (1980):

\[
o_{cc} C_{cc} = \sum_{nb=1}^{N} o_{nb} C_{nb} + S_0
\]

where the subscript \( cc \) represents cell centre and \( nb \) the neighbouring points. The number of neighbouring points, \( N \), the coefficients \( o_{cc}, o_{nb} \) and the source term, \( S_0 \), of the discretization equation depend on the used discretization schemes.

The computational stability and the correctness of the CFD solution depend very much on used discretization schemes, grid layout and under-relaxation factors given to the segregated solver. Because the CFD calculation contain non-linearities of the equation sets solved, it is necessary to control the change of \( \phi \). This is achieved by under-relaxation, which reduces the change of \( \phi \) produced in each iteration. In a simple form, the new value of the variable \( \phi \) within a cell depends upon the old value, \( \phi_{old} \), the computed change in \( \phi \), \( \Delta \phi \), and the under-relaxation factor, \( R \) (nd), as follows:

\[
\phi = \phi_{old} + R \Delta \phi
\]

Iteration number and the convergence criteria are interrelated. Because of these non-linearities in the problem the solution process is controlled via under-relaxation factors and all the governing equations are solved sequentially (i.e., segregated from one another). Typically 5-10 000 iterations were used to obtain converged solutions for all solved equations. Convergence criteria
were typically set to $10^{-4}$ for fluid as well as particle concentration equations and $10^{-7}$ for the energy equation.

### 6.9 Walls and solid boundaries

All the surfaces in an indoor space, such as walls, ceilings, floors and the furniture surfaces, are considered as walls. In the close region of the wall, the airflow is laminar and convective heat transfer occurs between the flow and the wall surfaces. For instance, in Paper II the wall function treatment in the numerical simulations was unable to fully deal with the convective heat transfer from the solid boundaries. In the region very close to the wall, the airflow is laminar, and often the convective heat transfer occurs between the flow and the surfaces in this region. This is still a problem for many turbulence models, such as the standard $k$-$\varepsilon$ model. In this thesis many of the investigations focused on fully turbulent flow motion, therefore one can understand that the current model predicted airflow behaviour near the tested diffusers well, but could have some limitations in correctly predicting the heat transfer from the walls, Paper II. The near-wall grid is also important for handling particle calculations as deposition treatment on solid boundaries is still grid-dependent in our calculations (Holmberg & Li, 1998). Additionally, it is necessary to specify wall functions for the description of friction and heat transfer. In most of the CFD calculations the wall temperatures are prescribed. The BCs are applied to wall surfaces by supplying the surface temperature. One can understand that the local heat transfer coefficient is an important parameter for expressing the heat flow between the wall and the first grid node. The heat flow, $P_cA_w$, between the wall and the first grid node is

$$P_c = \alpha_c (T_{nw} - T_w)$$

where $P_c$ (W/m$^2$) is the local convective heat transfer from the walls when $A_w$ (m$^2$) is set to 1, $\alpha_c$ (W/m$^2$K) is the local convective heat transfer coefficient from the fluid side, $T_{nw}$ (K) is the air temperature at the first grid node and $T_w$ (K) is the surface temperature at the wall. Only in Paper IV the temperature was not specified on room wall surfaces and adiabatic room conditions were used.

Radiation heat transfer, $P_{rad}$ (W/m$^2$), is considered indirectly by prescribing the surface temperatures of floor, ceiling and walls. In this way the temperature at the wall surface temperature adjacent to a fluid cell can be defined by using a heat flux, $P_c - P_{rad}$, at the wall surface as in the calculation example, Paper IX.

$$T_w = \frac{P_c - P_{rad}}{\alpha_c} + T_{nw}$$

Another important feature in wall treatment is choice of wall functions. Wall functions are a collection of semi-empirical formulas and functions that in effect link the solution variables in the near-wall cells and the corresponding quantities on the wall. The wall functions contain laws of the wall for mean velocity, temperature and turbulence quantities. The standard wall functions were used throughout the thesis (Versteeg & Malalasekera, 1995). More information about wall
dimensionless values such as non-dimensional velocity, $v^+$, and dimensionless length near wall, $y^+$, and wall functions can be found in several publications (Brohus, 1997, Chen & Srebric, 2001, Versteeg & Malalasekera, 1995). However, one has to understand the limitations of wall functions under certain flow conditions which depart too much from the ideal conditions. The software then provides enhanced wall treatment for such situations (Fluent Inc, 2003).

