Physical and numerical modelling of dust dispersion in the leeward zone of two single-standing buildings

Cornelia Wevers, Rüdiger Höffer

Wind Engineering and Fluid Mechanics, Ruhr-Universität Bochum, Universitätsstraße 150, Bochum, Germany

ABSTRACT: The aim of this work is to define a model setup for a suitable and economical prediction of dust/particle dispersion and deposition around buildings driven by an atmospheric boundary layer (ABL) flow. The dispersion behind two different single buildings is modelled physically and numerically. The numerical simulations with gas and particle dispersion show different results in comparison to the physical tracer gas experiments. The normalised concentrations behind the single cube are overpredicted and underpredicted behind the single-standing hall with an open leeward side. The used wind tunnel technique does not allow the simulation of particle settling, in contrast the numerical simulation is able to model particle deposition using different particle diameters in the gravity field, which is shown in a pre-study.

KEYWORDS: dispersion, particle transport, CFD, wind tunnel, Eulerian, Lagrangian

1 INTRODUCTION

To model dust/particle dispersion and deposition from diffuse sources in the atmospheric flow physical and numerical simulations were combined and used together in this study. In the past, several researchers investigated numerical simulation approaches for urban pollution dispersion in comparison to physical models [1], either for gaseous pollutants [2,3,4] or for particle dispersion [5,6]. Numerical CFD calculations need to be compared to physical experiments to ensure a proper prediction of the target values and to proof the suitability of the numerical model and the dispersion characteristics. But before adopting a physical model for validation purpose it needs to be validated and tested itself. For this reason first a geometrically simple test case, namely a cubic building with a pollution source on the building top is used to validate the experimental setup for dispersion modelling (cf. Fig. 1 Case1). The dispersion process itself depends on the flow field and in detail on the existent turbulence quantities. In a previous work the validation of the computed wind field around bluff buildings using the commercial code ANSYS CFX and the same simulation setup compared to this study were performed with the VDI Guideline 3783-9 (VDI = The Association of German Engineers), [7]. This validation shows a suitable agreement between the experimental and numerical predicted velocity components within a given range [8,9]. The target values of this work are the nondimensional concentration distributions. For that reason the validation test case from the wind tunnel model, the cube, is also used for CFD calculations in order to compare the computed concentration values with the performed experiments. As idealised case of use a leeward open industrial hall (Case 2 in Fig. 1) with a source inside was placed in the ABL-flow. In real live such buildings dusty goods like construction or soil materials are handled and storage. Due to the wind around and through the halls emitted particles are transported outwards and interact with the environment. The other way around, numerical calculations were used to find appropriate and optimal measurement positions in the wind tunnel for detect the concentration distribution behind the buildings.
One main disadvantage of the physical approach is the difficulty of modelling particle tracking because of the scaling requirements (see Chapt. 2.1.2). Thus, the physical experiments were performed using a tracer gas, assuming that very small dust particles are suspended in air and not affected by gravity. The same tracer gas approach (Eulerian model) is then used in the numerical calculation for comparison. In contrast, the advantage of the numerical model is the possibility to simulate particle transport in real scale while using a Lagrangian model approach. Therefore, at first, gravity-free dispersion simulations with uniform particles were performed and compared to the tracer gas approach. Afterwards, simulations with gravity and different particle diameters were done in order to model particle deposition. The physical plausibility of the simulated particle behaviour is analysed heuristically in a first step.

2 DESCRIPTION OF THE PHYSICAL AND NUMERICAL MODELS

2.1 Physical model

2.1.1 Boundary conditions and measurement techniques

The physical tracer gas experiments are performed in the boundary layer wind tunnel of the Ruhr-Universität Bochum. The oncoming turbulent flow is generated using a Couinhan-setup [10] and corresponds to an atmospheric wind over urban terrain with a real roughness length $z_0 = 0.1m$ (geometrical scale 1:200). In Figure 2 the dots show measured flow characteristics, like vertical velocity profile and turbulence quantities in x-direction [11].

