MISKAM

Manual for Version 6

On behalf of



environmental meteorological software

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Preface

During the last couple of years the flow and dispersion model MISKAM has become a highly respected expert tool for evaluations in sectors as e.g. road planning, environmental impact studies, and air hygiene.

This manual describes the MISKAM model version 6 (latest published version 6.3), which was improved and extended in comparison to the previous releases 3.x, 4.x and 5.x.

- Modified stationarity criteria for flow and dispersion calculations, resulting in a more consistent convergence.
- Time-step-splitting for calculating turbulence variables. All known problems with respect to convergence in complex obstacle configurations could be eliminated by processing each time-step in two halves. Optionally, the time-step for the turbulence model may even be sub-divided into four steps. Thus, instabilities which rarely occured connected to very high grid resolutions could be eliminated.
- Two-dimensional calculations with only one grid cell set in the *y*-direction, resulting in an greatly reduced calculation time, for instance for street canyons.
- Change to programming without fixed array sizes in all program sections. This eliminates the necessity to distribute different program versions depending on RAM availability.
- More consistent one-dimensional initialization, with more realistic z_0 -dependencies of the wind and turbulence profiles.
- Automatic internal generation of lateral up- and downstream flow zones. An equidistant
 or a spread grid can be used. Further, it can be distinguished between boundary zones
 without obstacles or a conversion to the boundaries of the last obstacle belonging to the
 inner model area.
- Optional setting of a vertical flow velocity for point sources. Stack emissions can thus be very realistically simulated.
- The influences of vegetation (flow deceleration and additional turbulence production) can optionally be considered.
- Controlled abortion of the simulation with a dump of partial results.

- Various possibilities of additional control dumps.
- Increased maximum number of grid points for vertical direction.
- Improved adcetion calculation by optional use of McCormack scheme for velocity components and MPDATA algorithm for all scalar quantities.

The model was vastly verified and validated while revising the code. The test calculations mainly oriented at the guidelines of the VDI-Code 3783/9 "Environmental meteorology - Prognostic microscale wind field models - Evaluation for flow around buildings and obstacles." More tests were run recalculating previous research by other authors, for instance within the PEF-projects.

MISKAM was mainly programmed in Fortran90. The compiler *Absoft Pro Fortran, Version 14* was used to generate the executables. A 32Bit-operating system is compulsory, we recommend using Windows 7 or newer. A usage under Linux or various Unix-systems is possible, some adjustments in the source code are needed, however. A model version for 64Bit Windows systems is currently in preparation.

This MISKAM-manual is structured as follows:

- In the first part, short information is given with respect to the MISKAM model, according to the requirements of the VDI-Code 3783/9.
- The ensuing chapter describes model concepts and usage limitations.
- The theory, upon which the model is based, as well as the numeric transformation are subject of chapters 3 and 4.
- Chapter 5 describes the installation as well as the usage of the model and of the help programs.
- Chapter 6 summarizes the validations of MISKAM's flow model according to VDI guideline 3783/9.

Calculations of verifications and validations are documented in scientific publications and results are openly published on the homepage of Lohmeyer GmbH & Co KG.

The data and results of all examples given in the manual are supplied with the MISKAM-CD.

Wackernheim, March 2014 Dr. Joachim Eichhorn

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1 Short information

Model name

MISKAM

Version

6.3 (as of November 2013)

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Model type

Non-hydrostatic, three-dimensional, obstacle-dissolving flow model; three-dimensional Eulerian dispersion model.

Scope of application, size of areas and resolution

Flow and dispersion calculations in build-up areas, area sizes up to about $1000 \times 1000 \times 300$ m, grid resolution of approximately 1 to 10 m.

Limitations of application

Not usable for steep topography, unstable thermal stratification and oversaturation (condensation).

Solution algorithms

Model equations:

- Three-dimensional momentum equations, non-elastic boussinesq-approximated
- E- ε -turbulence model
- Patrinos-splitting
- Advection equation of diffusion for mass concentrations

Numeric solutions using the following schemes:

- Forward differences in time
- Upstream-advection optional McCormack scheme (momentum) and Smolarkiewicz scheme (scalars) (mass transport)
- ADI-process for diffusion equations
- SOR-process for Poisson-equation

Input sizes

Model geometry: Cartesian coordinates, orientation of the model areas, position and height of buildings, roughness length of the terrain (or: type of surface per grid) and of building areas, optional flow-through building areas (e.g. passageways or arcades) Meteorology: wind speed, wind direction, stratification

Control parameter to run the program: number of time-steps to be calculated, abortion criteria, control of the advection calculation

Output sizes

Flow model: Three-dimensional arrays of the Cartesian wind components, of the dynamic pressure disturbance, of the turbulent kinetic energy, of the energy dissipation and of the diffusion coefficients

Dispersion model: mass concentrations, if needed the dry deposition rate

Previous Evaluations

The following verifications of the model were performed:

- Evaluation of the flow model according to the draft of the VDI-guideline 3783 sheet 9 (prognostic microscale wind field model), internal verification of consistency as well as comparison with wind tunnel data.
- Verification the dispersion model with wind tunnel data and natural data (Göttinger Straße, Hannover).
- Evaluation of the flow and dispersal model by comparison to wind tunnel data of the Mock Urban Setting Test (Yea and Biltoft, 2004).

Hard- and Software requirements

Standard PC

approx. 10 MB hard disk space for the standard installation, some hundred MB's for model results,

32 Bit-operating system (Windows 7 or newer, 64 Bit version upon request, Linux versions upon request)

Availability

The following versions can be obtained:

- Standard version (executable, manual, help programs), operating under WindowsXP or later. Obtainable through **giese-eichhorn, Wackernheim**.
- WinMISKAM (Standard version + Windows-surface), obtainable through Lohmeyer GmbH & Co. KG, Karlsruhe.
- Soundplan-Modul, obtainable through Braunstein + Berndt, GmbH, Backnang.

Literature

see Chapter 7.

2 Introduction

2.1 About MISKAM

The prediction of expected, traffic-related immissions will gain greater importance in the context of current discussions regarding new legal guidelines (for instance "Bundes-Immissionsschutzverordnung", VDI-guidelines).

No planning tasks, be it in the urban sector or in road design, are practically imaginable without considering the immission load. Measuring the most important air contaminants is very important to evaluate the existing pollution. However, measurements, due to their relatively high costs, cover only a small area, and, in addition, can only be performed during a short time-span.

Since several years, numeric methods have been developed as a supplement and an upgrade to the existing measurements. The fast technical development of the hardware sector allows us to run elaborate numeric models on a standard PC nowadays. High-end computers were required for these jobs until recently. It is even more surprising that current guidelines, as the TA-Air, only demand Gaussian models even though their weaknesses and limitations are well known. Just lately, the official interest has shifted to more complex models, which mainly consider the dispersion conditions of developed terrain.

The MISKAM model (microscale climatic and dispersion model) is one of the more sophisticated models with respect to its physical content within a wide range of available models in the meanwhile. It has been developed at the Institute for Atmospheric Physics at the University of Mainz. This institute had been working on the development of regional and local climate and dispersion models since several years.

MISKAM is suited for dealing with small-scale dispersion processes (typical model dimensions of several 100 m). Therefore, MISKAM is especially useful for tasks previously mentioned (road and urban planning), because it considers mainly the physical processes influencing the transport of pollutants within the direct environment of buildings.

MISKAM is a three-dimensional non-hydrostatc numeric flow and dispersion model for smallestscale forecasts of wind behavior and immission concentrations, e.g. in roads, as well as up to urban quarters. It was originally planned to treat microclimatic problems (Eichhorn, 1989). It was only after users expressed the desire for a PC solution to predict the immission in roads, that the current model version was further developed. MISKAM allows for the explicit treatment of buildings in the form of rectangular form structures, so that the particular flow around buildings can be realistically modeled. It was further desired to develop a model of a high physical standard avoiding as much as possible the usage of empiric-diagnostic relationships.

The physical basis of MISKAM are the three-dimensional equations of momentum (so-called primitive equations) to simulate the flow conditions as well as the advection-diffusion-equation based on the dispersion calculation of density-neutral substances.

2.2 Why prognostic modeling?

Even when using the most modern hardware resources, the use of prognostic flow and dispersion models is still combined with considerable computer time in comparison to the diagnostic models. Diagnostic flow models first estimate the wind field considering empirical assumptions regarding the flow pattern (Lee-circulations, flow separation at edges, etc.). This estimated field is then freed of flow divergencies by iterations. Mass-conserving wind fields are thus obtained also for large areas with many flow obstacles after a relatively short computational time. To prognostically calculate a wind field, as done by MISKAM, requires 10 to 20 times more computational time. However, various arguments support prognostic modeling:

- Prognostic models generate information on the wind and turbulence field, while diagnostic models do not allow to consistently calculate the turbulence. Especially the reciprocal influence of wind and turbulence is not considered with diagnostic models.
- Complex structures of obstacles are combined to single obstacles in the diagnostic model. However, the interaction of flow effects of single obstacles do not correspond with their real flow conditions.
- Diagnostic models do not consider the stratification effects, which are important for air hygienic investigations, especially the effects of a stable stratified atmosphere.

2.3 Scope and limitation of application

The possibility to gain secure conclusions about the expected atmospheric load via a validated numeric model seems to be promising. Cost-intensive measuring campaigns can be reduced. Further, numeric models also offer an area-wide, respectively space-wide construct of information being much more detailed regarding single points of immission then legally required.

As long as the numeric model can be used reasonably comfortably according to our present standards, the perspective is tempting at the first glance so as to obtain those results within a few steps on a standard PC which previously only could be obtained via complex interaction of measurements, calculations and meteorological knowledge.

