DYNAMIC DISPERSION MODELLING OF ODOURS AND AEROSOLS

Philipp Lodomez[1], Eberhard Rosenthal[1], J. Henseler[2], Wolfgang Buescher[2] and Bernd Diekmann[1]

[1]Institute of Physics, Bonn University, Nussallee 12, D-53115 Bonn, Germany
[2]Institute of Agricultural Engineering, Bonn University, Nussallee 5, D-53115 Bonn, Germany

Abstract: The transmission of dust particles is one of the interesting processes in the dispersion of aerosols. Due to the fact that it is impossible to follow the track of every single particle, a lot of effects and their parameters must be known to simulate the dispersion.
At the Harmo 7 conference a dynamic model to simulate the dispersion of odours was presented, before. This model is based on a numerical solution of the Navier-Strokes equation. Building upon this effort the dispersion model was enhanced, so that it is now possible to simulate the dispersion of aerosol particles. Extensive modifications were necessary to consider the aerodynamic and physical characteristics of polydisperse aerosols. Effects as sedimentation, deposition, resuspension and agglomeration of aerosols are or will be integrated into the simulation model.
In order to realize a validation of such a complex dispersion model, our research group is developing two independent aerosol tracer systems. Primary attention is paid to the environmental compatibility of the tracer dust. Both procedures are based on fluorescence marked particles, but they differ from each other with regard to their methods of detection. This enables us to practice both procedures at the same time. The dispersion model as well as the validation methods is objects of this paper.

***Key words**: dispersion modelling, aerosol tracer systems, Navier-Stokes-equation, aerosol transmission.*

1. 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 dissolved in air. The strength of the changes is related to the physical properties of the particles density, size and shape as well as external condition. The most important physical effects in this context are aerodynamics, sedimentation, agglomerationand furthermore adsorption and resuspension to surfaces.

To simulate the dispersion of odours or aerosols different models can be employed. One possibility is to use so-called Gaussian models (Zenger, A., 1998), another possibility is the use of statistical approaches, used in Austal2000 for example (Janicke Consulting, 2003). Our dispersion model is based on dynamic dispersion modelling, i.e. the form of the fluid field is calculated for every time step and is used subsequent to calculate the trajectories of the aerosol particles.

In the context of the research project "Dust emission from animal houses" funded by the DFG (Deutsche Forschungsgemeinschaft, German Research Foundation) the dispersion modelling of aerosol emissions from animal houses is studied. Therefore the dispersion model STAR3D is under development and should by evaluated by a field survey.

2. THE AEROSOL DISPERSION MODEL

The dispersion model STAR3D (abbreviation of **S**imulated **T**ransmission of **Ae**rosols, 3-dimensional) is a further development based of an odour dispersion model presented at a former conference (Boeker, P., Wallenfang, O. et. al., 2001). A characteristic is the dissociation of the calculation of particle trajectories from the calculation of the fluid field. To calculate the fluid field the software Nast3D is used, the obtained field is used afterwards to calculate the particle trajectories.

Nast3D
Nast3D (abbreviation of Navier-Stokes, 3-dimensional) is software for the numerical solution of the incompressible Navier-Stokes equations:

$$\frac{\partial \vec{u}}{\partial t} + (\vec{u} \cdot \nabla)\vec{u} + \nabla p = \frac{1}{\mathrm{Re}} \Delta \vec{u} + \frac{\vec{g}}{Fr} \qquad (1)$$
$$\nabla \vec{u} = 0$$

Here Re denotes the Reynolds-number and Fr the modified Froude-number $Fr = u^2/L$. Nast3D was developed by the Institute for Numerical Simulation at Bonn University (Griebel et. al., 1998). It is based on the technique of direct numeric simulation (DNS), so special assumptions on the sub-scale level as the k-ε model are avoided. Through the object-oriented program code it is feasible to use the software on parallel computer systems. Due to the time-resolved calculation of the fluid field the user can store the actual field in arbitrary time intervals.

STAR3D
After the calculation of the fluid field the dispersion of the aerosols is simulated. For this purpose the trajectories of the aerosol particles are calculated according to the following equation:

$$\frac{\partial \bar{x}}{\partial t} = \alpha_w \cdot \bar{u}(t) + \lambda \cdot \bar{e} + \bar{v}_s \qquad (2)$$

Here $\dot{x}(t)$ denotes the velocity of the particle at time the *t*, $\bar{u}(t)$ denotes the velocity of the fluid field at the position of the particle, α_w denotes the coupling between the particle and the fluid field due to the inertia of the particle. The second term considers the diffusion of the particle, λ is the diffusion length and $\bar{e}$ is a unit vector indicating the direction of diffusion. In this term not only the molecular diffusion is regarded but also the eddy diffusion, which is a few orders of magnitude larger, is considered. The last term considers the sedimentation of the particles due to gravitational force. If the time resolution t of the trajectory calculation is not too large, the position of the particle can be expressed as follows:

$$\bar{x} = \alpha_w \cdot \bar{u}(t) \cdot \Delta t + \lambda \cdot \bar{e} \cdot \Delta t + \bar{v}_s \cdot \Delta t \qquad (3)$$

The sedimentation velocities of different aerosols from agricultural emission sources were studied in detail at the institute of agriculture engineering, which is involved in project, too. These experimental results are used to calculate the particle trajectories, according to equitation 3 (Nannen, 2007).