### 6.10 CFD modelling based on integrated design process

Due to a lack of standardization of CFD simulation procedures the author proposes a static way to link different software packages to assist CFD simulations and to improve the quality of the final result. Through interoperability, different software tools used in the design process of buildings can provide some new features to the CFD simulation process. The amount of manual modelling and numerical input values can be decreased using computation results from other programs, as shown in Paper IX. Using already existing data generated in various stages of a building project can reduce both the time consumption and the cost. The integrated design process is a new method to systemise building projects in a way that earlier calculations and design processes could promote the quality of the CFD simulation. The earlier more primitive computations could help to identify where the rather complicated CFD simulation is required. Performing the airflow simulations based on reliable numerical BCs (boundary conditions) creates a unique possibility to optimise the indoor environment by comparing different system configurations. This new method helps the engineer to choose the best alternative ensuring certain design criteria and target levels concerning thermal or contamination aspects, Paper IX. The integrated CFD modelling approach is presented in Fig. 19.

![Fig. 19. CFD simulation procedure based on an integrated design process](image-url)
The integrated design process can be used for optimising the ventilation system’s layout by comparing the effect of distribution solutions, system layout constructions and source locations on contaminant concentrations.
7 RESULTS

The results from this thesis have revealed the full complexity of CFD simulations in buildings. The gathering of input data for modelling and generation of BCs for CFD is very complex and not fully understood. The current thesis used many different methods to promote CFD modelling. They are listed below:

- Literature studies of air diffuser BCs and particles
- Introducing simplified models of air diffusers
  - Low velocity devices
  - Swirl diffuser
  - Industrial air diffuser
- Validation of simplified models by laboratory measurements
- Full-scale measurements in the laboratories concerning
  - Particle behaviour
  - Airflow behaviour
  - Thermal behaviour
- New information on how the internal heat source location can influence the heat removal efficiency by using validated simplified diffuser models
  - Full-scale measurements of 10 different cases
  - CFD simulations of these cases
  - Comparison of simulation and measurement results
- Improved method for evaluating the ventilation efficiency in removing particles
  - By comparing different room ventilation configurations
    - Mixing ventilation
    - Displacement ventilation
    - Different positions of ATDs
  - Using combined multi-zone and CFD methods to evaluate particle concentrations in different parts of the room
  - Using a new type of sub-models for different-sized particles
- Presenting a new method for performing the CFD simulations – integrated design process

7.1 Literature studies

A quite extensive literature study on particles is presented in Paper III. Furthermore, part of the validation of the current particle model is based on measurements found in literature. The results from literature were used when developing the simplified models of air diffusers and comparing the results from different simulations to literature results and measurements, Papers V-VII. The results from literature reveal that the whole CFD modelling procedure needs more systematisation. CFD modelling needs a more systematic way of improving the modelling procedure and generation of BCs. This improvement could partially be achieved through an integrated design process where for instance design criteria and input values, as given in Paper IX, could be adopted from other building design disciplines. Furthermore, CFD-specific
modelling criteria discussed in Paper IX should be followed by the standard procedures given in CFD guidebooks (Casey & Wintergerste 2000, Chen & Srebric, 2001).