This way of thinking can be dangerous however, as shown. If a model – for instance the model software – takes over too much of the user's work, it can happen that the user overly emphasizes the model results and does not critically analyze them any longer. It is therefore important to point out the limitations of a numeric model very clearly. This is the purpose of this chapter.

2.3.1 Scope of application

MISKAM can be used for the following tasks:

- Calculation of quasi-stationary wind fields in the environment of isolated buildings or within a complex structured urban development. It has to be kept in mind that structured developments can only be considered with a limited accuracy depending on the selection of the grid of discretization.
- Simulation of the dispersion of density-neutral, non-reactive substances with a randomly assumed source distribution in previously calculated wind fields.
- Comparison of the calculated arithmetic mean and percentile of concentrations with the guideline and threshold values.

The dynamic effects of various ground conditions can be considered via the roughness length for the calculation of wind fields. The degree of roughness of the various grids is determined by setting a constant value for the whole model area or by entering a two-dimensional field of parameters assigning a certain type of surface (low or high vegetation, asphalt, non-explicitly assigned development, etc.) to each grid. In the last case, the classification of the lengths of roughness to the various surfaces is model internally determined.

The thermal stratification can be considered as a further critical value for the flow behavior. It will be considered as being constant in the model area and is specified as input parameter by the vertical gradient of the potential temperature. The influence of the thermal stratification consists of a reduction of the turbulent exchange for stable conditions as well as an increase for unstable conditions.

The simulation of the pollutant dispersion also considers the effect of the sedimentation besides the source dispersion, which also allows – at least approximately – the interpretation of non density-neutral substances as well as deposits. Both processes are recorded by setting constant characteristic velocities.

The sedimentation velocity is added to the vertical component of the wind field for the calculation of advection. The disposition velocity determines this portion of the transported substance which settles on the ground or on the surface of buildings out of the atmosphere. Both velocities have to be considered as material constants and have to be set by the user. Due to the possible usages mentioned above, the model MISKAM becomes a multi-functional tool for urban planning and road design.

However, the model should not be interpreted as a black box, its usage demands an intensive amount of work and thinking. This is intended to avoid any uncritical usage of the model. The following steps for numeric model simulations are thus *not* automatically taken care off by MISKAM:

- Generating an optimal grid of discretization specific for the area of investigation.
- Positioning of sources and determination of the source type.
- Setting emission rates.
- Construction of statistics based on several MISKAM runs.
- Conversion of calculated fields of immission into planning-relevant parameters (yearly average mean, 98-percentile, etc.).

The program KONFIG can be used to convert the selected grids, the containing buildings, as well as the sources of pollutants to a suited input file. It asks for all required values, performs a thorough verification for the data of its plausibility, and finally generates the MISKAM-readable input file.

Sophisticated instruments are available for some of the above mentioned tasks, as for instance the manual of emission factors which was developed on behalf of the Federal Environmental Agency. In addition, various implementations of the model also exist in the form of comprehensive program packages to work more comfortably with MISKAM.

Lohmeyer GmbH & Co. KG (Karlsruhe) offers the program WINMISKAM, adding a comfortable Windows interface to the MISKAM kernel. This can be used to generate the needed input files, to produce the diagrams of the results, to evaluate the statistics, and to produce the most important parameters.

MISKAM also was integrated in the widely-used program package SoundPLAN (Braunstein + Berndt GmbH, Backnang), allowing the SoundPLAN-users to work with their familiar surface for data entry and evaluation.

More information about both implementations can be directly obtained by the distributors or by **giese-eichhorn**.

2.3.2 Limitations

Besides the requirements mentioned in the previous chapter, several further, principal limitations exist, because certain actions cannot be simulated in MISKAM. Moreover, some limitations result from the adopted modeling assumptions as well as their numerical implementation.

- Thermodynamic processes (energy transformation at the surface of the terrain, along walls, and roofs of buildings, as well as thermal dispersion, buoyancy, water balance) are not considered, because this would cause a dramatic increase of computational time and disk space which cannot any longer be handled by a standard PC.
- MISKAM does not consider any chemical processes. The reactions of NO_x to NO₂ are particularly interesting for road traffic, for which various empirical relationships are available. This was not considered in the model equations, because the general validity of this relationship is questionable and a later consideration is possible by the appropriate conversion of the concentrations of immission.
- The approximation of slanted roofs by step shaped structures requires a critical evaluation of the results for the near field of the roofs (see Eichhorn, 2003).

Considering flow over buildings it is noticed that the height of recirculation zones is generally underestimated by MISKAM. This is a result of the E- ε turbulence closure which doesn't permit a realistic simulation of the flow separation at windward edges. This flaw of E- ε models is well-known and accepted, as the model otherwise represents a reasonable compromise of accuracy and applicability.

For dispersal simulations, e.g. for traffic induced emissions this property of the turbulence model is of no relevance. For emissions at roof level, however, it is not advisable to use MISKAM as long as the emission sources are not definitely located outside the recirculation zone. In particular, the model is not suitable to specify the optimal minimum height of an emission source. For this purpose, alternative data, e.g. from wind tunnel measurements or results from more elaborate models (LES) have to be adopted.

The usage of the model is restricted by neglecting the thermodynamics because certain conditions exist where thermodynamic influences on the flow field cannot be omitted (for instance street canyons with intensive asymmetric solar radiation). However, it can be assumed that these effects can hardly be identified in the yearly mean. Thus, one of the most important area of usage is not effected by this restriction.

The thermic effects can generally be excluded for calculating episodes, since these are mainly calculations of air-hygenic critical cases (so-called worst case studies). The most important thermal factors for near-ground immissions, stratification, is considered while calculating the turbulent diffusion coefficient.

This listing could lead to the assumption that the usage of MISKAM is very limited. However, its spectrum covers practically all air-hygenic aspects needed by planners as annual average value, percentile, and the maximum load. However, MISKAM expects a competent and diligent user producing finally reliable results for a particular scenario.

3 Theory

3.1 Preliminary note

Every numerical atmospheric prognostic model basically consists of a linked system of differential equations to predict the conditional variables (wind, temperature, air composition). These differential equations follow from known physical conservation equations of momentum (\Rightarrow momentum equations), mass (\Rightarrow continuity equations) and energy (\Rightarrow energy equation). Various simplifications and omissions are possible, depending on the complexity of the task and the size of the model area.

MISKAM is used to calculate wind fields and immission dispersions. Therefore, MISKAM does not consider the thermal exchange and the hydrologic process. This reduces all the prognostic variables to components of wind vectors and mass concentrations of the substances under investigation.

The elimination of sound waves, and the density as independent prognostic value are performed with the help of the Boussinesq-approximation. In addition, the equations are averaged, resulting in variables which have to be considered as microturbulent means. As a consequence of the averaging, the equations contain subscale processes for the turbulent transportation of momentum, heat and mass. The used closure of turbulences additionally requires the prognostic computation of turbulent kinetic energy as well as energy dissipation.

A detailed derivation of the system of equations is not given here. Details of the Boussinesqapproximation as well as of the averaging procedure are given by Eichhorn (1989).

3.2 The momentum equation

The prognostic system of the flow part of MISKAM consists of the Cartesian components of the Boussinesq-approximated momentum equations. Due to the small size of the model area, Coriolis force is neglected. In addition, buoyancy is also not considered.

The turbulent transportation of momentum is calculated by a first-order closure without any differences between horizontal and vertical exchange coefficients.

Using these assumptions, the momentum equation is the following:

$$\frac{\partial u_i}{\partial t} + \frac{\partial u_k u_i}{\partial x_k} = -\frac{1}{\rho_0} \frac{\partial p'}{\partial x_i} + \frac{\partial}{\partial x_k} \left[K_m \left(\frac{\partial u_i}{\partial x_k} + \frac{\partial u_k}{\partial x_i} \right) \right] - c_d n L \mathbf{v} u_i$$
(3.1)

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|----|--------|
|----|--------|

where

| $x_i = x, y, z$ | Cartesian coordinates | [m] |
|-----------------|--|-------------|
| $u_i=u,v,w$ | Cartesian components of the wind vector | [m/s] |
| t | time | [s] |
| $ ho_0$ | constant reference density at near-ground atmosphere | $[kg/m^3]$ |
| p' | dynamic pressure disturbance | [Pa] |
| K_m | exchange coefficient of momentum | $[m^2/s]$ |
| c_d | resistance coefficient | [-] |
| n | "degree of vegetation coverage" | [-] |
| L | one-sided leaf area density (LAD) | $[m^2/m^3]$ |
| v | wind velocity | [m/s] |

The last term on the right side describes the deceleration of the flow due to vegetation, i.e. the friction against leaf areas within a grid cells.

The normal convention of sums was applied in the momentum equation, which means that equal indices have to be summed up from 1 to 3.

This system of equations is enhanced by the requirement of a non-divergent wind field, which replaces the continuity equation for the total mass:

$$\frac{\partial u}{\partial x} + \frac{\partial v}{\partial y} + \frac{\partial w}{\partial z} = 0$$
(3.2)

To assure non-divergence at each time-step, an elliptical differential equation has to be solved for the dynamic pressure disturbance (condition of compatibility) in addition to solving the prognostic equations. It is only due to this additional computational load that economic timesteps can be used, since the requirement of a non-divergent wind field enables the elimination of sound waves from the system.

3.3 The turbulence model

The K-model, which was still provided in the previous version, and which is based on the classical boundary layer theory, calculated the required diffusion coefficients diagnostically with the help of the three-dimensional wind field, and the specified thermal stratification, as well as the so-called mixing length.