The dust phase is modelled with Sulfurhexafluorid (SF6) diluted in Nitrogen (N2) to achieve the same fluid capacity like air. The source is geometrically modelled in such a way, that the mo-
mentum flux densities of the tracer and of the air flow in source height are almost equal. For both cases, the concentrations were measured along three axes, two laterals and one longitudinal (see Figure 1) in certain heights with an Electron Capture Detector (ECD). Under consideration of all fluid parameters the local concentrations \( \rho_{SF6,i} \) are measured and normalised with a reference velocity \( u_{ref} \), height \( z_{ref} \) and the source mass flow \( \dot{m}_{Q, SF6} \) to a nondimensional concentration coefficient \( C_i \):

\[
C_i = \left( \frac{\rho_{SF6,i} u_{ref} z_{ref}^2}{\dot{m}_{Q, SF6}} \right)
\]

For testing the repeatability and independency from the measured values of the parameters variations of the experiments were made with different flow velocities, source strengths and measurement times.

2.1.2 Scaling requirements for particle simulation

The basic principle of a boundary layer wind tunnel test is to scale the wind field so that a certain similarity of wind velocity profile, turbulence intensity and turbulent length scales exists compared to the real wind [12]. One measure for similarity between real and model scale flow is the Flow-REYNOLDS-Number \( Re_F = \frac{\rho_t u L}{\eta} \), using a reference velocity \( u \), a characteristic building length \( L \) and the fluid density \( \rho_t \) as well as the dynamic fluid viscosity \( \eta \). It is usually not possible to match the real \( Re_F \)-Number in the experiments, but to ensure a similarity of the flow around bluff buildings \( Re_F \cdot 10^4 \geq 10000 \) is recommended in the literature for the experiments [13].

Physical experiments with particles were done in the past either for saltation of scaled snow [14,15] or for analysis of real sand motion [16,17,18]. In case of modelling aeolian particle motion requirements for particle scaling in a wind tunnel simulation are summarized e.g. by Kind [19], White [20] and Durán et al. [21]. Kind performed a similarity analysis and stated out, that “it will often be impracticable to simultaneously satisfy all the simulation requirements [...]”, therefore compromises are necessary [19, p. 219]. There are three particle movement modes which develop due to the wind shear stress on the grain surface and due to atmospheric turbulence: suspension (free flight), saltation (short jumps on a surface) and creep or reptation [22]. The main influence on the mode is given by the ratio between particle size, particle settling velocity, particle spin, wind shear stress and turbulence intensity. Therefore, as scaling requirement, e.g. the ratio between the particle settling velocity and a reference velocity should be equal in real and model scale [19]. The similarity of the aerodynamic behaviour of the free flying particles is characterized amongst others by the Particle-REYNOLDS-Number \( Re_p = \frac{\rho_t u_p d_p}{\eta} \), which describes the inertial and viscous effects at the scale of a grain. In case of fine sand (quartz, \( d = 300\mu m \)) the deposition velocity is \( u_p = 3m/s \) [21] and the corresponding Particle-REYNOLDS-Number is \( Re_p = 58.3 (\gg 1, \text{turbulent regime}) \).

The consideration of all requirements can make it nearly impossible to find a proper material, which matches all requirements for modelling suspension, deposition and saltation simultaneously in a scaled physical wind tunnel experiment. Therefore, in general, only physical gas simulations are performed and then in the numerical approach discrete particles are considered. The development of the numerical set up is still progressing.

