The Modelling of Odour Dispersion with Time-Resolved Models

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In connection with the methods used so far, this contribution describes a new approach for the modelling of odour dispersion.
Using the aid of example cases, the methodology of odour prognosis with different approaches is explained, and their advantages and disadvantages as well as their limitations are discussed.
Particular attention is given to close-range dispersion from odour emission sources with low source heights and a complex fluidic environment. Typical examples of such cases are agricultural sources or biological processing plants (composting, sewage treatment plants).
The new dispersion model is a further development of the NaSt3D model with two variants of improved dispersion modelling, an advection-diffusion approach (Euler model) and a Lagrange-particle model. This model is able to conduct time-resolved calculations of flows and dispersion and hence allows the question of concentration fluctuation, which is important for odour phenomena, to be integrated into the model. The parallelizing of the computer code enables terrain- and source configurations which have been too complex thus far to be calculated in a fine division of the calculation grid. At present, computer clusters and high-performance computers can be used for this purpose in anticipation of the fast further development of efficient personal computers.
The consistently analytical approach avoids empirical model supplements with adaptation parameters, such as the otherwise necessary models of exceeding probability, and can thus be calibrated on a physical basis.

Keywords
Odour, diffusion model, lagrange partikel model

Introduction

Odour immission is a difficult area with high potential for disputes. This is caused by the character of the sensation which, as a physiological phenomenon, eludes purely technical consideration. In contrast to the other senses, i.e. hearing, seeing, and sense of touch, the sense of smell is a so-called chemical sense, as is the related sense of taste. A series of sensory and neurological processes leads to a strong subjective component in the development of the sensation: the individual odour thresholds, the classification of odours in a range from pleasant to repulsive, and the adaptation to continuous exposure to odour are examples of this subjectivity.

Nevertheless, an objective methodology of odour measurement and -prognosis is called for in approval questions. The methods with their advantages and disadvantages are roughly described below, followed by the new developments towards realistic, time-resolved modelling.

Odour Measurement

The human sense of smell is the reference for odour impressions. Since no technical odour measurement instruments have been available so far, odours are determined by panelists in the laboratory at the so-called olfactometer and in the open using the method of odour inspection.

The panelists are selected using the criterion of average olfactory capability. At the olfactometer, the odour samples are diluted systematically and the threshold of perceptibility is established. The odour concentration of the samples is calculated back from the dilution. The olfactometric method [1] also defines the unit of odour: the odour unit 1 OU. If 50% of the panelists just barely perceive the odour, the sample has the odour strength 1 OU/m^3. The character of the odour unit as a physiological quantity prohibits the application of categories of gas measurement technology to odour. Even if the unit OU/m^3 is used as a quasi-concentration, like a gas concentration, it is impossible, for example, to superpose the odour strength of several components with known odour strength in a multi-component mixture. The individual odour components can mutually reinforce, weaken, or mask each other.
During inspections, odour perceptions are registered at defined grid points in certain points in time and time intervals and converted for prognosis using different statistical methods [2]. Due to the high variability of the meteorological conditions, a very large number of samples must be taken to obtain reliable results.

Odour Dispersion Calculation and Annual Input Prognoses

Between the olfactometric measurement of an emission source strength and the immission rate determined through inspections, the process of transmission takes place. This term comprises the transport and the distribution of the emitted substance in the air flow. In addition to all the difficulties caused by the physiological-subjective character of the odour impression, the high variability of the natural wind currents and weather situations also exerts an influence.
It is the goal of dispersion calculations to provide the basis for annual statistics of the odour pollution to be expected in the environment of emission sources. These calculations are based on the analysis of

the individual meteorological situations and their specific dispersion behaviour. Usually, these situations are classified threefold: in individual wind directions and the corresponding wind speed- and dispersion classes. These data are available at the meteorological district offices or at local weather stations.

This triple data basis serves to calculate the dispersion of substances with the aid of dispersion models. The models differ with regard to their structure and their range of validity.

