Physical aspects of aerosol particle dispersion

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Abstract

The dispersion of dust particles gives us the causal connection between particle emission and immission. Due to the fact that it is impossible to follow the track of a single particle through the air, a lot of effects and there parameters must be known to simulate the dispersion.

The usage of tracer-gases allows to compare (gas) dispersion models with measured data, but the dispersion of gases or odours is not comparable with the dispersion of aerosols. One reason for that is a factor 10 to the power of 10 in the weight of a one micron particle with the density of 1000kg/m³ and a SF6 molecule.

The best available technologies to determine the parameters of all participated effects are laboratory-confirmed experiments. At the Institute of Agriculture Engineering at Bonn University such experiments has been made and will be done further, supported by the DFG (German Research Foundation).

In our research we examine dust samples with agriculture background, mostly from animal farms. One major effect, which influences the dispersion of aerosols, is the sedimentation. The results of our experiments are that the sedimentation velocity and the aerodynamic behaviour of aerosol particles depends on the animal type, the feeding system and the animal house setup. Another important effect is the agglomeration, which is depending just as well on the dust source and meteorological parameters, basically from the humidity. Furthermore aerosol particles can interact with surfaces. Depending on the surface structure, the humidity and the particle attributes as well as the air velocity nearby the particle surface interface, the aerosol particles can be accumulated or displaced.

Difficulties occur in statistic dispersion simulations including all before described effects. At our institute a numerical dispersion model is developed. Every single track of all particles is computed, so that all participated physical effects which influence the behaviour of aerosol particles can be taken into account.

Keywords: aerosol transmission, dispersion models, sedimentation, agglomeration, adsorption, resuspension

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Introduction

The term "aerosol transmission" describes the transport of dust particles from the emission source to the immission point. During the transmission phase the emitted substance is subject to a number of processes which change the properties and the concentration of the substance in the air. Apart from the influence of chemical decomposition, the concentration of a substance at the immission point is primarily determined by physical effects and dilution during dispersion. The dispersion of dust particles differs in important respects from the dispersion of gases. Dust particles are subject to a variety of physical processes according to their density, size and shape. The most important physical effects in this context are sedimentation, agglomeration and aerodynamics as well as adsorption and resuspension. Statements about the transmission behaviour of an aerosol require particle-specific analysis of the dust in question.

Sedimentation

It is primarily the sedimentation effect, i.e. the influence of gravity on aerosol particles, that causes them to fall to the ground. The sedimentation velocity depends not only on the weight of the particle but also on meteorological parameters (temperature, air pressure, air humidity) and, of course, on the size of the particle. This is illustrated in figure 1, which shows the sedimentation velocities of different size classes in a dust sample from an aviary house with approximately 70,000 laying hens (Schmitt-Paukszat G. 2006).

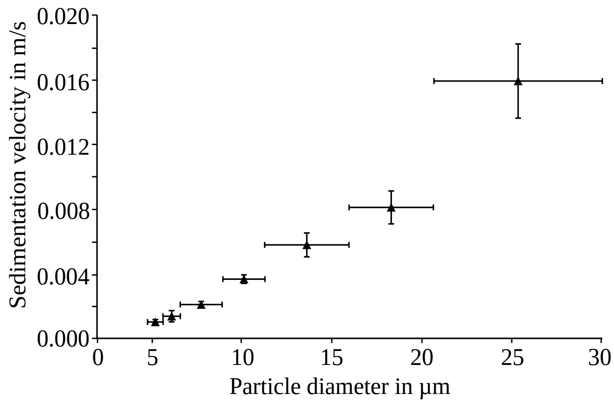

Figure. 1:
Measured sedimentation velocities of different particle size classes in a dust sample from an aviary house for laying hens (Schmitt-Paukszat G., 2006)

Measured sedimentation velocities and particle sizes can be used to calculate the ratio of particle density to particle shape. Figure 2 shows that the ratio of the density to the shape of the particles of the dust sample used in this example differs according to their diameter. In the same sample, the ratio is three times higher for small particles than for large particles.

