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Tracer particles for the validation of aerosol immission predictions

In approval procedures the prediction of the expected additional load of aerosols in the vicinity of livestock facilities gets more and more important. Dispersion models used for this purpose and the underlying algorithms reproduce insufficiently the natural conditions. A dynamic dispersion model based on the solution of the Navier-Stokes-equation was developed and successfully evaluated in a field survey. The course of the dispersion modelling and the results of the field survey are presented.

Keywords
Dispersion modelling, validation, aerosol, transmission, immission

Abstract
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Existing dispersion models often reach the limits of their capabilities when applied in structured agriculturally-associated areas. To take account of even small air eddies during throughflow of buildings and landscape elements dynamic dispersion models such as the STAR3D are increasingly applied. This model was developed within the Institute for Physics, University of Bonn in the Energy and Environmental Physics Working Group in cooperation with the Institute for Agricultural Engineering. Too test the forecasts made by STAR3D, validation measurements had to be conducted. The difficulty hereby: the normal procedure up until now, based on tracer gases, could not be applied for the dispersion simulation of dusts. This was because the particularly aerosol-specific physical characteristics with this procedure could not be verified. For this reason a new procedure was developed based on the application of a tracer aerosol.

Dispersion model

The developed STAR3D (Simulated Transmission of Aerosols in 3 Dimensions) dispersion model is characterised by the separation of dispersal procedure simulation into two steps. In the first step the fluid field is calculated with NaSt3D; this is responsible for the transport of the aerosol particles. Based on this, the flight paths of the aerosol particles are calculated as a second step. Here, sedimentation, adsorption and resuspension are taken into account. This separation has the advantage that both calculation steps are independent of one another and that the parameters of the particle trajectory calculation can be varied at any time without having to repeat the time-consuming calculation of the wind field.

Navier-Stokes in 3-Dimensions (NaSt3D)

The NaSt3D program was developed at the Institute for Applied Mathematics at the University of Bonn. It forms the basis of the dispersion model and has so far been applied in simulating dispersion of gaseous substances [1]. This program permits a time-dependant resolving of the Navier-Stokes equation on right-angled grids. It is possible to model the flow conditions in the simulation area as well as obstacles in the area (buildings, etc). The necessary stability of the calculation method compared with high Reynolds numbers has been realised through an adjusted discretization technique. The VONOS (Variable order non-oscillatory) scheme has enabled the carrying out of flow calculations with air as medium and a mesh width of one meter and inflow speeds of a number of meters per second without turbulence. The NaSt3D model has already been successfully applied [2] as odour dispersion model.

Simulated transmission of aerosols in 3-D

Following the wind field calculation comes the simulation of aerosol dispersion through calculation of the particle trajectories. Applied in this calculation is the Langevin equation that describes movement of particles under a partly stochastic force (in this case Brownian motion) (**equation 1**) [3].

$$m_p \dot{\vec{v}} = -f(\vec{v} - \vec{w}) + \sum \vec{F}_{ext} + \sum \vec{F}_{i,j} + \vec{F}_B \qquad \text{[Eq. 1]}$$

Hereby m_p stands for the mass of the particles, $\vec{v}$ die momentane Geschwindigkeit des Partikels, f the friction of the particle, $\vec{w}$ the wind speed at the particle location, $\vec{F}_{ext}$ the exterior forces acting on the particle, $\vec{F}_{i,j}$ the interparticle forces, $\vec{F}_B$ the stochastic force acting on the particle released by the particle's Brownian motion. Considered as exterior force in this case is gravity as well as the Saffman Lift force of the particle. When necessary, Coulomb forces can be integrated with the interparticle forces [4].

During the movement of the particle within the simulation volume there is a control after every time step to find if particles have escaped into a "forbidden" area: a building, tree or similar. If this turns out to be the case the particle is reinstated on the surface through which it had penetrated and marked as inherent. In the subsequent time step the particle is then released for possible resuspension according to the determined parameters.

Modelling the dispersion process breaks down as follows: In the first step the simulation volumes are defined. For this the mass of the simulation area and the size of the mesh are determined, on which the NaSt3D later calculates the wind field. In the next move buildings are included with any existing emission sources such as air emission chimneys. The positions of any trees in the area are also marked. Also given are characteristics of the aerosols (density, form) and those of the surfaces of objects in the simulation area. The wind field flow conditions and the source strength of the air emission chimney are then defined. Also determined are the total time to be simulated and the size of the time steps Δt.

In the next step the wind field is then calculated with NaSt3D. This part-step takes up most time and can last between a few hours and a few weeks, depending on the time span and complexity of the procedure that is to be modelled. When this is concluded the trajectories of the aerosol particles set free from the emission sources are then calculated. Taken into account hereby are the earlier-defined physical characteristics. This part of the calculations is in most cases able to be concluded in a few hours with a PC.

In the last step the results can be evaluated. It is possible to represent wind field and aerosol particle distribution in diagrams for determining particle numbers deposited on the ground surface of the simulation area. This allows the compilation of time series for particle numbers found in partial volumes of the simulation volume, and to represent the movement of the aerosol particles in animation sequences. These functions enable comparison of the results forecast by the dispersion model with the results collected by open-air measurements.