7.2 Full-scale laboratory measurements

An important goal for this work was to investigate how the air distribution influences the particle concentration in different parts of a ventilated room. The first goal was to develop an air diffuser or ventilation configuration which could efficiently control the airborne particle distribution in the occupied zone to an acceptable level. The tested diffuser was a low velocity diffuser called “Floormaster”.

Fig. 20. Full-scale laboratory room for measurements and numerical simulations

All the tests and CFD simulations were compared in full-scale assuming:

- Equality in geometry and co-ordinate system
- Equality in used boundary conditions. This means:
  - Equal air supply/exhaust terminal locations and source conditions
  - Equal room conditions, including surface temperatures in the room
- Equal flow conditions in the room. This means:
  - Identical temperature and velocity conditions
Identical particle concentration conditions

The main results from the tests in Fig. 20 are presented in Paper II. This paper revealed problems with generating constant particle concentration in the room, Fig. 21. The particle concentration varied considerably with time as shown in Fig. 10.

![Fig. 21. The particle generator located in the test chamber](image)

The low velocity diffuser Floormaster was tested in the ABB laboratory in Enköping. Additionally, different-sized particles were measured in the same laboratory hall. Some of the results of the particle measurements are presented in APPENDIX C. The measurements in test rooms verifying the CFD simulations are described in Papers II, V-VII.

The swirl diffuser and the industrial air diffuser simplified CFD models were validated by full-scale measurements done in a laboratory room of the Finnish Institute of Occupational Health.

![Fig. 22. Laboratory test hall in the Finnish Institute of Occupational Health, see also Papers V-VII](image)
In the test facility shown in Fig. 22 two types of air diffusers were used for testing the heat removal efficiency. Totally 10 different configurations were utilised to test the airflow and thermal behaviour in the laboratory test room, Paper VII. It is expected that contaminants behave in the same way as excess heat and therefore also contaminant removal efficiency was measured in parallel, Paper VII. The results revealed that the air distribution is rather important for an efficient design as to the heat and contaminant removal. Most of the measurements were performed as a collaboration work and one can acknowledge uncertainties during the computer-controlled measurements. Due to huge amounts of measurement data generated by the computer-controlled measurement equipment, the study focused more on handling data properly. For instance, near zone validation of the industrial air diffuser model in APPENDIX A used (17 x 4 = 68) measurement points for one measurement line. Three velocity components and temperature were measured simultaneously in one measurement point. Measurements of air velocity and temperature were time averaged over 60 s and the values were recorded with a data logger (in the swirl diffuser case 180 s), Paper VI. Totally 680 measurements points were used to validate the industrial air diffuser performance in the near zone, Paper V. In the swirl diffuser case, 34 x 4 = 136 points were used and totally 1360 points were utilised in the validation process in Paper VI and APPENDIX B. Totally 10 different ventilation configurations were tested in the same test facility, 5 cases for the industrial air diffuser and 5 cases for the swirl diffuser, Paper VII. 10 different test conditions used 28 x 24 x 4 = 2688 points for vertical plane measurements of three velocity components and the air temperature. Horizontal plane measurements used 11 x 28 x 4 = 1232 points. For that reason each tested case produced 3920 measurement points and totally 39200 points were used for visualisation and validation of all the cases. The time spent, for instance, measuring the industrial air diffuser cases was 327 hours, approximately two weeks around the clock. The cases with the swirl diffuser took three times longer, because of the extended measurement time of 180 seconds for one measurement point. This kind of measurements cannot be performed by humans, but was achieved by a computer-controlled traversing system and with a data logger. An example of the measurement results is presented in APPENDIX D; it was used for validating the swirl diffuser model in Paper VI.