Further effects, which will be prospective included into our dispersion model, are the deposition of aerosol particles on surfaces, the resuspension, i.e. the raise of deposited dust and the agglomeration of particles during the transmission time. Laboratory researches of the effects mentioned above are currently under way, the results will be available in summer 2009 at the end of the DFG-project.

The aim is to simulate the whole dispersion process from animal house. Therefore the following approach is applied:

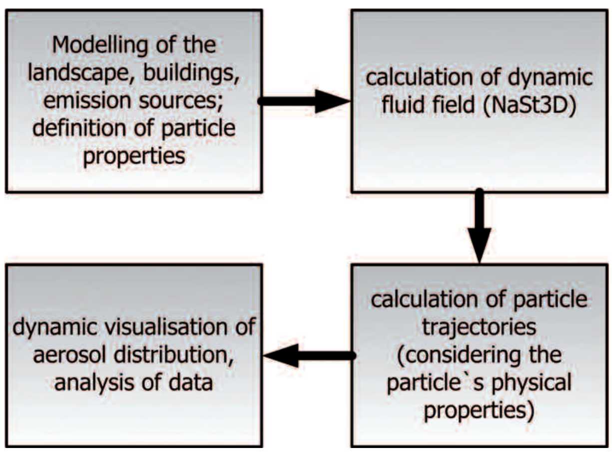

Figure 1. Flow chart of STAR3D

In Figure 1 a flow chart of the software STAR3D is shown. In the first step the modelling of the simulation terrain is done. Buildings, obstacles and emission sources can be added to the simulation scenario as well as the properties of the aerosol particles can be defined. Also the constraints for the fluid field like the direction and the velocity of the inflowing wind field can be set. In the next step the fluid field is calculated by Nast3D. This process can take a few days depending on the complexity of the created scenario. In the following step the dispersion of the aerosol particles is simulated referring to Equation 3. In this stage the physical properties of the particles as the sedimentation velocity are considered. Finally it is possible to visualise the results. On one hand it is possible to visualize the aerosol flow in a 3D scene rendered with OpenGL, and on the other diagrams can be created to show the distribution of the aerosols in every time step.

3. FIRST RESULTS OF THE DISPERSION MODEL

In this section the results of a first test done with our dispersion model are described. Doing first tests, a dispersion scenario of aerosols in a 100 x 100 x 25 metres large simulation volume is studied. A barn in the left lower corner with 5 chimneys having a height of 6m acts as emission source. A second building in the middle of the terrain is inserted as an obstacle. The amount of dust escaping from every chimney is chosen to be 10 μgm^{-3} (PM10) and the escape velocity of the exhaust air is 5 m/s corresponding to a typical scenario in agriculture. The wind inflows from the left lower corner, i.e. from the south-west direction, the actual direction is changing randomly in every time step of the simulation in an interval of 15° around the main wind direction. The wind velocity is set to 5 ms^{-1} varying in an interval of +- 1 ms^{-1} randomly for ever time step. The total simulated time period was 600s and from this short period the daily immission rate was extrapolated. In Figure 2 a snapshot of the dispersion modelling is shown. The aerosol cloud is clearly visible moving from the emission source in the north eastern direction. This result is also shown in Figure 3. Here the amount of immited particles is presented as a surface plot. One can see that most of the immission occurs in the direction of the wind. Furthermore a large amount of particles deposit on the building in the middle of the terrain (the obstacle).