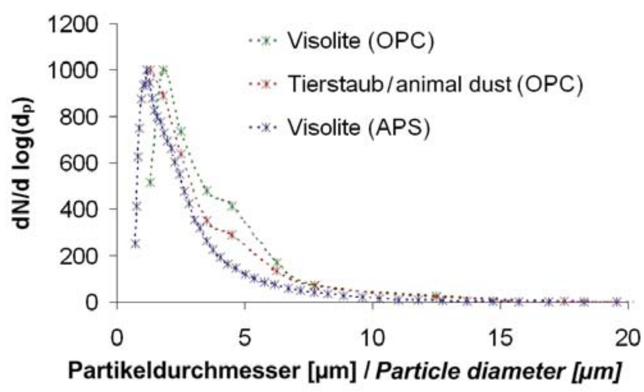
The validation process

In determining the dispersion of aerosols outdoors it is not possible to track the trajectory of individual particles nor to definitely attribute individual particles to a source. This means a validation of the dispersion models cannot be realised without further input. In order to validate the STAR3D dispersion model, a process has been developed based on a special aerosol tracer and an appropriate verification method.

Applied as tracer is BHA Visolite from General Electrics, a fluorescent powder based on calcium carbonate. Presented in **figure 1** is a comparison of particle characteristics of typical animal dust and that of Visolite. The characteristics are similar and this means Visolite can be applied for animal dust dispersion simulations. Fluorescence is activated through scanning with 390-400 nm wavelength light. The emission spectrum of the selected tracer has a wavelength of 590-650 nm.

The APMS (Aerosol Particle Measurement System) has been developed for verifying tracer particles. This comprises a measurement system for examination of particles adhering to surfaces with particular consideration of the fluorescent characteristics of the Visolite tracer. APMS is already described

Fig. 1



Comparison of tracer dust with dust from animal housings in detail in [5]. It is based on a lens that can be moved mechanically in three dimensions over any formed surface whereby particles adhering to the surface are depicted and measured in the measurement calculator. Following processing of the images the APMS delivers information leading to determination of number of particles as well as the size range of both total particles and tracer particles. In this way it is possible in field trails to compare the results of dispersal models with the APMS experimental data.

For verifying emitted tracer particles there have to be suitable measurement positions on the dispersion area. These comprise 1 m high stands each with attachments for two collection surfaces. Each stand is surrounded by a windbreak so that the deposited particles cannot be re-agitated by any wind. The collection surfaces comprise a Polysine® object support measuring 76 x 26 mm already coated so that particles can be affixed to the surface both electrostatically and chemically.

The validation measurement

The STAR3D validation procedure can be divided into 4 different sections:

- Dispersion of the Visolite tracer at the emission point
- Recording the meteorological conditions
- Deposition measurements at different positions on the dispersion area
- Evaluation of measurement results and their comparison with STAR3D simulation results

The validation measurements were carried out on the experimental fields of the Dikopshof estate, University of Bonn. There was a southeasterly wind on the recording day. The trial method was as depicted in **figure 2**. Three measurement beams were defined along which the deposition measurement points were positioned at a distance of 50 m in each case. Opening angle between the measurement beams was 11.3°. The air emission chimney described in [5] was used as emission source. Measurement time was 60 minutes.

Used for recording the weather data were two ultrasonic METEK USA-1 anemometers. These were sited in the positions shown in **figure 2** identified by the markings USA-1 and USA-2 and positioned on a stand at 3 m height. The first position was in the immediate vicinity of the emission air chimney. To avoid any influence of the chimney on the wind field recording, the second ultrasonic anemometer was placed out in the field. Through comparing measurements from both instruments possible influences from the chimney could be determined. The average wind speed on site as recorded by USA-1 (3.20 ± 0.74) m/s and at the SAT-2 location (3.18 ± 0.74) m/s agreed with each other within error limits. Airflow speed out of the chimney during recording was 5.97 m/s.

Within a period of one hour 14 mg/s tracer dust was continually emitted. Subsequently the collection surfaces from the deposition measurement locations were automatically evaluated in the laboratory with the assistance of the APMS. At the same time the measured wind speeds and emission data, recorded every second, the average emission air speed and the tracer particle characteristics as determined in the laboratory and the STAR3D simulated dispersal process were all taken account of. Established hereby was a 220 m broad, 220 m long and 40 m high simulation site. The mesh size was 1 m so that 1.94 million cells had to be calculated per time step. The simulation of the aerosol transmission required in this case a PC calculation time of 3 months.