In the context of a PEF¹-program promoted project (Röckle and Richter, 1995), validation runs were performed for several models available at that time, amongst them was a previous version of MISKAM. The comparison was based on wind tunnel data on the one hand flowing

¹PEF = Projekt Europäisches Forschungszentrum

around a U-shaped building and on the other hand through a complex arrangement of buildings representing a section of the BASF factory site in Ludwigshafen. The results of MISKAM were partially unsatisfactory concerning the flow around the single building due to the above mentioned diagnostic treatment of turbulences. Therefore, a more sophisticated method of closures, the so-called E- ε -closure, was integrated for further developing the model. The obsolete diagnostic closure is no longer used by MISKAM since version 4.

Due to the E- ε -closure, the model results are based on a much more sound physical foundation. The exchange and diffusion coefficients are now obtained from the local values of the turbulent kinetic energy and the turbulent energy dissipation. These fields have to be calculated by solving two additional prognostic equations.

The mixing problem existing in the K-model is bypassed with this closure. The distance to the ground of the single grids is only needed to initialize the turbulent energy dissipation. In addition, several empirical constants have to be specified as external values. Broadly accepted values can be obtained from literature.

Instationary phenomena, as for instance the instationary separation of lee turbulence and the separation of so-called wakes, are not considered by this method. In principle, there are models available for this simulation, however, the time of computation needed does not make them feasible for a standard PC. The E- ε -closure seems to be appropriate to simulate quasi-stationary conditions corresponding to a temporal mean of the flow regimes (see, for instance, Paterson and Appelt, 1986, 1989). However the computational complexity is significantly higher than with the K-model.

3.3.1 Calculation of the diffusion coefficients

The diffusion coefficients for the transportation of momentum, K_m , are calculated as follows for the E- ε -closure:

$$K_m = c_\mu \frac{E^2}{\varepsilon} \tag{3.3}$$

where

| E | turbulent kinetic energy | $[m^2/s^2]$ |
|-----------|------------------------------|-------------|
| ε | turbulent energy dissipation | $[m^2/s^3]$ |
| c_{μ} | = 0.09 empirical constant | [-] |

For simplification, the relationship valid for neutral stratification is used for the diffusion coefficient for heat K_h

$$K_h = 1.35 K_m \tag{3.4}$$

3.3.2 The prognostic equations for *E* and ε

The following prognostic equations have to be solved to determine the kinetic energy of turbulence:

$$\frac{\partial E}{\partial t} + \frac{\partial u_k E}{\partial x_k} = \frac{\partial}{\partial x_k} \left(K_m \frac{\partial E}{\partial x_k} \right) + K_m \left(\frac{\partial u_i}{\partial x_k} + \frac{\partial u_k}{\partial x_i} \right) \frac{\partial u_i}{\partial x_k} - K_h \frac{g}{\Theta_0} \frac{\partial \Theta}{\partial x_k} \delta_{3k} - \varepsilon + c_d n L \mathbf{v}^3 - 4c_d n L \mathbf{v} E$$
(3.5)

$$\frac{\partial \varepsilon}{\partial t} + \frac{\partial u_k \varepsilon}{\partial x_k} = \frac{\partial}{\partial x_k} \left(\frac{K_m}{\sigma} \frac{\partial \varepsilon}{\partial x_k} \right) + c_1 \frac{\varepsilon}{E} \left[K_m \left(\frac{\partial u_i}{\partial x_k} + \frac{\partial u_k}{\partial x_i} \right) \frac{\partial u_i}{\partial x_k} - K_h \frac{g}{\Theta_0} \frac{\partial \Theta}{\partial x_k} \delta_{3k} \right] - c_2 \frac{\varepsilon^2}{E} + \frac{3}{2} \frac{\varepsilon}{E} c_d n L \mathbf{v}^3 - 6 c_d n L \mathbf{v} \varepsilon$$
(3.6)

where

 $c_1 = 1.44$ empirical constant [-] $c_2 = 1.92$ empirical constant [-] $\sigma = 1.3$ empirical constant [-]

The numerical values of the empirical constants correspond to the "classical" $E - \varepsilon$ -model (for instance Rodi, 1980). The validity of atmospheric calculations of turbulence was verified for instance by Ramanathan (1995).

The quantities $P_{E,m}$ and $P_{\varepsilon,m}$ denote the mechanical production of turbulent kinetic energy and energy dissipation, respectively, for which MISKAM offers diverse computation methods. In the classic model, both are computed from the deformation of the wind field:

$$P_{E,m} = P_{\varepsilon,m} = c_{\mu} \varepsilon S^2 \tag{3.7}$$

with the deformation S given as

$$S = \frac{E}{\varepsilon} \sqrt{\frac{1}{2} \left(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i}\right)^2}$$

This version of the $E - \varepsilon$ closure is known to overestimate turbulent kinetic energy and, as a consequence, diffusion coefficients near windward obstacle edges. Kato and Launder (1993) suggested to compute the production terms from deformation and rotation of the wind field:

$$P_{E,m} = P_{\varepsilon,m} = c_{\mu} \varepsilon S\Omega \tag{3.8}$$

with

$$\Omega = \frac{E}{\varepsilon} \sqrt{\frac{1}{2} \left(\frac{\partial u_i}{\partial x_j} - \frac{\partial u_j}{\partial x_i} \right)^2}$$

This reduces the production terms near edges, but likewise reduces energy dissipation. Lopez et al. (2005) use KAto and Launder's formula only in the equation for E but stay with the original form for the computation of ε :

$$P_{E,m} = c_{\mu} \varepsilon S\Omega; \qquad P_{\varepsilon,m} = c_{\mu} \varepsilon S^2 \tag{3.9}$$

Using this closure, Lopez et al. obtain best results for the flow over simple obstacles. Therefore, (3.9) is recommended for the application of MISKAM as well. The standard closure (3.7) and the Kato-Launder closure (3.8), however, are optionally available too.

The term P_t denotes thermal production of turbulence quantities and accounts for the fact, that stable stratification inhibits, unstable stratification enhances turbulence:

$$P_t = -K_h \frac{g}{\Theta_0} \frac{\partial \Theta}{\partial x_k} \delta_{3k}$$
(3.10)

It should be noted that this closure with the required stationarity can only lead to plausible results for neutral and stable thermal stratification. With unstable stratification, the thermal production leads to a steady increase of the turbulence energy and of the diffusion coefficient. But this contradicts the requirement of quasi-stationary conditions, like in reality, where an unstable stratification cannot be kept upright for a prolonged time due to the increased exchange. Therefore, unstable stratification, if specified by the user, is reset to 'neutral' for **MISKAM** simulations.

The last two terms contain the parameterization of the influence of vegetation. The positive terms describe the increased mechanical production of turbulence energy and dissipation because of leaves. The last term was derived from a suggestion by Greene (1992), leading to a significantly better correlation between simulated and observed wind fields of trees (see for instance Lauerbach and Eichhorn, 2004).

E and ε are diagnostically calculated via

$$E_1 = \frac{u_*^2}{\sqrt{c_\mu}}$$
 (3.11)

$$\varepsilon_1 = \frac{u_*^3}{\kappa z_1} \tag{3.12}$$

in the lowest grids with the help of the friction velocity u_* . z_1 is the height of the first grid above ground or building. Equal relationships are formally applied for vertical walls, however, z_1 is replaced by the roughness length of the building wall.

These boundary conditions are strictly valid only for neutral stratification. The influence of thermal stratification on the turbulence along the horizontal boundary areas is taken into account via the calculation of u_* . This is calculated by

$$u_* = \frac{|\mathbf{v}_{\parallel}(\zeta)|}{C_m(\frac{\zeta+z_0}{z_0}, \frac{\zeta+z_0}{\lambda})}$$
(3.13)

 C_m is the Clarke-function for momentum, whose values are taken from existing tables (Panhans und Schrodin, 1980). ζ is the minimal distance of the considered grid point to the fixed boundaries of the model, λ is the stability length. Details of the Clarke-function are given by Eichhorn (1989). To calculate u_* along building walls, a neutral stratification is assumed referring to a logarithmic wind profile vertically along the wall.

3.4 The splitting method according to Patrinos

The splitting method of Patrinos und Kistler (1977) is used to solve the prognostic system. Here, the momentum equations are first numerically solved by neglecting the pressure disturbances, resulting in temporary wind components \tilde{u} , \tilde{v} , \tilde{w} :

$$\frac{\partial \tilde{u}_i}{\partial t} = \frac{\partial u_i}{\partial t} + \frac{1}{\rho_0} \frac{\partial p'}{\partial x_i}$$
(3.14)

The following equation is obtained by applying the divergence operator and temporal forward discretization

$$\frac{\partial \tilde{u}_k^{n+1}}{\partial x_k} - \frac{\partial \tilde{u}_k^n}{\partial x_k} = \frac{\Delta t}{\rho_0} \frac{\partial^2 p'}{\partial x_k^2}$$
(3.15)

where Δt is the time-step, n and n+1 denote time t and $t+\Delta t$. The compatibility conditions have to be fulfilled before starting with a time-step. Therefore, the second term on the left side is zero and the following Poisson-equation remains for the pressure disturbance

$$\frac{\partial^2 p'}{\partial x_k^2} = \frac{\rho_0}{\Delta t} \frac{\partial \tilde{u}_k}{\partial x_k}$$
(3.16)

After solving and inserting into

$$u_i = \tilde{u}_i \frac{\Delta t}{\rho_0} \frac{\partial p'}{\partial x_i},\tag{3.17}$$

the desired non-divergent velocity field is obtained.

3.5 The dispersion model

3.5.1 The prognostic equation

The dispersion model mainly consists of the prognostic equation for a density-neutral air constituent with the mass concentration m:

$$\frac{\partial m}{\partial t} + \frac{\partial u_k m}{\partial x_k} = \frac{\partial}{\partial x_k} \left(K_h \frac{\partial m}{\partial x_k} \right) + Q \tag{3.18}$$

 ${\it Q}$ refers to the sum of the sources and sinks of the considered air constituents.