2.2 Numerical model

2.2.1 Meshes, flow boundary conditions and simulation settings

For both Case 1 and Case 2, the geometries and meshes were build regarding the used wind tunnel models and following the recommendations of Franke et al. [23]. In Case 1 the height of the cube is \( H_{C1} = 25cm \), the width \( W_{C1} \) and the length \( L_{C1} \) are equal. For Case 2 the building height is \( H_{C2} = 12cm \) and the size ratio is \( H_{C2} : W_{C2} : L_{C2} = 1:2:4 \). Block-structured hexahedral
volume meshes are generated with a maximum cell-growing ratio of 1:1. The meshes were refined iteratively until the target values did not change much anymore. For the particle simulation in real scale the mesh was exported with a building height \( H_{C2} = 24 \) m. Therefore Case 1 has c.a. 1.4Mio cells and Case 2 has c.a. 5.3Mio cells. The inlet profiles for velocity, turbulent kinetic energy (TKE) and its dissipation are modelled according to the method proposed by Richards et al. [24] to match the results of the performed physical simulations, see Figure 2. The lateral sides, the bottom and the building surfaces are defined as walls. The top boundary has a constant shear velocity in order to keep the vertical velocity profile as much as possible constant in horizontal direction [25]. The outlet has a relative static pressure of 0Pa. All numerical simulations were performed as Reynolds-Averaged Navier-Stokes (RANS) simulations with the Standard k-\( \varepsilon \) turbulence model using the commercial code ANSYS CFX 12.1. For the approximation of the convective terms the High-Resolution scheme is used, and the truncation error is set for the maximum residuals to 10\(^{-6}\) within 1000 iteration steps. The iteration convergence is observed using monitor probes behind the buildings.

2.2.2 Modelling the dust dispersion

The physical experiments for modelling the transport of the dust material use a tracer gas method as mentioned before. In order to use these experiments for comparison the dust in the numerical simulations is modelled in two ways. The first way describes the tracer as gas, like in the physical model, using an additional transported scalar variable (Eulerian approach) and the standard gradient-diffusion-hypothesis (SGDH) for the scalar fluxes [26]. They are modelled amongst others using the turbulent eddy viscosity \( v_t \) and the turbulent Schmidt-number \( S_{ct} \). The latter one describes the scale between the turbulent viscosity and turbulent diffusivity, thus the scale of transport values between momentum exchange and mass exchange [27]. Although \( S_{ct} \) is not a constant [28,29], it is used as a constant in the gradient-diffusion-hypothesis. A proper value choice is an actual discussion of research [3,4,29,30]. The choice should be made case dependent. In this study the turbulent Schmidt-number is \( S_{ct} = 0.9 \) and will be not vary for this study. The transport properties for the scalar are the same like for air at 25°C, which is defined as fluid for the whole domain. The source mass flow and velocity of the tracer are set with respect to the wind tunnel experiments. For analysis the nondimensional concentration is calculated with Equation (1). The second way to model the tracer is to track discrete particles in the continuous air phase using the RANS-calculated flow field (Lagrangian approach). With Euler-forward integration of the particle velocity in discrete points the particles are moved along paths through the domain. The particle velocity itself is calculated from an analytical solution of the particle momentum equation, which sums all forces acting on a spherical particle [31]. The most relevant force is the drag force, which is calculated using Stokes-law in Equation (2). This includes the velocities of the fluid \( u_f \) and of the particle \( u_p \) as well as the particle diameter \( d_p \), the dynamic viscosity \( \eta \) and the correction factor \( C_{cor} \), which depends on the Particle-Reynolds-Number, used model from Schiller & Naumann in [32,31].

\[
m_p \frac{dt}{dt} = 3 \pi \eta d_p C_{cor} (u_f - u_p)
\]

Additionally the stochastic “discrete droplet” model from Gosman and Ioannides [33] is used to calculate the turbulent diffusion of each particle due to turbulent eddies with a characteristic fluctuation velocity \( u'_t \), length \( \ell_e \) and lifetime \( \tau_e \):

\[
  u'_t = \Gamma \left( \frac{u_i^2}{\ell_e} \right)^{1/2} = \Gamma (2k/3)^{1/2} \quad ; \quad \ell_e = \left( C_{\mu}^{3/4} k^{3/2} / \epsilon \right)^{1/3} \quad ; \quad \tau_e = \ell_e / (2k/3)^{1/2}.
\]
The variable $\Gamma$ denotes a normal distributed random number, $k$ the local TKE, its dissipation $\varepsilon$ and $C_u$ a constant [31]. For suspension modelling 80,000 numbers of positions with particles of diameter $d_p = 2.5\mu m$ (quartz $p_r = 2650kg/m^3$) and a mass flow of $m_{Q,P} = 0.2kg/s$ were injected inside the hall (real scale sized). The maximum tracking time was set to 24 hours with an integration time step per particle of $\Delta t = 1s$. The nondimensional concentration $C_i$ (Equ. (4)) is calculated comparable to Equation (1) using the averaged volume fraction from Equation (4). The summation is performed over all particles and time steps in a control volume $CV$ and stored in each vertex; $\Delta t$ is the particle integration step, $N_P$ is the particle number rate, $m_P$ is the particle mass and $\Phi_P$ the volume fraction [31].