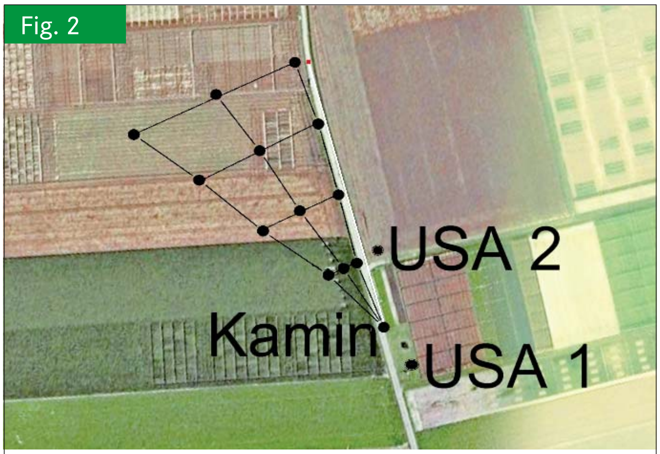
In conclusion there took place the comparison between the particle numbers on the 12 measurement points from the APMS measurements and the forecast from the dispersion model.

In **figure 3 a** can be seen the STAR3D-forecasted distribution of deposited particles. Inserted are the positions of the chimney and the 12 measurement points. The total number of deposited particles forecast by the dispersion model in the simulation area was 9.87 ± 0.01 bn tracer particles. This means: Around 2 % of particles from the emission particle flow were deposited within the simulation area.

Presented in **figure 3 b** is a comparison of particle numbers measured with APMS and forecast by the model. Also shown is the total number of particles deposited per square metre. On most measurement points there was a good agreement between measurement and model. Only the positions 1, 3 and 5 show deviations. On 1 the measured particle deposition is approx 1/3 higher than that forecast by the dispersion model. The situation was reversed at points 3 and 5 where the model forecast values were 2–3 times higher than those determined through APMS. A reason for the deviations at these measurement points has not been able to be found so far. Deviations between measurement and model on all measurement points were 27 %. Hereby it was possible to do without using a global scale factor as in [5].

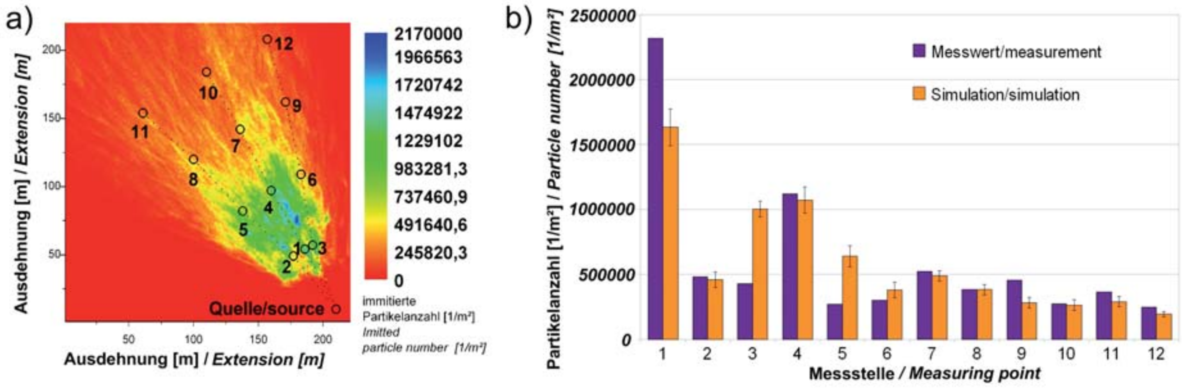
For comparison, simulation of the dispersal behaviour was additionally carried out with the AUSTAL2000 program. A comparison of the recorded deposited particle numbers can be seen in **figure 4**. The colour scale of both presentations was in each case standardised based on the maximum deposited particle amount.

Fig. 2



Positioning of the measurement equipment [6]

Fig. 3



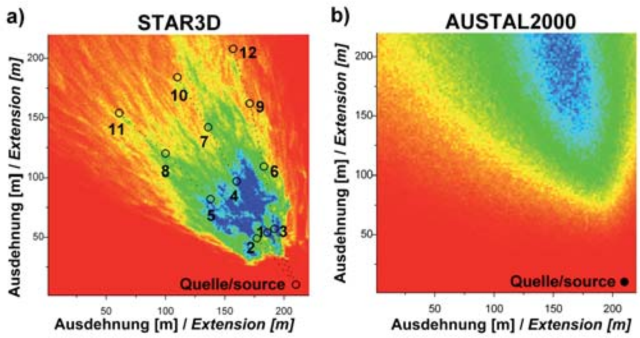
(a) Deposited particle number; (b) Comparison APMS-simulation

Conclusions

In a field trial it could be shown that the described procedure for validation of an aerosol dispersion model could be applied. The trial location was a level area and the emission source could be freely subjected to airflows. However, STAR3D was developed to simulate the dispersion of aerosols in complex, built-up areas. In this respect the field trial represented a very simple situation where similarly simple dispersion models delivered results with significantly reduced computer calculation time.

The results of the field trial could offer a contribution to solving the problem of (fine) dust and germ emissions. A limitation for such applications which, so far, has not been satisfactorily solved is the problem of computer costs and the associated calculation times. Assistance here could come from the use of mainframe computers.

Fig. 4



Comparison of the results achieved by STAR3D and AUSTAL2000 in arbitrary units

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