As normally, the heat exchange coefficient, K_h , is also used for the mass transportation.

3.5.2 Sedimentation and deposition

A constant sedimentation velocity can be set to consider the sedimentation of substances with a greater density than air. It is added to the vertical wind for the advection calculation.

Dry deposition on horizontal planes can be considered by setting a deposition velocity. The amount which is deposited on the ground per time unit is proportionally added to the deposition velocity and the mass concentration in the grid cell located above.

Both velocities are set as material constants of the considered air additives, values can be obtained from literature.

3.5.3 Momentum sources

A fixed vertical velocity (velocity of air emission, for instance out of a stack) can be set for point sources. This is already incorporated in the flow calculation, so that wind and turbulence fields close to a stack outlet can react to the additional momentum. This results in much more realistic pollutant plumes than without considering the emission velocity or application of the effective height of the source.

3.6 Initial and boundary conditions

3.6.1 Initializing the flow model

The three-dimensional model calculations are preceded by a one-dimensional initialization. For this purpose, wind and turbulence profiles are calculated up to a height of 2000 m.

To implement the MISKAM model thereafter, the three-dimensional profiles are converted in such a way that the simulated wind velocities at the height of the used anemometer correspond to the set value at all times.

Before starting the 3D-simulation, the profiles of the wind velocity and the turbulence energy are homogeneously transferred to the three-dimensional model area. To incorporate the elevated energy dissipation around buildings already in the initial distribution, an increase, depending on the distance to the model's boundaries, is applied while implementing the dissipation:

$$\varepsilon_{3D}(x, y, z) = \varepsilon_{1D}(z) \frac{z}{\xi(x, y, z)}$$
(3.19)

 ε_{3D} is the energy dissipation used in the initial distribution of the 3D-simulation, ε_{1D} is the one-dimensional profile which was simulated in advance. ξ is the minimal distance of each model point to the solid model boundary.

3.6.2 Boundary conditions for the flow model

The profiles resulting from the 1D-initialization of the wind components and the turbulence variables are temporally kept constant on the inflow areas and the upper boundary.

So-called no-flux-boundary conditions are valid on the lateral outflow boundaries which means that the disappearance of the normal gradients on these boundaries is required.

The outflow boundary values are corrected for the solution of the Poisson-equation of the dynamic pressure disturbance in such a way that the conservation of the total mass is assured for the entire model area. An extensive discussion of the boundary conditions is given by Eichhorn (1989) as well as by Eichhorn et al. (1997).

All wind components disappear on the lower boundary as well as along the building walls. Consequently, the disappearance of the pressure gradient perpendicular to the relevant planes is required there as well as at the upper boundary.

The values of the lower boundary of the diffusion coefficients are - as already mentioned - calculated by applying the Clarke-function. This also determines the corresponding friction velocity u_* , which again can be used for the calculation of the boundary values of turbulence energy and dissipation.

3.6.3 Initialization of the dispersion model

A wind field, which was calculated before, is read to initialize the dispersion calculations, including its exchange coefficients. The mass concentrations are set to zero at the start of the simulation.

An optionally added background level is not considered during the simulation, it is only added to the results.

3.6.4 Boundary conditions for the dispersion model

Inflow and outflow grid cells are treated differently in the lateral boundary conditions of mass concentrations. Clear air from outside of the model area is assumed at the inflow boundaries which means that the concentration value is kept at its initial value of 0.

The boundary value of the inner field is extrapolated for outflow grid cells with the assumption that the concentration gradient along the area normal remains constant.

In the case of a non-disappearing disposition velocity, the mass concentration at the lower model boundary is diagnostically calculated for each time-step, otherwise m is set to zero at the surface and walls, respectively.

4.1 Discretization and grid configuration

A staggered discretization grid of the type Arakawa C is used in MISKAM. The components of the wind vectors are defined on the corresponding grid surfaces, while the components u_i are set on the center points of the cell planes, being perpendicularly oriented to the direction *i*. All scalar prognostic variables (p', E, ε) as well as the exchange coefficients are defined at the cell center points. Figure 4.1 illustrates the grid configuration.

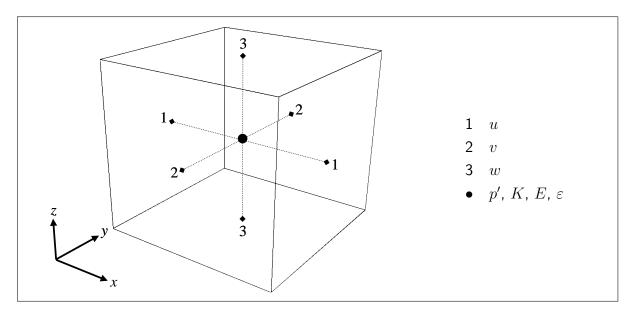


Figure 4.1: Grid configuration

The selected grid structure allows a simple usage of flow obstacles. Assuming that the grid box is located either completely free or completely within an obstacle, it is sufficient to define fields of multipliers which define whether a grid wall belongs to an obstacle (value of the multiplier is 0) or not (1). These multipliers are used for the Cartesian wind components as well as for the pressure gradient, and therefore assure that wind components will always disappear on building areas.

A modeling of overhanging obstacles (bridges, driveways, or similar) is also possible in MISKAM via this procedure, because the multipliers contain the entire information about the obstacles in the model area. It only has to be assured that the configuration will be clearly interpreted by the model and the calculation program respectively. This has to be done via input files which have to be set according to well-defined rules. More details can be found in chapter 5.

4.2 Treatment of the advection terms

4.2.1 Momentum advection

To discretize advection terms of the momentum equations, up to version 5.x simple so-called upstream-differences have been adopted. Even though the upstream-method contains a high numeric diffusion, it is quite acceptable for the purpose of MISKAM - the simulation of quasistationary flow fields - and due to the smaller computational requirements, it is superior to the numerically more precise but far more complex methods.

A significant improvement of the accuracy of computed momentum advection can be achieved mith the help of McCormack's (1969) predictor-corrector-algorithm. This combines the advected momentum as arithmetic mean of an upstream and a susequent downstream step.

4.2.2 Advection of scalar quantities

For the computation of advection of positive definite scalar quantities (turbulent kinetic energy, energy dissipation, mass concentrations) the MPDATA algorithm (Smolarkiewicz and Grabowski, 1989) may be adopted instead of the upstream scheme. This method is based on an upstream step, followed by one or more corrective steps to reduce in part the numerical diffusion. To keep computational requirements reasonable, the number of corrective steps in MISKAM is limited to 1 for turbulence variables.

For dispersal simulations it is suggested to use the MPDATA scheme for point sources. For line sources (e.g. streets) usually the upstream scheme should be sufficient.

During flow and dispersal models for complex obstacle configurations, Balczo and Eichhorn (2009) found the best over all model performance using the combination of McCormack and MPDATA schemes for the flow model, whereas differences between upstream and MPDATA where less pronounced for the dispersal model.

Treatment of the diffusion term 4.3

The diffusion term is numerically evaluated by the ADI (Alternating Direction Implicit)-method of Douglas and Rachford (1956). The values of a variable Ψ at time n+1 are calculated via two interim solutions Ψ^* and Ψ^{**} . Implicit calculations are performed in one space direction which means that the derivatives of the variables Ψ with respect to the space coordinate have to be applied at the new. The method can be described in the following form:

$$\frac{\Psi^* - \Psi^n}{\Delta t} = \Delta_z(\Psi^*) + \Delta_x(\Psi^n) + \Delta_y(\Psi^n) + R^{\Psi}$$

$$\frac{\Psi^{**} - \Psi^{*}}{\Delta t} = \Delta_{x}(\Psi^{**}) - \Delta_{x}(\Psi^{n})$$

$$\frac{\Psi^{n+1} - \Psi^{**}}{\Delta t} = \Delta_{y}(\Psi^{n+1}) - \Delta_{y}(\Psi^{n})$$
(4.1)

The abbreviations Δ_x , Δ_y , Δ_z stand for differential operators which are applied to the particular quantity Ψ . The remaining parts of the prognostic equation are summarized in the remaining term R^{Ψ} .

In principle, the working order is extraneous in the direction of the space. The order specified here is used because other boundary conditions are formally used in the vertical (closed boundaries, i.e. prognostic variables are prescribed) versus along the lateral boundaries (open boundaries).

The inversion of a tridiagonal matrix is only respectively needed to calculate the various interim solutions, for which a simple standard-algorithm is used.

4.4 Solution of the Poisson-equation

A so-called *Red-Black-SOR*-method is used to solve the Poisson-equation. The pressure values of the six adjacent cells are needed, in addition to the pressure value of the considered grid cell in order to discretize the Laplace-operators in the Arakawa-C-grid. If the discrete equation is solved for the pressure value of the central grid, the following is obtained:

$$p'_{i,j,k} = \frac{A_x p'_{i-1,j,k} + B_x p'_{i+1,j,k} + A_y p'_{i,j-1,k} + B_y p'_{i,j+1,k} + A_z p'_{i,j,k-1} + B_z p'_{i,j,k+1} + D}{A_x + B_x + A_y + B_y + A_z + B_z}$$
(4.2)

where

$$D = \frac{\rho_0}{\Delta t} \frac{\partial \tilde{u}_k}{\partial x_k}$$

The coefficients A_x , B_x , A_y , ... are obtained by discretizing the Laplace-Operators, they contain the multipliers described in chapter 4.1, to assure the disappearance of the normal gradient of the pressure disturbance on and in obstacles.