All models are based on the Navier-Stokes equations [3, 4]:

$$\frac{\partial}{\partial t^*}(\vec{u}^*) + (\vec{u}^* \cdot grad)(\vec{u}^*) + grad^* p^* = \frac{1}{\mathrm{Re}}\Delta^* \vec{u}^* + \vec{g}^* \quad (1)$$

where:

$\vec{u}^*$	wind speed field
p^*	pressure
$\vec{g}^*$	external forces
Re	Reynold´s number

The Navier-Stokes equations provide a generally valid description of the flow. A dispersion model which describes the actual distribution of substances in the wind field is connected with these equations in different ways. Since there is no closed analytical solution for this set of equations in natural wind currents, either a solution under radically simplified boundary conditions must be employed, or the solution must be established using numerical methods. The first case leads to the so-called Gauss model. In the second case, grid-based models are used which are divided into Euler models and Lagrange models.

The currently employed dispersion models furnish average values of the immission concentrations. Due to fluctuations around the mean value, however, odour events above the threshold occur in reality even if the average values are below the odour threshold of 1 OU. For the evaluation of annoyance, a period is rated polluted if the odour threshold is exceeded during 10% of the time. To draw the conclusion from the calculated mean values to the probability for exceeding, the so-called factor 10 model [5] is employed frequently. This model defines a period as odour-polluted if the mean odour value during this period is 0.1 OU. The factor 10 model is considered an (intentional) over-estimation in terms of a safety distance required by the approval regulations.

An alternative is the BAGEG model [6]. Instead of a rigid odour limit of 0.1 OU, a variable transition of the exceeding probability is assumed to occur in the BAGEG model in keeping with the mean calculated odour concentration. Average values below 0.1 OU have a small probability for exceeding, while the exceeding probability is high if the mean values are above this limit. The advantage of the BAGEG model is the possibility to calibrate the probability for exceeding using the individual case to be examined. During a plume inspection, a parameter of the curve of the probability for exceeding is established and used for the annual prognosis.

The different approaches of the two models are shown in **figure 1**.

Gauss Models

Gauss models use a closed solution of the advection-diffusion equation in a collinear wind field.

According to this approach, the dispersion is explained by two phenomena: pure transport in the wind field (advection) and distribution at right angles to the wind direction (diffusion). Here, diffusion is not understood as molecular diffusion, but as the distribution of substances caused by microturbulence, which is larger by dimensions.

$$\frac{\partial C}{\partial t} = \lambda \Delta C - \vec{u} \cdot gradC + Q \quad (2)$$

where:

C	concentration
λ	diffusion coefficient
$\vec{u}$	wind speed field
Q	source
$\lambda \Delta C$	(turbulent) diffusion
$\vec{u} \cdot gradC$	advection

The Gauss dispersion equation derived from this equation describes the average value of the concentration distribution under idealized conditions (no buildings, undisturbed dispersion) if the emission mass flow, the wind speed, and the dispersion class are given. The employed solution has the following structure:

$$C(x,y,z) = \frac{Q}{2\pi u_h \sigma_y \sigma_z} \cdot e^{-\frac{y^2}{2\sigma_y^2}} \cdot \left(e^{-\frac{(z-h)^2}{2\sigma_z^2}} + e^{-\frac{(z+h)^2}{2\sigma_z^2}} \right) \quad (3)$$

where:

$C(x,y,z)$	concentration at the location (x,y,z) in OU/m³
Q	source strength in kOU/h
u_h	wind speed in m/s in the direction of the x axis
σ_y, σ_z	horizontal, vertical dispersion parameters in m
h	effective source height in m

The formula describes the shape of a dispersion plume with double Gaussian concentration distribution. For the observation of mass conservation, a second term has been inserted into the equation which causes a reflection of the concentration distribution when below ground level.

The advantage of the Gauss model is its fast calculability within odour predictions. For every dispersion situation, the solution for the entire area is directly included analytically. For this reason, Gauss models were the only method of making immission prognoses before efficient computer systems became available.