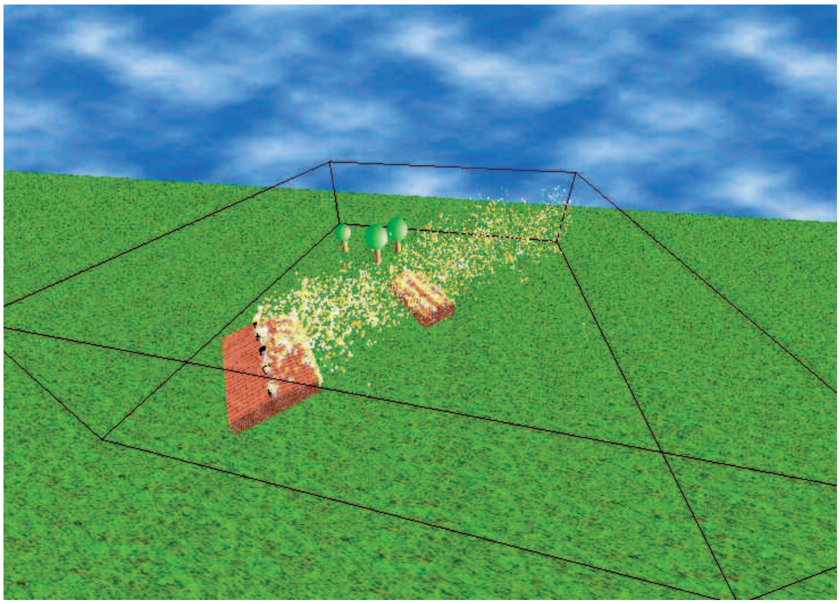

Figure 2. Visualisation of the particle distribution for an arbitrary time step.

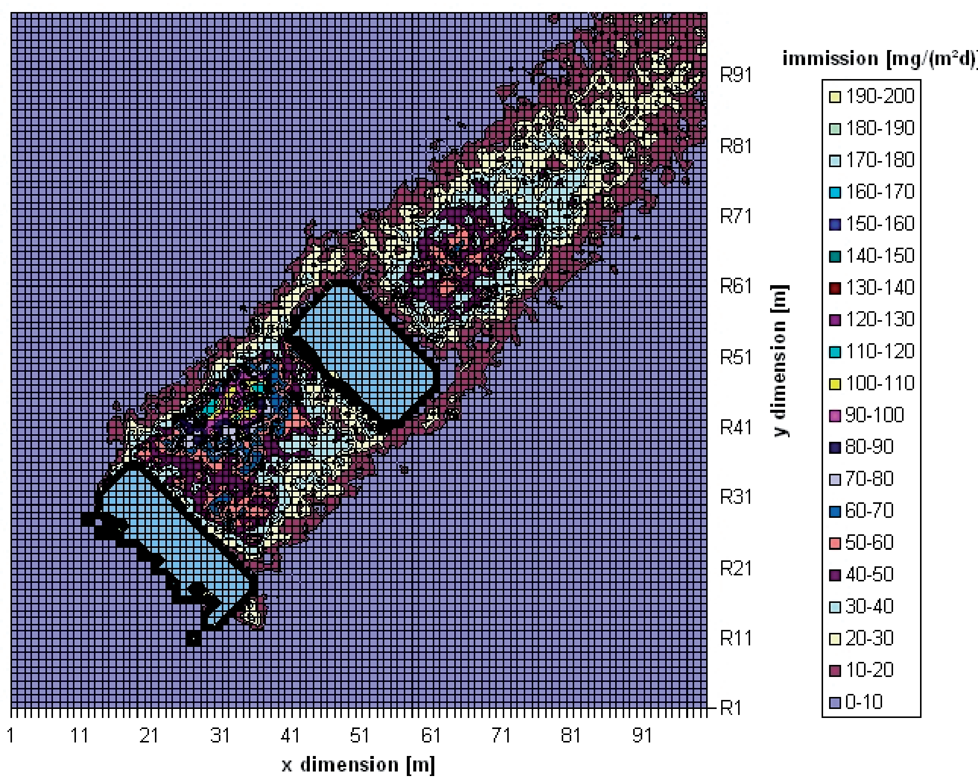

Figure 3. Immission of PM10 in simulation area.

4. VALIDATION

To be able to validate dispersion models and to estimate certain field parameters measurements are essential. In order to do these experiments a special aerosol, as well as an adequate detector system is needed. The time resolved measurement of the aerosol concentration is posing a further challenge.

To enable the comparison of STAR3D results with field measurements, the working group energy and environmental physic at the institute of physics, Bonn University, is developing two different detection systems. Both systems are based on a common fluorescent tracer aerosol. Releasing the tracer, it is possible to detect the aerosol tracer concentration and additionally the naturally existing aerosol concentration all over the spread out area. The systems can be split-up into two categories: Online- and Offline-System.

The Offline-System bases on the proven methods releasing, collecting and measuring. At the point of emission a tracer dust sample is dispersed by a common aerosol generator. Collecting the dust in the field, could be done time resolved or not. Measuring non time resolved means that you have to collect the dust particles over a defined time span. In this manner a medial aerosol concentration or a medial deposition rate can be estimated. Time resolved measurements stand for an additional complexity. Stirring the collector plate comparatively to the impaction point, it is possible to get information about the aerosol concentration or the deposition rate per time unit. Dynamic aerosol dispersion models, such as STAR3D, compute the aerosol concentration at each node per time unit. Accordingly especially time resolved measurements are suitable to validate this type of model.

The analysis of collected dust samples is the major disadvantage of existing methods. In order to enhance this method, an automatic analysing device was constructed.