At first, in order to solve this, a first approximation of the pressure disturbance is used in the right side of the equation (4.2). The pressure field is set to zero at the beginning of the simulation. For future time-steps, the pressure field of the preceding time-step is used as an initial approximation.

The solution itself is obtained in two half-steps for each iteration step ν . In the first step, new pressure values are calculated for each second point on the grid. Thereby, those points on the grid obtain new pressure values which take over the adjacent values on the right side of the equation (4.2) in the second half-step. The name of this treatment is based on the checkered

arrangement of the grids containing the new values of the half-steps, however why *red* is used and not *white* is unknown to the author.

The two half-steps result in a interim solution p^* , which is combined with the pressure field of the previous iteration step $\nu - 1$ according to

$$p^{\nu} = \omega p^{*(\nu)} + (1 - \omega) p^{(\nu - 1)}.$$
(4.3)

 ω is a relaxation parameter without dimension, whose optimal value depends on the grid geometry. The iteration is stopped when the maximal divergence of a wind field (corrected for the calculated pressure values) falls below a previously set value. This threshold is successively decreased during the simulation to increase the precision of the wind field calculation.

5 Operating instructions

5.1 Conventions

Special fonts are used for the following descriptions / actions in the following chapters:

command line *cd miskam*

file, directory name NAME.INI

MISKAM refers to the model itself as well as to the total program package. The various executable program parts are **MISKAM?.EXE¹**, **KONFIG.EXE** and **DATXYZ.EXE**. A Demo version of the visualization program **MISVIS.EXE** is also part of the package.

Attention: The hyphen in a file name at the end of a line has to be ignored.

5.2 Hardware- and software requirements

To run MISKAM, a 32Bit operating system is mandatory, Windows 7 or later is recommended. A 64 bit version is available upon request.

The available memory limits the number of processed grid points. A RAM size of 2 GByte allows model domains of approximately $200 \times 200 \times 50$ points.

5.3 The MISKAM-CD

The MISKAM-CD contains all files needed to run the model MISKAM in a self-extracting ZIP-archiv **M?SETUP.EXE**.

The input files as well as the results of the sample calculations are in the directories **BEISPIEL****EIN** and, respectively, **BEISPIEL****AUS** on the CD. The files **GOETTING.*** contain the input data as well as the results of a simulation for the Göttinger Straße (Hannover). The input file is a revised version of the afore mentioned PEF-project.

The results saved under the name **QUERU.*** contain the flow and the concentration field around a single building with a flow through (for instance passageway). The file **QUER.INP** describes the basic configuration, the flow-through areas are defined in **QUER.001**.

¹The **?** in the program name stands for its actual version number at the time of printing.

All input files as well as the most important results of all validation calculations are finally put together in the directory VALIDIERUNG with a separate subdirectory for each calculated case. Descriptions and results of the various calculations are given in chapter 6.

Installation 5.4

5.4.1 Extracting the program files

The following steps are required for a new installation under Windows:

- 1. Starting of M?SETUP.EXE in the root directory of the MISKAM-CD.
- 2. Setting of the target directory to unzip the program files.

Further subdirectories below the target directory are created while unzipping. The directory **MISKAM** contains the executable program as well as the needed control files. The subdirectory **MISKAM****EIN** is created for input files and **MISKAM****AUS** for model results. A copy of this manual is stored in the directory **MISKAM****DOC** as as PDF file.

5.4.2 Installed files

After executing M?SETUP.EXE according to the instructions above given, the files listed in table 1 are stored in the MISKAM-directories, assuming an installation on drive C: as well as in the directory **MISKAM**.

The batch file **MSTART.BAT** is used to start MISKAM with the help of a pre-generated INI file, more details can be found in chapter 5.8.

The files **STROEM1.INI** and **STROEM0.INI** contain the necessary startup information for the flow calculations (STROEM1: new run, STROEM0: serial run with using the previous results), AUSBR1.INI and AUSBR0.INI are the corresponding startup files for the dispersion calculations.

The file **README.TXT** contains the most important information on how to install and use MISKAM. Program changes which are implemented after the printing of this manual are described in the text file **WHATSNEW.TXT**.

The configuration files *.INP 5.5

MISKAM needs information about the grid structure and the layout of the model area regarding obstacles (buildings). This information has to be delivered via an ASCII file in a fixed structure

| 5.5. | The configuration | files *.INP | 33 |
|------|-------------------|-------------|----|
|------|-------------------|-------------|----|

| File name | Explanation |
|--------------------------|--|
| C:\MISKAM\MISKAM?.EXE | MISKAM - main program |
| C:\MISKAM\MSTOP.BAT | batch program to interrupt MISKAM runs |
| C:\MISKAM\STOPTEXT | help file for MSTOP.BAT |
| C:\MISKAM\KONFIG.EXE | producing INP-files |
| C:\MISKAM\MISVIS-D.EXE | plot routines to evaluate the results |
| | (demo version) |
| C:\MISKAM\README.TXT | general information regarding MISKAM |
| C:\MISKAM\STROEM1.INI | startup file for the flow calculation, |
| | new run |
| C:\MISKAM\STROEM0.INI | startup file for the flow calculation, |
| | restarted run |
| C:\MISKAM\AUSBR1.INI | startup file for the dispersion calculation, |
| | new run |
| C:\MISKAM\AUSBR0.INI | startup file for the dispersion calculation, |
| | restarted run |
| C:\MISKAM\EIN\KONFIG.INP | Example of the configuration file |
| C:\MISKAM\AUS\STROEM.PRS | results of the sample files, |
| | log file of the flow calculations |
| C:\MISKAM\AUS\STROEM.UVW | results of the sample files, |
| | table of wind components, pressure irritations |
| C:\MISKAM\AUS\STROEM.TUR | results of the sample files, |
| | table of turbulence variables |
| C:\MISKAM\AUS\STROEM.ZWU | results of the sample files, |
| | binary file of wind field |
| C:\MISKAM\AUS\STROEM.ZWT | results of the sample files, |
| | binary file of turbulence field |
| C:\MISKAM\AUS\AUSBR.PRA | results of the sample files, |
| | log file of dispersion calculation |
| C:\MISKAM\AUS\AUSBR.KON | results of the sample files, |
| | table of mass concentrations |
| C:\MISKAM\AUS\AUSBR.ZWK | results of the sample files, |
| | binary file of concentration field |
| C:\MISKAM\DOC\MANUAL.PDF | MISKAM manual |

Table 5.1: Content of the self-extracting archive $\ensuremath{\mathsf{M?SETUP.EXE}}$

(**NAME.INP**, **NAME** variable, DOS compatibility is required). Form and content of the configuration files are described in this chapter.

5.5.1 Structure of the configuration files

As an example, the file **KONFIG.INP** of the **M?SETUP.ZIP** archive is illustrated in figure 5.1. Further examples are given in the configuration files on the CD directory **BEISPIEL****EIN** as already mentioned, as well as in various subdirectories of the directory **VALIDIERUNG**.

The different parts of the configuration file contain the following information:

Cartesian grid: The first 4 rows of the configuration file define the number of used grid boxes as well as the grid resolution.

The number of grid boxes in each of the three dimensions (sequence x, y, z) is set in the first row, the fourth number in this row refers to the angle between the x axis of the model area and the northern direction. The three following rows contain the Cartesian coordinates of the cell walls in the three dimensions. Hence, one more value has to be set in each row than grid boxes were defined in each dimension.

- **Arrangement of buildings:** The size of the following data blocks depends on the number of grid boxes in the *x* and *y* directions which was set before. The following rows represent a top view of the model area, where the number of cells, being filled in the vertical direction with flow obstacles (buildings), are given for each horizontal grid surface. 0 thus means no obstacle.
- **Roughness length:** Either a unique value for the roughness length z_0 of the ground or a two-dimensional field for the surfaces with internally determined roughness lengths can be set in MISKAM. In addition, a roughness length for building walls and roofs has to be set in any case, which is identical for all buildings recorded in the model area.

To set a unique roughness length, "j" has to be inserted in the row after the building configuration. The next row thus contains the roughness length of the ground as well as of the building areas. In previous versions (up to 5.x) no distinction has been made between building walls and roofs. This inconsistency has been eliminated with MISKAM 6, $z_{=}$ for roofs has to be specified as third number within the same row of the input file. To ensure backward compatibility, MISKAM will accept configuration files with only one value specified for building surfaces, which will then be used for both, walls and roofs. All values of $z_{=}$ have to be specified in cm.

To use an inhomogeneous roughness distribution, "n" has to be set in the row following the building configuration. Only the values for building surfaces then have to be entered in the following row.