The drawbacks lie in the simplifications which led to the development of the approach [7]. Generally, dispersion is not undisturbed. At best, this could be assumed by approximation for dispersion from high chimneys which were actually used to calibrate the Gauss model. In a more complex terrain, the flow- and dispersion conditions are entirely different, and effects such as turbulence and streaming around obstacles must be taken into

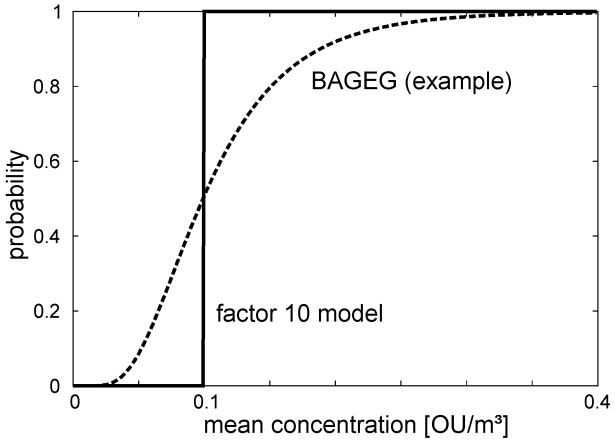

Figure 1: Probability of the odour threshold being exceeded by 10% according to the factor 10 model (leap at 0.1 OU) and the BAGEG model (functional connection)

account. The model cannot be employed properly, especially in close range and if source heights are low. The mathematical structure of the solution leads to a systematic under-estimation of the close-range concentrations because, from a mere geometric viewpoint, the dispersion plume reaches ground level only at a larger distance. Especially if air flows around a building, however, emissions are actually particularly high due to the „downwash“ effect [8], especially behind the source and close to it. Dispersion in each wind- and dispersion class is determined with a set of parameters which were obtained using high sources for calibration. In principle, their application to low, close-range sources is impossible. For this reason, varied sets of parameters have meanwhile been proposed [5].

A consideration of the dispersion calculation errors of the Gauss model with varying dispersion parameters shows that the proper range of validity first begins at a distance of approximately 100 m. **Figure 2** shows the relative error in the concentration distribution calculated with error propagation calculation using a dispersion class as an example. Given a 10% variation in the dispersion parameters, which approximately corresponds to the change from one class to the next, the relative error in the calculated concentration first falls below 50% at a distance of approximately 90 m.

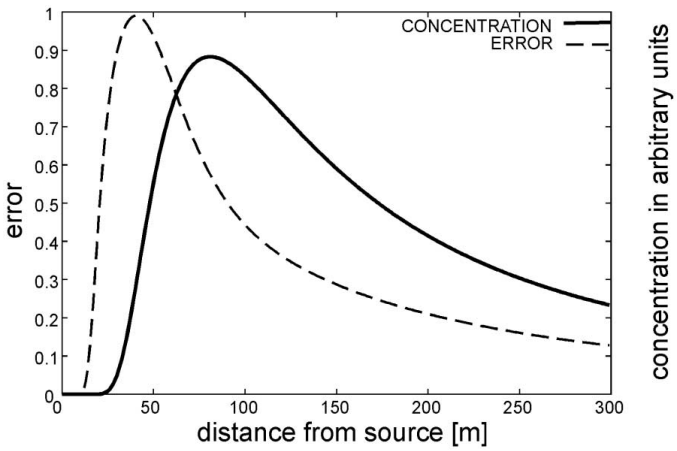

Figure 2: Development of the concentration with the relative error of the Gauss model, calculated using the dispersion class III/1 at a height of 2 m as an example

Numerical Models

The characteristic of numerical models is that the area to be examined is divided into individual cells. Instead of a closed solution, the model equations are solved for each cell and time interval. The refinement of the grid as well as intelligent approximations and equation resolvers allow very high calculation precision to be achieved. However, this requires the availability of high computer- and memory capacity. For this reason, the development of numerical models is linked to computer development.

With regard to the numerical models, a distinction is made between Euler models and Lagrange models [9]. The former calculate the dispersion in the flow field with the advection-diffusion approach (equation 2) using the grid. Lagrange models simulate the flow by calculating the trajectories of particles which are subject to the laws of point mechanics in the flow field. Lagrange models have some advantages over Euler models. The numerical treatment of the advection-diffusion approach leads to the effect of *numerical diffusion* [7] in Euler models. With the aid of Lagrange models, the behaviour of particles with a mass, as well as ongoing chemical processes, can be described well. However, they need very large computing and storage capacity [8].

Using two representatives of models as examples, the possibilities and limitations of such models at different levels of development are discussed.