7.3 Simulation results

Original simulation results are presented in all papers except in Paper III which was almost entirely focused on literature research. All the results indicated that the air diffusion in a room is a complex combination of many factors such as supply airflow profile, diffuser type, location of heat sources, heat source strength and internal obstructions. Room ventilation is caused partly by the airflow supplied from air diffusers and additionally by the buoyancy-driven flows from heat or cold surfaces, Figs. 23-24 and Papers V & VII. That is why it is essential to model the air diffusers for the CFD simulation case as accurately as possible, Papers V-VII. Contaminant or particle behaviour within a ventilated space is entirely a function of air diffusion which is discussed in Papers I-II, IV & VIII.
Large particles settle in the regions where low velocity conditions occur. This is proven both by measurements and simulations. Due to the complex nature of the CFD modelling even the evaluation of the results is difficult. The results from simulation are given in all cells in the computational domain. The usual surface cuts are not always the best method to present the results. In this thesis a new type of evaluation method for particle behaviour is presented in
Paper VIII. Particle simulation results in CFD combined with multi-zone modelling approach represent a powerful method to understand how particles actually behave in airflow and where they are to be found in a room. This method can assist in finding the best ventilation configuration by performing comparative simulations. For instance, the position of the diffuser can be tested to find out how it influences the breathing zone concentration, $C_{bz}$. The simulation results of testing the influence of diffuser location at isothermal conditions for particle concentration in the occupied zone are presented in Paper IV. The comparison of different simulations is a way to optimise the system layout to ensure certain design criteria and target levels. The design criteria presented in Fig. 11 are important from the architect’s point of view concerning the room layout and spatial relationships of internal obstructions. The design of a ventilated room is important for room airflow distribution as well as particle behaviour. That is why it is necessary to use sophisticated methods and procedures to optimise the ventilation system’s performance, as in Paper IX. In Paper IX the ventilation performance in an office was optimised by using cooled beam air distribution.

7.4 Quality and evaluation of the results

The quality of the simulation results was assured by various means. When comparing the results either a single point value or a whole set of points was assessed. When validating, principally measurement value and simulation value were compared, as in Paper V. The quality of the simulation results was achieved by:

- Comparing a single point measurement value to the simulation value, Papers V-VI
- Comparing a whole set of values in the graph in a given comparison area, Paper V-VI
- Visualisation of measurement results and simulation results, Papers V-VI
- Smoke visualisation in the full-scale laboratory hall, Paper V

The particle simulation results were reported and assessed in numerous articles. Additionally, for typical graphs and surface cuts the simulation results were calculated by:

- Integrating over the supply and exhaust openings to calculate the particle flux, Papers I-II, IV, VII-VIII
- Volume integration over certain volumes such as the breathing zone, $H = 1.5 – 1.8$ m, and the occupied zone, $H = 0 – 1.8$ m, above the floor height, Paper IV
- Reporting results in iso-surfaces with certain concentration, as in Paper I.
- Dividing the room into different zones and reporting the concentration in these zones. This was a way to evaluate the particle mass transfer in different parts of a room, Paper VIII.
- Comparing the room average concentration to the concentration in the investigated location, Papers II, IV, VIII.

7.5 Accuracy of the results

The deficiencies or inaccuracies of CFD simulations can be related to a variety of errors and uncertainties. These can be generation of BCs, CFD-related models and methods, human lack of
knowledge and so on. This thesis mainly focuses on integrating simulation-related procedures and to recognise and overcome the problems during the CFD modelling.

There are two main problem categories when performing the simulations and they can be divided into:

- **Errors**: Recognizable deficiency that is not due to lack of knowledge
- **Uncertainly**: A potential deficiency that is due to lack of knowledge (Casey & Wintergerste, 2000). In other words, unknown problems appearing during the simulation.