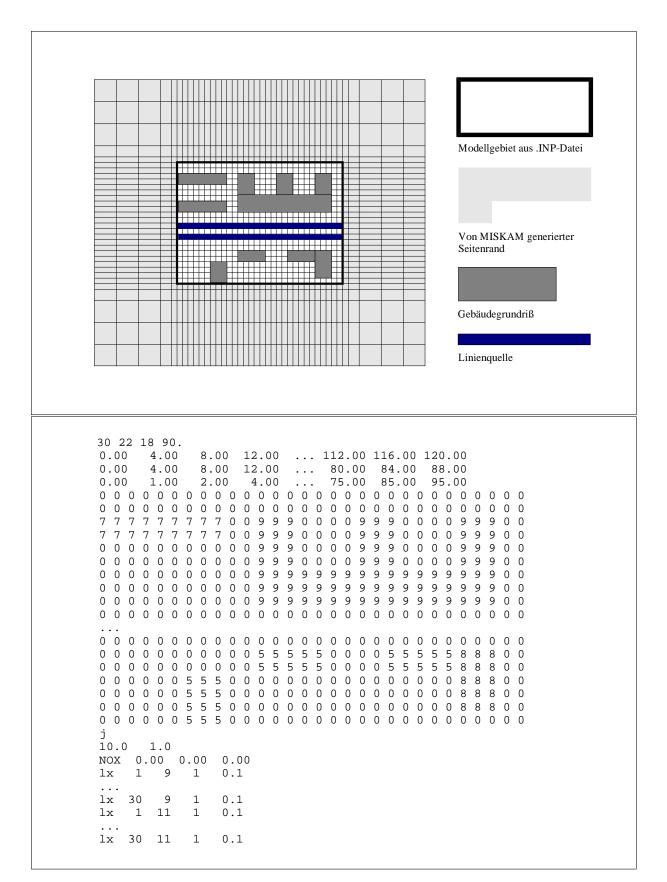


Figure 5.1: Example for MISKAM configuration as top view (top) and in form of the INP file (bottom, not completed). In this case, no value for roughness of roofs is included, MISKAM will therefore use the value specified for walls.

| value | kind of land allocation | \mathbf{z}_0 in cm |
|-------|---|----------------------|
| 0 | roof of a building | $z_{0,w}$ |
| 1 | asphalt or similar without obstacles | 1 |
| 2 | meadow | 5 |
| 3 | meadow with single trees, shrubs | 10 |
| 4 | more dense low vegetation | 25 |
| 5 | low buildings, not explicitly resolved | 50 |
| 6 | higher buildings, not explicitly resolved | 100 |

Table 5.2: Kind of ground and roughness lengths in MISKAM. The set value of walls and roofs is used for $z_{0,w}$.

A two-dimensional data field follows, in which each grid area is assigned a value between 0 and 6. The values of the corresponding surface types as well as the corresponding roughness lengths are given in table 2.

Distribution of sources: The INP file lists the considered pollutant sources after the geometry of obstacles as well as the specifications of the roughness of the ground.

The name of the considered substance, its background values (in mg/m^3), as well as, if applicable, sedimentation velocity and deposition velocity (each in m/s, a positive sedimentation velocity refers to a sinking of the considered substance!) have to be set here.

Then, a table follows describing source type, grid positions, and the strength of the source. Roads are normally represented as line sources. However, attention has to be paid, if the considered road's orientation is not parallel to one of the horizontal coordinate axes. In those cases, appropriately corrected emissions have to be set, because a description as a source parallel to one axis would result in an overestimated total extent of the source. Alternatively, the intensity of a source can be converted into a point source and specified in the configuration file accordingly.

It has to be mentioned that each grid cell can contain multiple sources. The strength of the sources are converted into volume sources within the model, multiple sources will be summed up.

Instead of the point-wise definiton of sources, regions of grid points to which identical source strengths will be assigned, may be specified. To do this, the input row specifying the substance has to be extended by an 'm' (for 'multiple'). In the subsequent table each row then must contain six $(i_{left}, i_{right}, j_{front}, j_{back}, k_{lower}, k_{upper})$ instead of three grid indices. The file **QUER.INP** shows an example of this type of source definition.

5.5.2 Precision requirements

The following settings are absolutely required during configuration of the buildings:

- The height of the highest building is not allowed to exceed 30 % of the model height.
- The blockage coefficient as defined in the VDI guideline 3783/9 must not exceed 10 %.
- Investigation points (points for which results should be deducted according to 23. BIm-SchV) should be located at least 10 grid cells away from lateral model boundaries.
- Investigation points must not be located within grid cells containing sources as well as in their neighboring cells.
- Investigation points must not be located in direct neighboring cells of buildings and must have a minimal distance of two grid cells to the ground.
- Relevant street canyons have to be divided into at least 6, better into 8 grid boxes perpendicular to their longitudinal axis.
- A precise representation of the buildings is needed in the area of investigation, some uncertainties can be allowed in the boundary zones. The geometry of the buildings should be recorded with a precision of ≤ 1 m in the area of investigation, in order to decrease errors as much as possible which can occur in the Cartesian grid.

Within the limits of the possible grid resolution, the shape of the roofs can be considered while grating the buildings.

 The geometric dimension of buildings in the upstream area has to be determined with a precision of ≤ 20 %. It is not required - and also impossible for the somewhat less precise grid resolution in the upstream area - to consider the shape of the roofs, the buildings can be considered as cuboids with an averaged eaves height.

Regarding the position of investigation points, the mentioned restrictions imply, that, near the ground, vertical mesh sizes of e.g. 0.5 m - 0.6 m - 0.8 m - 1.1 m can be used accordingly to 23. BImSchV. This assures that the center of a cell is located at the height of 1.5 m and that there are two further grid cells in between the point and the ground.

5.5.3 Storing of minimum distance to the ground

The minimal distance of each grid point to the fixed boundaries of the model is calculated after launching an INP file. This value is needed to initialize the turbulence model. This calculation can be very time consuming for complex configurations. Therefore, the distances

to the ground are written into a separate file called **NAME.XXL** after the calculation. For further simulations (for instance for other wind directions), only this file is then read. This shortens the startup phase of the flow model considerably.

If changes to the building configuration have been made, the file must be updated. MISKAM automatically determines if this is necessary by comparing the date stamps of both, the INP- and XXL-file.

5.6 Additional configuration files

MISKAM recognizes up to 999 additional configuration files, whose name consist of the prefix of the INP file and the ending nnn (001 < nnn < 999). Additional information about the configuration is given to the model via these files. Flow-throughs and obstacles with overhangs, vegetation, momentum-containing sources can thus be defined in MISKAM.

Furthermore, MISKAM 6 allows to limit the part of the model domain for which stationarity of the flow fields will be checked.

5.6.1 Flow-through

The used configuration file has to contain the string "Durchstroemung" (please note: small and capital letters!) in the first row. Any number of flowable cell areas can be assigned in the following rows. In the layer perpendicular to the flow direction, the extension of the flowable area has to be at least two grid cells wide in each direction.

The following example defines a flow in the x-direction, which should be spread over the grid cells 6 to 8 in the x-, 4 to 7 in the y- and 1 to 4 in the z-direction. The corresponding input file would then look as follows:

```
Durchstroemung
x 6 8 4 7 1 4
```

Figure 5.2: Configuration file to define the flow-through area

Setting the direction of the flow-through is important for the correct internal processing, because it determines which cell walls have to be freed again.

The results, under the consideration of the flow-through defined in the file BEISPIEL\EIN\QUER.001, are given in the files BEISPIEL\AUS\QUER-1.*. The files BEISPIEL\AUS\QUER-2.* contain the appropriate model results of a non-flowable building.

5.6.2 Vegetation

The influence of vegetation could only be considered in the model via the roughness length z_0 up to now. This, however, does not lead to realistic results, because the part which is influenced by the vegetation is explicitly dissolved by MISKAM, but z_0 only includes those surface roughnesses that cannot be directly described as flow obstacles. The implemented concept simulates the influence of vegetation via an additional restraining force in the momentum equations, as well as via modified production rates of turbulent kinetic energy and energy dissipation. This leads to a realistic simulation of of the flow retardation and the turbulence increase through trees and hedges.

The user has to provide information in an additional input file (naming convention as with flow-through, which means name.00x with x in the range 1...5) concerning the position of the leaf-containing grids, the degree of vegetation coverage (top view), as well as the leaf area density in (m^2 of leaf area)/(m^3 of air). Values for leaf area density of various forest species are given in the literature, for instance Groß (1993).

Sample data of an explicitly dissolved solitary tree (BAUM1.INP, BAUM1.001 in

BEISPIELE(N) are given. The following table shows a part of the file **BAUM1.001**. The value "Vegetation" (please note: small and capital letters!) in the first row is mandatory. The columns of the further rows contain the following information:

| 1st column | type of vegetation, "L" or "I" are mandatory. |
|--------------------|---|
| 2nd + 3rd column | index-area in x-direction |
| 4th $+$ 5th column | index-area in y-direction |
| 6th $+$ 7th column | index-area in z-direction |
| 8th column | leaf area density in (m 2 of leaf area)/(m 3 of air) of the cell area |
| | defined in columns 2–7 |
| 9th column | degree of vegetation coverage of the cell area. |

Vegetation

| 108000000 | | | | | | | | |
|-----------|-----|-----|----|-------|-------|-------|-------|-------|
| L | 22 | 22 | 19 | 19 | 6 | 6 | 8.400 | 1.000 |
| L | 23 | 23 | 25 | 25 | 7 | 7 | 0.781 | 1.000 |
| ••• | ••• | ••• | | • • • | • • • | • • • | | |

Figure 5.3: Configuration file to define the cell areas with vegetation

5.6.3 Sources with preset exit velocity

A fixed vertical velocity (outlet air velocity, for instance out of a stack) can be set for point sources. This is already integrated in the flow calculation, so that wind and turbulence field close to stack exits can respond to the additional momentum.

Much more realistic pollutant plumes are obtained with this method than without considering the escaping velocity or with using the effective source height.

Please note:

- The results are not any longer independent of the flow velocity, because the wind field which is close to the source directly depends on the exit velocity or, respectively, on its ratio to the undisturbed flow velocity.
- The time needed to calculate a stationary wind field can increase considerably.

A further input file is needed to set the exit velocity, the files **KONFIG.INP** and **KONFIG.001** contain an example. The additional file has to contain "Quellen" (please note: small and capital letters!) as a first value, thereafter exit velocities (column 4, in m/s) can be allocated to several grids (column 1 to 3 contain grid indices in x-, y-, and z-direction). The source position has to be consistent with the one of the .INP file (see source position in **KONFIG.INP**).