MISKAM

The MISKAM model [10] is a flow- and dispersion model of the Euler type for urban climate calculation, especially for the prognosis of air pollution caused by traffic. MISKAM uses a rectangular, non-equidistant grid on which the flow field is calculated in the first step. For reasons of computing economy, the emission conditions are set invariably. This and the limited possible number of grid points lead to the suppression of whirls, turbulence, and unsteadiness. Therefore, the calculated wind field is always stationary. Of course, this „pseudo-laminarity“ is not realistic. The dispersion calculation of MISKAM employs the advection-diffusion approach on the wind field calculated before. Not only is the flow calculation unrealistic, but an additional difficulty ensues with the advection-diffusion approach on a rectangular grid, namely numerical diffusion. This effect is particularly obvious when calculating the dispersion from a point source in an undisturbed area. If the flow is chosen at right angles or at an angle to the grid, the shape of the dispersion plume should not change. Due to the effect of numerical diffusion, however, very strong widening of the plume is observed if the grid is askew (**figure 3**). The explanation for this effect lies in the number of neighbouring cells into which substances are transported by the advection component if the flow is askew. If the flow is straight, only the weaker diffusion causes substances to stream into cells lateral to the main direction. Compensating approaches use a back-transporting step such as Smolarkievicz advection. When calculating annual prognoses, the effect of numerical diffusion leads to an asymmetry of the immission prognoses. **Figure 4** shows an annual prediction using a symmetric compass rose and a central point source as an example. The result is a pronounced cross form with higher values in the axial direction. Therefore, the input rate depends on the direction of the axes in the area to be examined, which in principle is arbitrary. This, however, is incompatible with the required objectivity of the prognoses.

NaSt3D

The flow- and dispersion model NaSt3D [11] (abbreviation of Navier-Stokes, 3-dimensional) is a further developed model, whose outstanding characteristic is its ability to be used on parallel computer systems. For this purpose, the program code is consistently object-oriented, which allows decisive modifications and program

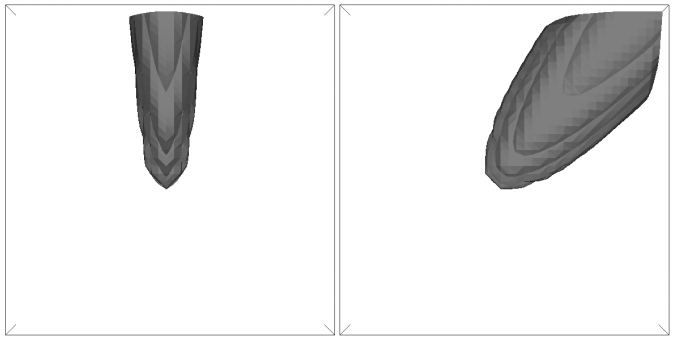

Figure 3: Numerical diffusion caused by a flow at 45° to the grid direction, as compared with a flow parallel to the axis, calculated with MISKAM (iso-area for concentration 1 OU/m^3; odour source: central area source 11 MOU/h at a height of 8 m; wind speed 1 m/s)

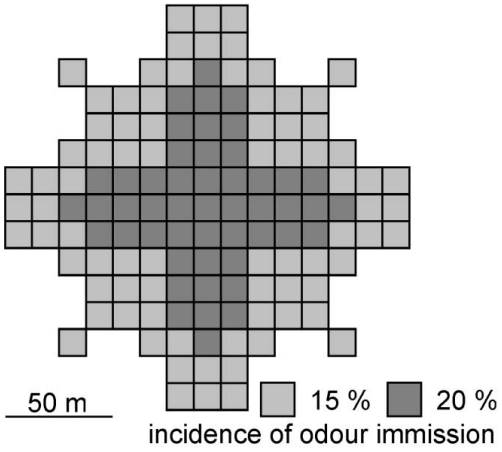

Figure 4: Influence of numerical diffusion on the annual prediction of the odour input of a central point source if wind statistics are symmetrical, calculated with MISKAM and the factor 10 model (wind speed 1 m/s in 36 directions; source see above)

extensions with regard to the problem of odour dispersion. Through dynamic memory allocation, NaSt3D makes the calculation of significantly larger grids possible.
In NaSt3D, the calculation of the flow and the dispersion is not carried out in two separate steps, but simultaneously at every point in time during the simulation. This also opens up the possibility of simulating the fluctuation of concentration, which is important for the problem of odour prognosis. Therefore, the conclusion from the mean concentration to the exceeding frequency (factor 10 model or BAGEG), which leads to disputes, can be avoided.