A possible explanation for the large differences between the individual particle sizes is not so much the variance of the particle densities as the different shapes of the particles. The density of smaller particles with a diameter of 3-5µm is in the same range as concrete, which has a density of 2000 to 3000 kg/m³ depending on the admixtures used, whereas the density of larger particles is in the range of organic material such as feed fines, epidermal scales or feather fragments. Moreover, in mineral particles the form factor is usually smaller than in organic particles so that the denominator and the numerator can lower or raise the ratio at the same time. Therefore, it is possible to gain information on the possible origin of dust particles by measuring the sedimentation velocity of a dust sample and calculating the ratio of particle density to particle shape.

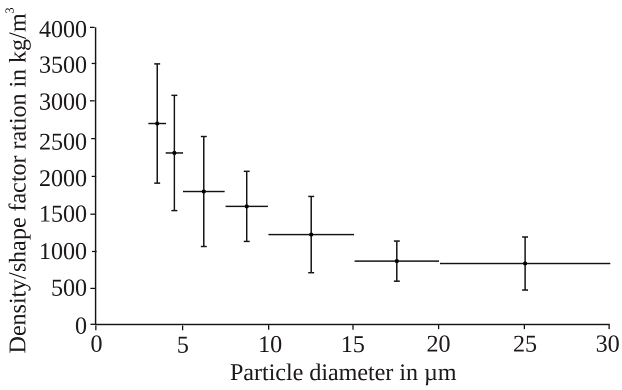

Figure 2:
Ratio of particle density to particle shape factor for different particle size classes in a dust sample from an aviary house for laying hens, calculated from experimental data

Agglomeration

Another important effect in relation to the transmission of aerosols is agglomeration. Agglomeration is the association of individual aerosol particles in so-called agglomerates as a result of attractive, binding forces. As the range of the forces between individual aerosol particles is very limited, agglomerates are formed almost exclusively as the result of two particles colliding. The collision of particles due to their thermal movement is called thermal coagulation. The binding forces between particles are mainly electromagnetic and hydrostatic forces. Differing from other particles in terms of diameter and shape, aerosols also have different aerodynamic properties and different sedimentation velocities. Experiments have shown that air humidity in particular has a great influence on the agglomeration behaviour of aerosols. Due to electrostatic forces the agglomeration rate is high at low air humidity, whereas hydrostatic forces stimulate agglomeration at high air humidity. Moreover, agglomeration depends on the material properties of the particles so that the variables describing the agglomeration process may vary for different aerosols from different kinds of sources (Rosenthal E. 2006).

Particle shape

Another important parameter in aerosol dispersion is the geometry or the shape of the particles. Microscopic studies show that dust from agricultural sources consists of highly structured particles of various shapes and densities (fig. 3).

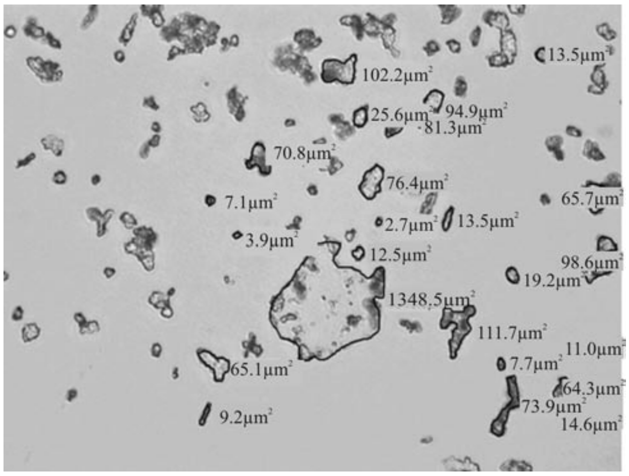

Figure 3:
Microscopic image of aerosol particles; the figures next to the particles specify their respective size (Nannen C., 2005)