Quellen 14 15 11 5.0

Figure 5.4: Configuration file to define momentum containing sources

5.6.4 Limitation of stationarity check to inner model domain

Computation times to achieve stationary flow fields can be reduced significantly by restricting the stationarity check to the inner parts of the model domain. To do so, in an additional configuration file the range of x- and y-coordinates for which the check shall be performed, must be specified.

```
Kerngebiet
250 750 200 800
```

Figure 5.5: Configuration file to define inner model domain for stationarity check. The header 'Kerngebiet' is mandatory. All coordinates in m.

In this example, stationarity would be checked within an inner domain of 500 m \times 600 m.

Test runs for the configuration file of Göttinger Straße, Hannover, showed that in that case computation times can be reduced by as much as 50 % without changing the results within the inner domain. Actually, the amount of time saved can vary in both directions, there is no general rule of thumb. Tests for each case considered are therefore requisite.

```
Settings for flow calculations
                         ΝΕW
                               START
      -----
                         -----
Controling parameter (s: flow model, a: dispersion model) .....s
configuration file (prefix) ..... konfig
isteps (number of time-steps until intermediate storage) ...... 1000
z0ein (roughness length for 1d-initialization in cm) ..... 10.0
zanem (Anemometer height in m) ..... 10.0
uv0 (wind velocity in m/s in anemometer height) ..... 5.0
winku (wind direction in degree against N in anemometer height) ..... 225.
dtdz (stratification in K/100m, 0: neutral, >0: stabile, <0: unstable) 0.
eeps (closure, e: E-eps-model, k: K-model) .....e
abbr (termination criterion, s for stationarity or number of seconds) s
output file (prefix) ..... stroem
Input folder
                                                    \ldots
Output folder
                                                    \ldots
When changing defaults, make sure the all values start in 70th column! ^
```

Figure 5.6: Example of a MISKAM initialization file for the flow calculation. The specification of input and output folder is optional

5.7 Parameters to control program flow and meteorology

MISKAM needs a number of control parameters to steer the program, as well as for the meteorological initialization. These parameters will be explained in the following chapter 5.7.1, "confidence intervals" are additionally given for the various values.

Lateral up- and downstream zones are program internally defined by default. These default values can be modified via an additional control file being described in chapter 5.7.2.

5.7.1 The initialization file MISKAM.INI

The parameter values to be used are transferred to MISKAM via the file **MISKAM.INI**. The file **STROEM1.INI** of the installation archive is shown in Figure 5.6. The results obtained by the program settings given in the file **STROEM1.INI** correspond to the installed files **EIN****STROEM.***.

The meaning of the various parameters, including those of other possible INI files is listed below. A \bigcirc preceding the text refers to parameters needed exlusively for flow calculations, a \bigcirc to those needed only for dispersion calculations.

Control parameter (s: flow model, a: dispersal model)

Self-explanatory, specifies if a flow or dispersal simulation shall be run.

To switch on the diverse advection schemes for flow simulations, instead of "s" also "s1" or "s2" can be entered.

"s": Upstream advection for both, momentum components and turbulence variables

"s1": McCormack scheme for momentum components, upstream scheme for turbulence variables

"s2": McCormack scheme for momentum components, MPDATA scheme for turbulence variables

Configuration file (prefix):

Specification of INP-file to be used. The file PREFIX.INP must be located in the folder **EIN**, unless an alternative path for input files is specified (see below).

New start (1) or consecutive run (0):

This parameter tells the program, whether a new calculation of all fields should be started (one-dimensional initialization for the flow model, start with a "clean" atmosphere for the dispersion model), or whether a still to be specified batch of existing result files of a previous run should be used.

Values other than 0 and 1 are not allowed.

Number of time-steps needed up to the intermediate storage:

The binary files are created at latest after the number of time-steps which was set here, and the calculation is terminated. The calculation is terminated earlier, if the defined stationarity criterion is reached before.

Turbulence closure (e, ek or es):

S This parameter controls which version of the $E-\varepsilon$ closure shall be adopted. To use the model suggested by MISKAM's developer (modified Kato-Launder closure, Lopez et al. 2005)) the option "e" is valid. Alternatively "ek" and "es" can be specified to use the Kato-Launder version or the standard version, respectively.

In rare cases, numerical instabilities of the turbulence model may occur. Up to now, all instabilities could be eliminated by a modification of the time-step splitting applied to the turbulence model. The default is a splitting into two steps, which, in case of numerical instabilities, can be extended to four steps by renaming the file **MISKAM_SPL**, located in the main MISKAM folder. to MISKAM.SPL.

Roughness length of 1d-initialization:

S This is used to calculate the one-dimensional wind profile, which is transferred to the three-dimensional model area after the required scaling.

As already mentioned, five additional grid cells are internally added to the lateral model boundaries. The outer three of these cells obtain the z_0 -value of the 1d-initialization, an interpolation to the first value of the actual model area is performed for the two inner grid rows.

The roughness length has to be given in cm.

Flow direction:

S The angle of the given flow is set according to the common notation (N = 0°, O = 90° and so on) in meteorology.

Flow velocity:

S Wind velocity at anemometer height, setting in m/s. It is principally sufficient in most cases to calculate one single flow velocity and to determine the distribution of immission for other velocities by an appropriate scaling, because the concentration values calculated by MISKAM are inversely proportional to the wind velocity.

Anemometer height:

S Optionally available wind measurements (for instance roof-level measurements) can be considered in the model calculation by setting the anemometer height (setting in m) explicitly. The pre-calculated wind profile is scaled in such a way that the settings of the wind velocity and the anemometer height are kept.

Thermal stratification:

S The stratification is set as vertical gradient (K/100m) of the potential temperature. The value 0 refers to neutral conditions, positive values characterize stable stratification.

Special attention is needed to set the non-neutral thermal stratification to produce physically reasonable combinations of wind velocity and stratification. Difficulties can arise when thermal stable stratification is combined with relatively high near-ground wind velocities (for instance > 1 m/s in 2 m height), because this produces unrealistically high wind velocities in high altitudes. It makes more sense to set low near-ground wind velocities in the case of stable stratification, or a large anemometer height, for instance at the upper boundary of the model. The gradient of the potential temperature should not be more than 1 K/100m.

Negative values of the temperature gradient (unstable stratification) are internally set back to 0 (neutral stratification), because the combination of unstable stratification \Leftrightarrow stationarity is physically not reasonable as mentioned above.

Number of corrective steps for advection calculation:

A To calculate the mass advection in the dispersion model, either the simple upstreamscheme or the MPDATA scheme of Smolarkiewicz and Grabowski (1989) is used, where numeric diffusion effects are partially reversed by one or more correction steps. The upstream-scheme is used if 0 is set, a maximum of two correction steps can be calculated. Values > 2 are set to 2.

It is generally justified to use the upstream-scheme for traffic emission (line sources). It has to be noted that each Smolarkiewicz correction-step increases the computational effort for the dispersion model by about 80 %.

Termination criterion ("s" or number of seconds):

Optionally, different termination criteria can be used for the simulations of flow and dispersion.

The fixed time termination criterion is identically handled in both parts of the model, the user has to set the number of seconds. This number is directly written in the INI files as an termination criterion (see example on the distribution disk).

It is especially advisable to set a fixed time for dispersion calculations, where various building variants are compared, because it assures that the same total mass is emitted for each model calculation.

The stationarity criterion is differently interpreted depending on the kind of simulation:

For flow calculations, the simulation is terminated, when the following unique criteria are fulfilled:

- The maximum of the relative changes (change per time-step / inflow velocity in 10 m height) of the three wind components,
- as well as the maximum change of the diffusion coefficient, also related to an inflow value in 10 m height

Both have to drop below 0.1 %. According to this stationarity criterion, stationarity should normally be reached after approximately 1000 to 2000 time-steps depending on the complexity of the model construction.

The dispersion calculations offer a further criterion. The setting of "s" implies a termination of the calculation as soon as the concentration changes do not exceed 0.01 % of the maximum concentration value in any grid. This needs approximately the same number of time-steps as the one for flow calculations. This criterion assures that no concentration changes occur close to sources any longer. It is therefore usable if, for instance, immission concentrations have to be analyzed close to roads.

This criterion is not sufficient to investigate the pollutant concentration in a larger distance of sources, the stationarity criterion "s2" can be set in this case. The termination occurs in the latter case when the concentration value of any cell is not changed by more than 0.1 % comparing with the cell's own value. Approximately 2 to 4 times more time-steps are needed for this criterion depending on the configuration of the buildings.

Output files (prefix):

Specification of the file prefix for model results **.PRS .UVW .TUR .ZWU .ZWT** for flow simulations, **.PRA .KON .ZWK** for dispersal simulations. The files will be created in the folder **AUS**, unless another path for output files (see below) is specified.

Folder for input files:

Optional specification of a folder containing the configuration file. The name can be specified either as a relative or an absolute path. The file name must end with a \setminus . Folder names containing blanks must be enclosed in quotation marks.

Folder for output files:

Optional specification of a folder for output files, name specification as for input folder.

5.7.2 The control file MISKAM.BND

An additional lateral boundary zone consisting of five respective grid rows is used by default for MISKAM simulations. The grid resolution is extrapolated from the model area, the three outermost grid cells are equidistant. All boundary cells are free of obstacles. Other settings of the lateral boundaries can possibly make sense in different scenarios. For instance, additional boundary cells are not needed, if the actual model area already contains sufficient up- and downstream zones. It also can be suitable to extend the flow obstacles beyond the lateral boundaries to regard them as being quasi infinite (for instance situations in street canyons, which should not be treated as being two-dimensional due to existing road crossings, approximative consideration of the topography). The file **MISKAM.BND** in the MISKAM directory can be used to overwrite the default values in these cases. The structure of the file is given as follows in Figure 5.7.