Modifications and New Developments regarding NaSt3D

In principle, the dispersion of gases and odorants in the NaSt3D model can be calculated using two different approaches. The built-in Euler approach uses an improved advection-diffusion model, and the alternative, additionally implemented Lagrange approach calculates the dispersion by following particle trajectories.

The Advection-Diffusion Approach

Through an approximation of a higher order, the VONOS method (Variable-Order Non-Oscillatory Scheme), the effect of numerical diffusion in NaSt3D has been reduced. **Figure 5** shows three dispersion plumes calculated with NaSt3D. The left figure shows the dispersion plume in the main grid direction and the middle figure the dispersion diagonal to the grid. The widening effect of numerical diffusion is clearly visible. The right figure shows the calculation with the VONOS method. The dispersion plume now corresponds to the shape in the left figure.

The Lagrange Approach

The Lagrange approach for the modelling of dispersion is based on the calculation of the spatial trajectories of virtual particles which are moved along in the flow field. In principle, the Lagrange approach avoids the problems of numerical diffusion. On the other hand, however, the calculation of the particle trajectories requires additional memory, especially if the particle densities are assumed to be sufficiently high. In order to be able to calculate statistically reliable concentrations using particle density at a larger distance from an emission source, a number in the order of several 100,000 particles must continuously be included in the calculations.
The decisive advantage of the Lagrange approach lies in the possibility to attribute a mass to the calculated particles and hence to describe the specific behaviour of such particles realistically. Especially in the case of odour emissions, it is assumed that a considerable portion of the odorants is transported by dust- or aerosol particles. Their behaviour cannot be described adequately with the aid of the classic gas dispersion calculation.
Figure 6 shows the calculation of the dispersion behind a low, wide source and a high source (chimney). The realistic representation of the „downwash“ effect and the whirl behind the low source can be seen in the diagram. Due to the back-flow, emitted substances accumulate in the back-flow area behind the obstacle.
The simultaneous calculation of the flow and the dispersion allows variable input wind directions and -forces to be taken into account in the calculations. This also enables meandering dispersion plumes to be simulated, which in reality result in heavily fluctuating odour impressions. **Figure 7** shows the calculation of the dispersion plume based on data measured during a tracer experiment. SF_6 was released as a tracer and measured in the environment using a mobile measuring equipment. The input wind data were measured at the source and employed in the model as a representative flow into the calculation area. In **figure 8**, the comparison between the calculated and the measured data for an input location at a distance of approximately 100 m shows a high degree of consistency between the measured heavy concentration fluctuations and the calculated passing of the meandering tracer plume over the input location. Further tracer measurements are being conducted for the parameterization [12] of the turbulent diffusion.

Summary and Future Prospects

The odour dispersion program NaSt3D allows time-resolved simulations of odorant dispersion to be carried out. The Lagrange particle modelling of the dispersion enables the specific behaviour of odorants with a mass to be described. The question of odour impressions above the threshold, which is important for the evaluation of annoyance caused by odour, can be addressed directly using the time-resolved calculation of the input concentrations without further auxiliary assumptions.

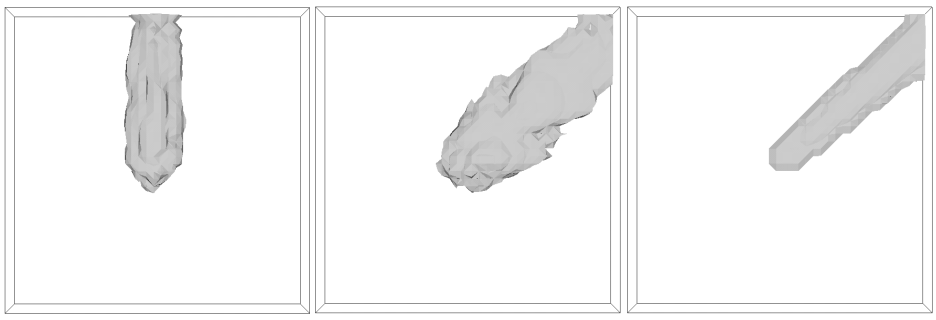

Figure 5: Comparison of the dispersion in different directions and with the improved approximation (iso-area for concentration 1 OU/m^3; central point source 5 MOU/h at a height of 8 m; wind speed 2 m/s)

For a comparison of the models, **table 1** lists the calculation time for one wind direction. In contrast to the Gauss model, the calculation time required by the numerical models seems very long. Therefore, the multi-processor compatibility of NaSt3D is a prerequisite for an acceptable total simulation time (given a certain wind distribution, different wind speed- and dispersion classes). The last line shows the performance of the current computer cluster in Bonn with 128 single processors (Pentium II 400 Mhz) as an example.
At present, tracer trials are being carried out for the calibration of turbulent diffusion and the subsequent validation [13] of the model in different dispersion situations.