It is assumed that the current thesis can contribute to improved knowledge so as to decrease the errors in the CFD process. Uncertainty issues are left out as there are no straightforward methods on how to assess uncertainties in CFD simulation. One needs to be aware of the limitations and capabilities of CFD in modelling an indoor environment. The end result of any CFD simulation is dependent on

- **Choice of BCs**
  - Numerical values for physical wall boundaries
  - Numerical values for supply/exhaust openings
- **Geometrical uncertainties**
  - Geometrical representation of objects within the modelling
  - Oversimplification is not recommended as the geometrical objects alter the indoor airflow field. This concerns all the objects embedded in the modelling such as ATDs, furniture, walls, humans and other objects
- **Mesh quality in the computational domain**
  - Numerical diffusion
  - Grid design close to ATDs
  - Grid dependence tests should be performed
- **Choice of models**
  - Turbulence modelling
  - Code errors
  - Specific model errors known by solving a specific problem with an unsuitable model
- **Choice of discretization technique**
  - Numerical error represented in each cell because of discretization of governing equations
  - First order vs. higher order schemes
- **Numerical values as under-relaxation factors for segregated solver and others**
- **Convergence criteria**
  - Caused by iterative solution technique
  - Scaled residuals should reach pre-given limits. In the normal case $10^{-4}$ for flow equations. The residual $R_\phi$ computed by segregated solver in Eq. (53) is the imbalance in the concentration equation summed over all the computational cells. This is referred to as the unscaled residual. The scaled residuals are computed by comparing a scaling factor representative of scalar quantity, $\phi$, through the computational domain.

- **User errors**
  - Depends very much on the person who actually performs the simulation
In indoor environment, the airflow diffusion is typically driven by natural convection, forced convection or mixed convection. The calculation of airflow field coupled with solid contaminants makes the indoor problem very complex. Conclusively, particle calculation in indoor air is dependent on all the factors mentioned above and the quality of the particle model itself. That was the main reason why the current thesis used similar numerical methods throughout all the papers, because for instance the limitations of the $k$-$\varepsilon$ turbulence model are known, but still it seemed to be the most suitable model for simulating indoor air turbulence. Accuracy of the results was assessed by simplified means:

- Comparing simulated results to results found in the literature, **Paper III**
- Comparing simulated results to the measurement results, **Papers II & V-VII**
- Comparing different simulation results with each other, **Paper IX**

If the simulation results are compared to each other it is necessary to recognise the limitations of the simulated results. Still, when an acceptable quality of CFD simulation results is maintained CFD can be used for optimizing the ventilation system’s performance, as in **Paper IX**. This is the main reason why the accuracy of the simulation should always be maintained at an acceptable level. If one considers using the particle model presented in this thesis it needs to be recognised that the model only accounts for the particle settling and the deposition at physical boundaries by simplified means. To capture the dynamic behaviour of particles in indoor air one needs to use a more sophisticated model. At the moment there are very few CFD models which can account for particle coagulation, nucleation, Brownian diffusion. Even if such a model exists it is always a problem to evaluate the results in a proper way, because of problems of 3D space-time representation.

In general, the accuracy of simulated results was assessed by comparing them to measurement results, as in **Papers V-VII**. The results quantitatively showed some deficiencies in modelling air diffusers. The grid layout was a very important factor for the accuracy as the BCs were represented on the boundary of the simplified model. If the grid was too coarse numerical diffusion took place and the simulated velocity in the near zone of the diffuser was unacceptably low compared to the measured values. Additionally, the grid layout close to heat sources was important because it had a strong impact on the plume generated above the heat source, **Paper VIII**. The accuracy of particle simulations was assessed mainly based on results found in the literature and previous validations.
8 GENERAL DISCUSSION AND CONCLUSIONS