$$C_i = \left(\Phi_{P,i} u_{ref} z_{ref}^2\right) / \left(m_{Q,P} / \rho_P\right)$$

with

$$\Phi_{P,i} = \sum(\Delta t m_p, N_p) \Phi_P / \sum(\Delta t m_p, N_p)$$

3 RESULTS AND DISCUSSION

3.1 Independence of the flow-REYNOLDS-number and of the model scale

The dependency of the inflow velocity, more precisely of the flow-REYNOLDS-number $Re$, and of the model-scaling was tested and analysed. The physical experiments were performed with a $Re$-number around $Re = 42000$ with $u_{ref} \approx 5m/s$ ($> 10000$, cf. 2.1.2). The normalised numerical results for gas and particle dispersion are not affected by different inlet velocities above a critical minimum velocity (e.g. model scale: $u_{ref} \approx 2.5m/s$ results in an undeveloped flow field). The normalised results of the gas dispersion are also not influenced by different scaling (model scale = wind tunnel scale and real scale). But, as expected, the particle simulations show clearly the necessity of particle scaling. When using the same particles (size and material) the normalised concentration distributions show higher values in model scale simulations compared to the real scale simulations. The particle size is too huge in the ratio to the model scale domain size and yields to higher concentrations by calculation of the volume fraction in Equation (4). Therefore, all numerical simulations were performed in real scale and not in wind tunnel model scale.

3.2 Comparison of the normalised concentrations

3.2.1 Cubic building (Case 1)

The flow and dispersion around the cubic building is one of the benchmark geometries in the German VDI Guideline 3783-12 for physical wind tunnel tests. Figure 3 demonstrate the concentration distributions behind the cube along the measurement axes, and Figure 4 shows the normalised concentration contours in the middle vertical plane. The conducted physical experiments give almost satisfying results compared to this guideline. It can be stated that the physical wind tunnel set up is able to reproduce the dispersion process behind the cube. In contrast to this, the numerical approaches overestimate the concentration by far in longitudinal direction and underestimate the lateral dispersion. Similar results were also found for isolated sources e.g. by Blocken et al. [4] and Gousseau et al. [34] and seem to be characteristically for a RANS SGDH approach. On the one hand several researchers found a high dependency of such results on the turbulent SCHMIDT-number $Sc_t$, as discussed in Chapter 2.2.2, so that a variation of $Sc_t$ could lead to some improvement of the results. But on the other hand, to vary this number is not always a solution. For example Rossi et al. [29] pointed out, that the discrepancies “may reflect the inadequacy of the SGDH model in capturing the complex features of the scalar dispersion process, which cannot be compensated by adjusting the Schmidt number value.” [29, p. 3]. In addition, the source on the top lies in a highly turbulent zone where an unsteady recirculation bubble influences the source, which cannot be captured by a RANS model.
3.2.2 Leeward open hall (Case 2)

Behind the hall with an open leeward side the normalised concentrations are compared along the three axes. Figure 5 shows in the first row the concentrations at height $z = 0.5H$ and in the second row at height $z = 0.25H$. In general, the quantitative concentration distribution characteristics can be predict by the numerical approaches, but the gas simulation as well as the particle simulation underestimates the concentration values of the physical experiment, particularly inside the building (Figure 5 first column, negative x direction). This is strongly in contrast to the results of Case 1, where all numerical results are overpredicted compared to the physical measurements.

The dispersion in and outside the hall is mainly influenced by the recirculation zone behind the building, which leads to an interaction of the outer and inner flow field. Inside the hall the velocity and the pressure is low compared to the outer regime. The wake is pulling the dust out from the interior along the building walls (Fig. 6) and most of the dust (gas or particle mass) escapes the hall in the upper corners as well as close to the bottom (Fig. 7).
Figure 5. Comparison of normalised concentration distribution behind building “Case 2” along three measurement axes in two different measurement heights; all numerical simulations are run in real scale.