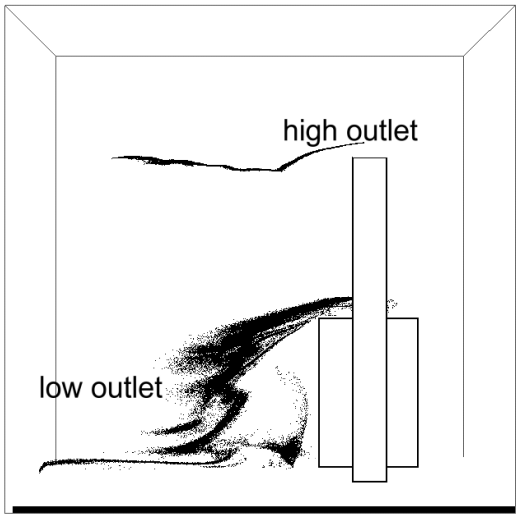

Figure 6: Comparison of the dispersion of substances behind a low and a high emission source, calculated with NaSt3D and the Lagrange particle model

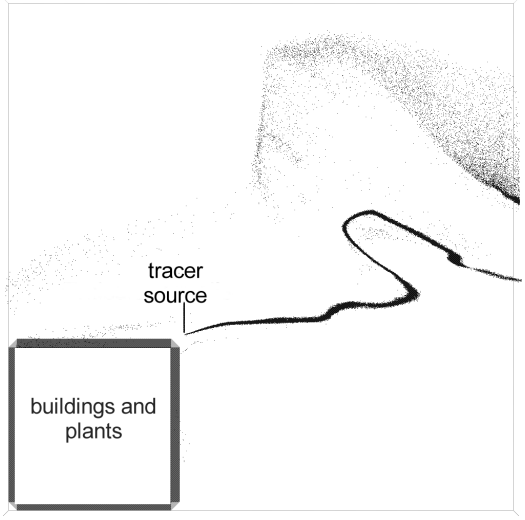

Figure 7: Meandering dispersion plume of a point source, calculated with the NaSt3D model and the Lagrange dispersion approach

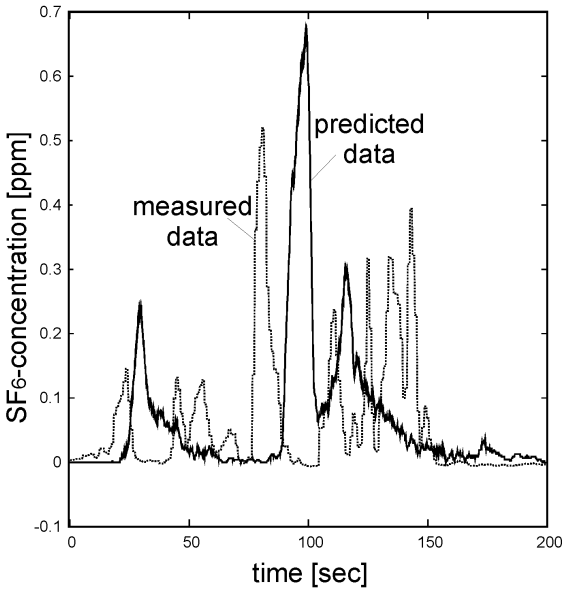

Figure 8: Comparison of measured and predicted immission concentrations

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Table 1: Simulation time with different models

Model	Number of cells	Simulation time – one wind direction
Gauß	40 x 40	~ 1 second
MISKAM	40 x 40 x 20	~ 1 hour
NaSt3D	40 x 40 x 20	~ 45 minutes (1 Processor)
NaSt3D	40 x 40 x 20	~ 2 minutes (128 Processors)

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