The results from this thesis reveal the full complexity of performing CFD simulations of an indoor airflow field coupled with solid particles. The thesis emphasises the importance of the many aspects of modelling. The quality of particle simulation results is partly determined by the quality of the indoor airflow field simulation. As the indoor airflow field is greatly dependent on air supply conditions it is necessary to have high quality models of air diffusers. The current thesis suffered limitations in the full-scale laboratory measurements for airborne particles. The laboratory measurements partly failed and the simulation results were partly validated by the results found in the literature. Nevertheless, measurements, literature and the simulation results revealed that the locations contaminated by particles in a room are where the low air velocity conditions occur. That was the main reason why airflow simulations were extensively performed to numerically test different design alternatives. As the heat sources generate plumes which are a crucial part of the indoor airflow field, mainly non-isothermal conditions were simulated except in one paper. All the simulations revealed that the air distribution to the space is important as it determines the occupied zone temperature, the concentration of contaminants and is a variable for the energy efficiency via use of the airflow rate. In this thesis CFD simulation is introduced as a design tool to improve the system layouts in pre-design. It is expected that with validated numerical tools, system designs may be significantly improved before the actual construction phase. At the same time it is important to follow the guidelines to assure a certain quality of these simulations. Still, the literature study has revealed, for instance, that there is no standard way to generate the BCs for air diffusers, because of their geometrical complexity. This is why the CFD simulations still are extensively used by universities, but have gained rather low popularity among engineering companies. The amount of parameters given to simulations and methods should be more standardised. Lately, some guidebooks on how to follow certain quality criteria in performing the simulations have been published (Casey & Wintergerste, 2000, Chen & Srebric, 2001). The gathering of input data and generation of BCs is still given small attention which prevents CFD usage becoming widespread. Future studies should improve the modelling, considering all aspects of CFD modelling to make it a more feasible tool in the normal building design process. That is why all the design disciplines should be integrated into one core to improve the data exchange and to reduce the manual data input. Future studies should integrate and standardise most of the procedures for CFD modelling. This will enable the use of CFD modelling more widely among people who do not have a deep knowledge in fluid and mathematical modelling, without compromising the modelling accuracy.
9 REFERENCES


Davidson, L., 2003: *An Introduction to Turbulence Models*. Department of Thermo and Fluid Dynamics, Chalmers University of Technology, Göteborg.


Lange, C., 1995: Indoor Deposition and the Protective Effect of Houses against Airborne Pollution, National Laboratory Risø, Denmark, PhD thesis.


Nagasawa, Y. and Y. Kondo, 2002: Modeling of Complex Air Diffuser for CFD simulation Part I and II. RoomVent 2002: 8th International Conference on Air Distribution in Rooms, Copenhagen, Denmark, pp. 105-112.


APPENDIX A

Boundary conditions for industrial air diffuser

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Measurement and simulation results in one comparison point

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Comparison of measurement and simulation results with industrial air diffuser
APPENDIX B

Boundary conditions for swirl diffuser

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<tr>
<td>( s )</td>
<td>0.0625 m</td>
</tr>
<tr>
<td>( V )</td>
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<td>( \theta )</td>
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**132.5 l/s case**

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**100 l/s case**

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Air Diffusion and Solid Contaminant Behaviour in Room Ventilation – a CFD Based Integrated Approach

**Measurement and simulation results in one comparison point**

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**Graph:**
- **Top graph:** Air velocity V, m/s vs Height, m
- **Bottom graph:** Temperature, °C vs Height, m
Comparison of measurement and simulation results with swirl diffuser
APPENDIX C

Particle measurements in displacement ventilated room at 2.0 meters

Particle measurements in displacement ventilated room at 1.3 meters

Particle measurements in displacement ventilated room at 0.4 meters
Particle measurements in mixing ventilation at 2.0 meters

Particle measurements in mixing ventilation at 0.4 meters

Particle measurements at exhaust outlet
APPENDIX D

Measurement results for swirl diffuser case in a vertical plane $Q_m = 380$ l/s. All the 10 measurement cases were measured in a similar way. See also Paper VII.

Velocity vectors in vertical plane

Velocity vectors in horizontal plane
Velocity conditions $V_a, \text{m/s}$

Velocity conditions $v_x, \text{m/s}$
Velocity conditions $v_x$, m/s

Velocity conditions $v_z$, m/s
Temperature conditions $T, ^\circ C$
APPENDED PAPERS