Figure 6. Bird eyes view on simulated normalised concentration contours in horizontal plane in height z/H=2, left: gas concentration, right: particle concentration; the straight lines determine the position of measurement axes.

Figure 7. Simulated normalised concentration contours in vertical plane x/H = 1 behind the opening, left: gas concentration, right: particle concentration; the straight lines determine the measurement axes z/H = 0.5 and z/H = 0.25.
The wake re-enters the building from all sides in the middle and lower area of the opening and transports air and partially dust back into the hall. Inside of this recirculation, particularly in the two lateral vortices, the dust is stored and the concentration is higher, see middle column in Figure 5. This recirculation is a highly turbulent and non stationary process, occurring and collapsing or meandering, as could be seen in laser light sheets during the physical experiments. This unsteadiness may cause the high discrepancies, especially along the lateral axes, between the physical and numerical approach, because in the performed RANS simulation the recirculation is of steady state. So there is less lateral mixing and more dilution of the concentration from the building interior to the outer region compared to the physical results.

3.3 Retention time of the particles and particle deposition

The Lagrangian approach is able to provide information about the time resolved particle motion and particle deposition, when gravity is acting on the particles. In Case 2 the particles moves from the source to the opening in about 10 minutes, for $u_{ref} = 10\text{m/s}$. The longest retention time is about 30 minutes. In the presented results no gravity was activated and all particles had the same size. Figure 8 shows particle tracks of a performed numerical sand simulation with gravity and different particle diameter. Particles in suspension mode are usually smaller than 20µm and are kept aloft by turbulent eddies, grains between 20-70µm develop short term suspension which reaches distances of tens to hundred meters [35]. Sand grains with a size of 70-100µm are transported mainly in a series of short jumps (saltation) in a layer close to the bottom, in which the vertical component of wind velocity due to turbulence has no effect on the particle trajectories [36]. If the particle size is larger than 500µm the grains are moved in contact with the surface by reptation and creep. This physical behaviour was reproduced in a first numerical approach and shows acceptable results compared to literature (Fig. 8 right).

![Figure 8. Particle tracks of aeolian sand, left: numerical simulation of sand particles in an empty domain (light = small 50µm – dark = large 250-500µm diameter, right: scheme of aeolian particle transport [Pye, 1987].](image)

4 CONCLUSION AND OUTLOOK

The comparison of the numerically calculated concentration distributions in the leeward zones of two different buildings with results from wind tunnel measurements indicates a completely different behaviour of the models while using almost the same simulation settings. In case of a cubic building with one local source on the top a high overestimation of the concentrations in longitudinal direction and an underestimation of the lateral dispersion are found. In contrast to this, the numerical results of the concentration distribution behind the open hall show better agreement but underestimate the concentration distribution in longitudinal direction. It can be stated that the dispersion behind an idealised geometry with a locally placed source in a highly turbu-
lent zone is more difficult to predict than the dispersion behind a more complex case. Such results were also found by other researchers, e.g. [4]. In case of an open hall the source itself is diffuse and the dispersion process is affected mainly by the recirculation behind the hall. It is not possible to generalise the suitability of a RANS model for dispersion modelling. It depends on the type, location and surrounding of the source. Large Eddy Simulation gives better results compared to physical experiments for pollution dispersion [37,38], but it is not a useful alternative until today because of the required high expenses in calculation time and computer power. The comparison of the flow field and turbulence quantities is matter of future works in order to define more precisely the transport mechanisms. The time resolved LAGRANGIAN particle model provides more detailed information about the particle transport compared to the EULERIAN approach, like tracking time or particle-wall interaction. In future work, the deposition and interaction of the particles with the walls shall be modelled/improved, to analyse e.g. the retention effect of dust in such a hall. But particle erosion and accumulation is difficult or rather impossible to model. One alternative to the LAGRANGIAN approach could be the use of an EULERIAN Multi-phase model, like the Algebraic Slip Model, which is commonly used for snow modelling [39,40].

5 REFERENCES


19. R. Kind, A critical examination of the requirements for model simulation of wind-induced erosion/deposition phenomena such as snow drifting, Atmospheric Environment 10 (1976), pp. 219–227.