The aerodynamic behaviour of a particle is influenced by its shape in the same manner as that of a car. To do justice to the various surface shapes of particles, a number of approaches to describing the aerodynamic properties of particles have been developed. The dynamic shape factor is a parameter that is used to adapt the Stokes friction term for irregularly shaped particles. Very much like the Cd factor (cars), the shape factor is very difficult to calculate and is therefore usually determined by experiments. Another way of adapting the Stokes term is by using the aerodynamic diameter, which is defined as the diameter of a spherical particle of unit density (1000 kg/m³) which has the same sedimentation velocity as the irregularly shaped particle under consideration (Hinds W. C. 1992). The Stokes diameter, which is used less frequently than the aerodynamic diameter, is the diameter of a spherical particle that has the same density and the same sedimentation velocity as the irregularly shaped particle under consideration. With a procedure developed at the Institute for Agricultural Engineering of Bonn University the ratio of particle density to particle shape can be determined experimentally. This measuring procedure is based on a comparison of experimentally determined sedimentation velocities with the corresponding optically measured size classes. Thus, the aerodynamic behaviour of particles of any shape can be taken into account in transmission simulationss (Schmitt-Pauksztat G. 2006). Analyses of the dispersion behaviour of aerosols must also take into account the interface behaviour between aerosol particles and various kinds of surface. The process of particles settling on a surface is called adsorption. The process of particles being detached again from the surface by airflow is called resuspension. Adsorption and resuspension both depend on the surface structure (roughness, physical and chemical properties) and on the properties of the particle under consideration. For precise predictions of the dynamic dispersion of aerosols it is necessary to parameterize the adsorption and resuspension processes with suitable variables, which have to be determined experimentally.

Immission and dispersion modelling

By means of flow simulations based on the physical effects described above and on parameters which have to be determined experimentally in advance, it is possible to analyse and predict the dynamic distribution of aerosols in the exhaust plumes of livestock houses. Dispersion simulations are often based on statistical plume models, the main advantages of which are short computing times and low computing performance requirements. Moreover, such models produce reliable predictions for areas further away from livestock houses, provided that the ground is level and that the meteorological conditions are stable. Statistical models have clear drawbacks, however, if the focus is on an area within only a few kilometres from the emission source. For example, turbulences caused by the animal houses themselves, by neighbouring buildings or by natural obstacles (trees, hedgerows, etc.) cannot, or can only insufficiently, be integrated in statistical models. This is partly due to the inertia of dust particles, which makes itself felt especially in turbulent airflows. Lagrange models seem to be more suitable for aerosol dispersion simulations. They use a stationary flow field on which the trajectories of the articles are calculated; averaged turbulences can be used as parameters in the calculation. For determining the travel distance of bioaerosols and the influence of neighbouring facilities it is important to look at the immediate vicinity of the source buildings and any turbulences that might occur there. Experimental findings by the State Environmental Agency of North Rhine-Westphalia have shown that the travel distance of aerosols depends strongly on the design and the resulting flow conditions of buildings on the immission side (Heller D. 2004). In order to be able to predict the dispersal of aerosols within a few kilometres while taking the buildings in that area into account, a numerical dispersion simulation for near-surface aerosols was developed at the Institute for Agricultural Engineering in co-operation with the Physics Institute of Bonn University (Wallenfang W. et al. 2002).

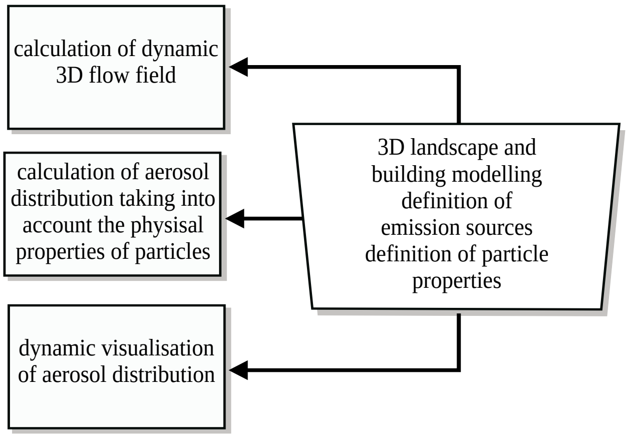

Figure 4:

Functional blocks of the NAAS 3D numerical dispersion simulation program

In a research project funded by the German Research Foundation (DFG – Deutsche Forschungsgemeinschaft) the three-dimensional aerosol dispersion simulation program (NAAS 3D – Numerische Aerosol Ausbreitungssimulation in drei Dimensionen) is being developed further. In contrast to statistical models, in NAAS 3D the trajectories of individual aerosol particles are calculated on the basis of a dynamic flow simulation. The simulation process can be divided into three functional blocks (fig. 4). In the first step, a dynamic flow vector field is created on the basis of three-dimensional information regarding buildings, the terrain and meteorological data. The relevant airflow calculations can be carried out with any meteorological or flow-dynamical simulation program with an ASCII Tecplot interface. The dispersion behaviour of aerosols in the vicinity of buildings and natural obstacles is influenced strongly by turbulences. Therefore, a program called NaSt3DGB, which was developed by the Institute for Numerical Simulation of Bonn University, is used in the simulation; it offers a numerical solution for incompressible Navier-Stokes equations (Griebel et al. 1995). In the next step, the trajectories of the aerosol particles are calculated on the basis of the dynamic vector field. This step is based on the physical parameters of the individual particles. Here the great advantage of the numerical calculation of the particle trajectories becomes evident; for instance, the agglomeration behaviour of the particles can be modelled with a high degree of precision. Moreover, the characteristic shape of each particle and the interaction between particles and surfaces are taken into account by using the aerodynamic diameter and experimentally determined variables, respectively. In the third and last functional block of the dispersion simulation the particle trajectories are visualised and the immission data are represented graphically. The representation of the aerosol distribution is generated by the computer in real time. This means that the computer continuously computes every individual image from the available geometrical data and from the behaviour and movement of the 'observer' (fig. 5). Thus, the user is provided with a three-dimensional insight into the spatial distribution of an aerosol from one or more sources in the vicinity of a building.

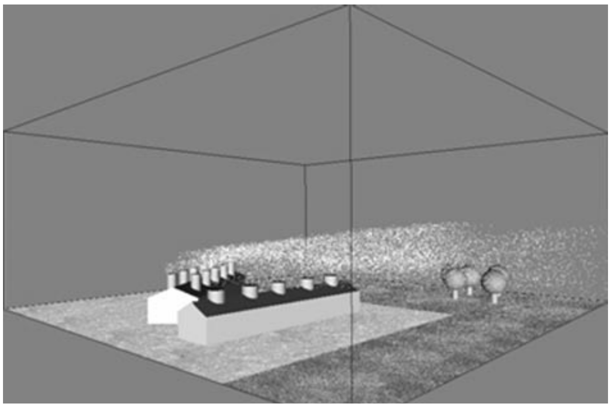

Figure 5:
Visual representation of a time step in a NAAS 3D numerical dispersion simulation

The three model variants presented in this paper can be classified as follows:

- Statistical programs
- Lagrange model
- Dynamic dispersion models

Statistical programs show their advantages in the prediction of odours if the immission point is a few kilometres removed from the emission source in less structured terrain. The Lagrange model strikes a compromise between the required calculation time and the precision of the prediction. It is only of limited use in the closer vicinity of emission sources. If the focus is on the dispersal of aerosols in complex terrain a few hundred metres around the source, then numerical calculation methods based on dynamic flow fields are the best choice.

Suitable tracer systems for the validation of aerosol dispersal simulations are currently being researched at the Institute for Agricultural Engineering. Tracer gases, such as SF6 which is used to validate odour dispersal models, are unsuitable because they do not replicate the particle-specific properties of aerosols. The difficulty in developing a suitable aerosol tracer system lies in linking measured dusts to particular emission sources. The two approaches taken to the problem of identifying dusts can be divided into online and offline methods.

The use of modified two-stage optical particle counter suggests itself fort he online approach. In the first stage, the size of a particle is measured by means of scattered light. On the basis of additional information on the number of particles it is possible to calculate the development of the concentrations of different particle size class. In the second stage, the particle counter checks if the particle can be attributed to the tracer source.

In the second approach, offline evaluation, particle samplers are used to collect the dust load together with the tracer dust at different times and at a specified distance from the source. In a laboratory the particles are examined with a light microscope in order to determine their size and distribution. One suitable kind of tracer dust can be pollen from plants which do not occur in the natural surroundings of the area under scrutiny at the time of the measurements. Fluorescent particles, which are easy to identify under the microscope in suitable light conditions, are another option, and they are also suitable for use in online methods.

Yet another option is the detection of released radioactive nuclide (Müller H.-J. 2001). Being much more sensitive than methods based on tracer particles, this method requires only small amounts of radioactive material to be released. Suitable radionuclides are pure gamma emitters with short half-life periods in the range of a few hours. Due to its environmental impact, however, this method is suitable only for sporadic research and validation measurements and not for use on a routine basis.

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