A special optical device, mounted at a 3dimentional numerical control machine is used to scan the dust sample. So it is possible to analyse each collected particle. To separate the tracer particles from the common dust particles the dust sample is irradiated with a 375nm wavelengths light source. This brings clearly out the fluorescent tracer particle as shown in Figure 4.

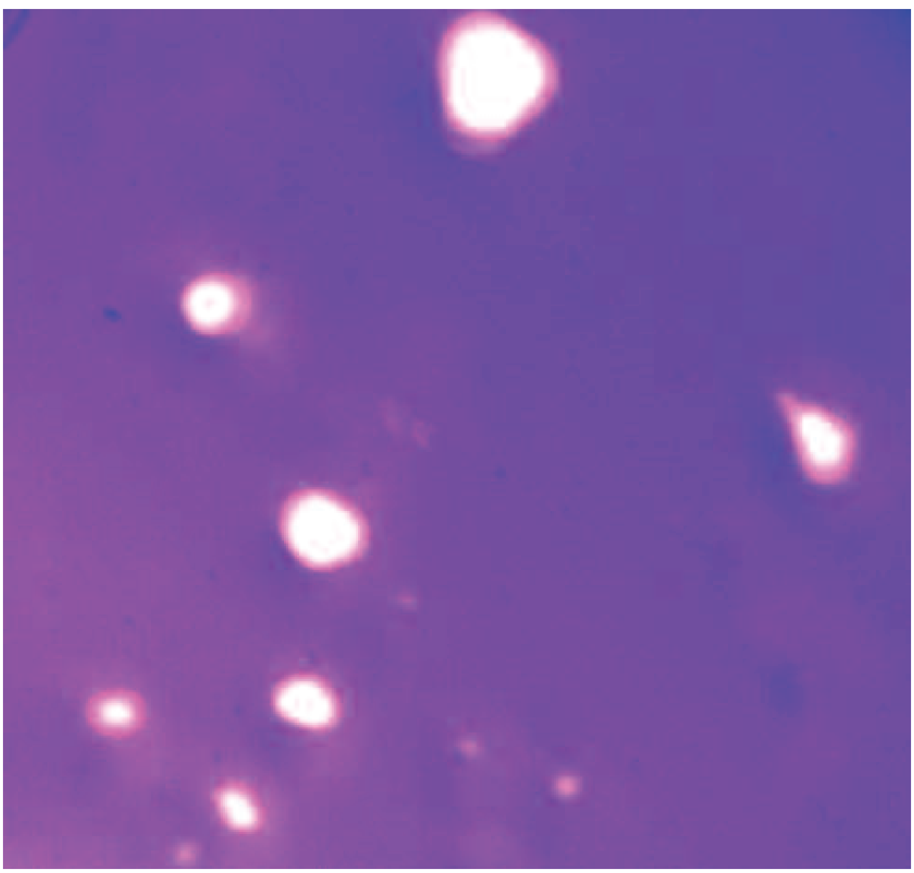

Figure 4. Collected aerosol tracer particles, illuminated with light of 375nm wavelength.

At each illumination wavelength an absolute gradient autofocus function (Groen, Young, Ligthart, 1984) is used to sharpen the pictures. Knowing the sampling time and the feed motion of the collector plate it is now possible to make a statement about the tracer particle concentration/deposition per time unit. These experimental values can be compared to the results of dynamic dispersion models.

In comparison with the Offline-System the Online-System is designed to deliver results right in the field. This system consists of an aerodynamic particle sizer (APS) in combination with a fluorescent light detector. The interaction of both methods allows a reliably detection of fluorescent tracer particle. The APS consists of two parallel laser beams. The accelerated aerosol particles cross the beams in an angle of 90 degrees. Detecting the scattered light, you will get two different pulses. The time difference between the two signals is a measure of the particle size. At the same time the particle will be illuminated with a UV light beam. A second detector measures the quantity and wavelength of possible fluorescent light. In this way the particle size distribution of all aerosol particles and the quantity of aerosol tracer particles can be estimated.

5. CONCLUSIONS

The first results of the dispersion simulation STAR3D, using the test scenario described above are promising. Varying the exhaust air velocity show the relevance of this parameter on the prognostic of immissions in the immediate vicinity of the emission sources. As expected, it is recognizable that with increasing exhaust air velocities a reduction of immissions nearby the emissions sources comes along. Doing field surveys these results should be proved.

At present the offline system is under test. First measurements show that it is possible to separate the aerosol tracer particles clearly from the background particles. Furthermore the automatic particle size recognition works satisfactorily. The online system is currently under development. In laboratory experiments first scattering pattern of the aerosol particles can be seen. The integration of the tracer particle recognition system is ongoing.

The experimental results for the parameters used by STAR3D will be available soon, so that the validation process of the software can be finalised in the near future.

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