In the given example, the first three additional grid cells obtain a higher grid spacing by the factor of 1.2, respectively. The fourth and fifth cell receive the same resolution as the third one. The boundary cells would be free of flow obstacles in this case.

The variable **igeb** is responsible not only for the obstacle height but also for the roughness of the ground and the sources of the pollutants at the lateral boundaries, these values also become "infinite" if **igeb**=1.

The boundary cells remain free of sources by default. The roughness of the ground is set for the three outer cells to this value, which is also used for one-dimensional initialization of the flow calculations. These cells are supposed to be representative of an undisturbed environment. For the two remaining rows of cells, the roughness length is interpolated between the value of initialization and the value of the boundary cell of the inner model area.

For two-dimensional calculations, the variable **igeb** is utilized only for the x-direction, homogeneous conditions are assumed for the y-direction.

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```
# Usage of the lateral boundaries
±
# Extrapolation of the grid spacing
# xyfact = 0 <==> 1 additional boundary cells as in MISKAM3.6
# xyfact = 1 <==> equidistant continuation of the grid over 5 cells
# xyfact > 1 <==> spread continuation of the grid over 5 cells
# xyfact is program internally limited to 2.
#
# Extrapolation of the obstacle structure
# igeb = 0 <==> no obstacles on boundaries
# igeb = 1 <==> last inner obstacle height is transfered to boundaries.
# igeb should ONLY be set to 1 to approximate the topography.
# Exceptions are two-dimensional calculations, igeb=1 is automatically set
#
xyfact
       1.2
igeb
       0
#
Ende
```

Figure 5.7: File **MISKAM.BND** to set the lateral boundaries.

To return to the default setting, the file **MISKAM.BND** has to be arbitrarily renamed or moved to a different directory.

5.8 Utilization steps

The model calculation is started with MISKAM via the command prompt. The program obtains the necessary information about program control and the meteorology from the file **MISKAM.INI**, as mentioned above. Results are stored in binary files and ASCII tables. Because no interactive processes have to be worked through to start, MISKAM can be used for batch processes, for instance to produce statistics.

5.8.1 Initialization and program start

Before MISKAM can be started, the appropriate INI file for the planned run has to be produced. The files **STROEM1.INI**, **STROEM0.INI**, **AUSBR1.INI**, and **AUSBR0.INI** are copied as "templates" into the program directory during the installation. The purpose of an initialization file is stated in its first line.

The command to launch the model MISKAM reads

[installpath\]MISKAM? ["'inipath\ininame"']

For "?" the version number included in the name of the executable must be inserted. MISKAM can be launched from any arbitrary folder, as long as the location of the executable is specified via the optional parameter installpath. The second optional command line argument *inipath**ininame* specifies location and name of the INI file. If the optional argument is omitted, MISKAM will request a file MISKAM.INI located in the installation folder.

Folders may be specified either as relative or absolute paths.

Examples:

- Launch MISKAM? from installation folder C:\PROGRAMME\MISKAM using INIfile **MISKAM.INI** located in the same folder cd PROGRAMME\MISKAM MISKAM?
- Launch MISKAM? from folder C:\PROJEKTDIR, EXE located in C:\PROGRAMME\MISKAM, use INI-file FLOWSTART.INI, located in folder C:\PROJEKTDIR\FLOW:

cd PROJEKTDIR

C:\PROGRAMME\MISKAM\MISKAM? FLOW\FLOWSTART

Depending on the kind of simulation to be run, different parameters are required (see 5.7), resulting in different structures of the INI files. Examples can be found in the installation folder. Names and contents of the examplary files are self-explanatory, therefore a detailed description is omitted here. The meanings of the various parameters has already been explained in section 5.7.1.

Terminating the program 5.8.2

MISKAM runs can be terminated in a controlled manner with the help of a provided text file **STOPTEXT** as well as the batch file **MSTOP.BAT**, both being copied into the MISKAM directory during installation. The execution of the batch file causes the termination after the next soft copy on the screen, i.e. latest after another 10 time-steps for flow calculations, 100 time-steps for the dispersion calculations, respectively. Results are stored to the usual output files.

5.8.3 **Result output**

All data which is needed for further runs (for instance the continuation of the simulation, for which the stationarity criterion was not reached yet) are saved in an unformatted binary file at the end of a model calculation. These files are produced at every 100. time step for flow calculations.

The binary files of the previous flow calculation are used as input files for dispersal simulations.

The binary files contain all the coordinates and building configurations, the distribution of roughness, and the positions and intensities of the pollutant sources, respectively. The complete wind field and the field of the pressure disturbance are additionally saved in the files *.ZWU, the diffusion coefficients, the kinetic turbulence energy, and the turbulent energy dissipation in the files ***.ZWT**.

A "readable" result output is additionally given in the form of ASCII tables.

The Cartesian wind components, the amount of wind velocity as well as the pressure disturbance are saved in form of horizontal cross sections in the files *.UVW. The files *.TUR contain the variables of the turbulence model (diffusion coefficient turbulence energy, and energy dissipation). The calculated mass concentrations are finally saved in the files ***.KON**.

A scaling is performed for all output values except the wind components. The scaling results in the domain maximum of each variable being printed to the file as a four digit number. The wind components as well as the value of the wind velocity are saved in mm/s.

To control the program, log files *.PRS (flow model) or *.PRA (dispersion model) are produced, where all information is saved about the simulation run (input and output files, parameter values, information about the calculated time-steps).

5.8.4 Control output

The logging of flow calculations was considerably improved already in MISKAM 5. The logs are controlled by the file **MISKAM.PRO**, which has to be located in the MISKAM directory.

If MISKAM.PRO does not exist, the log file NAME.PRS is normally generated. If MIS-KAM.PRO exists regardless of its content, a detailed protocol is generated with the name NAME.PRS. Besides the maximal residual divergence, the individual changes of the wind components, as well as the turbulent diffusion coefficient together with their respective grid positions are also given in the table. To add this detailed logging is useful, if convergence problems arise which still cannot be excluded for complex, extensive building configurations.

Time series of model variables at individual grid points can be used as a further online-control. The file **MISKAM.CTR** in the MISKAM directory is needed for this purpose. The grid point indices of up to nine grid points can be listed in this file, the time series of u, v, w, p', E, ε ,

and K_m are then written to a file **CONTROL-n.OUT**. The files are numbered, the **n**-th file contains the results of the **n**-th grid point of the input file **MISKAM.CTR**.

```
# MISKAM-Control
 _____
#
#
# Up to 9 tripels (i,j,k) can be set,
# indices must be entered flush right as four digit numbers.
#
 25
      7
         10
  25
      8
         12
  25
      9 11
# END
```

Figure 5.8: File **MISKAM.CTR** to control time series, as an example of three grid points.

5.9 Utilities

5.9.1 KONFIG: Interactive setting of configuration files

The program **KONFIG** belonging to MISKAM allows the generation of the INP files without the detour via an ASCII-editor. However, it is currently only possible to set the roughness length in this way, the setting of inhomogeneous surfaces has to be done by hand in the INP file afterwards.

KONFIG is a dialog program which successively prompts the necessary information to construct a MISKAM-suited input file. An extensive plausibility verification of the required data is performed. The following settings are rejected or questioned:

- Not strictly monotonic increasing coordinates of cell walls (new setting is required)
- Change of the grid resolution from one to the next cell by more than a factor of 2 (program asks, whether the user is sure about the setting)
- Only two free grid boxes above an obstacle (new setting is required)
- Less than 6 free grid boxes above an obstacle (program asks, whether the user is sure about the setting)

5.9.2 MISVIS: Visualization of MISKAM results

The previous versions of MISKAM used rudimentary graphic functions provided by MS-DOS to visualize model results and input files. Since the needed program libraries are not available any longer, a new visualization program became necessary with the introduction of pure 32-Bit Windows environments. The result of this development by **giese-eichhorn** is MISVIS. The graphic library DISLIN² was used.

MISVIS can be purchased from giese-eichhorn either as 32Bit or 64Bit version.

MISVIS reads the binary files (*.ZWU *.ZWT *.ZWK) and allows graphic display of the following data:

- three-dimensional view of the building configuration from various view points. When dispersal simulations are evaluated, positions of sources are additionally displayed.
- flow simulations:
 - wind vectors
 - contour plots of Cartesian wind components
 - contour plots of total velocity
 - contour plots of pressure disturbance
 - stream lines
 - contour plots of diffusion coeffizients
 - contour plots of turbulent kinetic energy
 - contour plots of turbulent energy dissipation
- dispersal simulations
 - contour plots of additional pollution due to sources within model domain
 - contour plots of total concentration, including background
 - contour plots of mass deposited on the ground

All plots can be created for horizontal as well as vertical (x - z or y - z) cross sections, either showing the complete plane or zoomed-in excerpts to be specified by the user.

The following figures show a screenshot of MISVIS as well as examples of various visualisations.

| 5.9. | D. Utilities | |
|------|--------------|--|
|------|--------------|--|

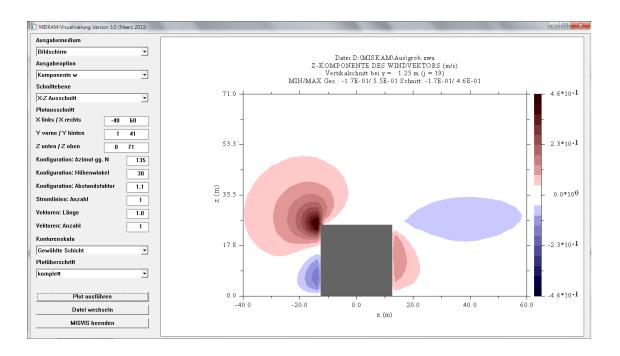


Figure 5.9: Screenshot of the program MISVIS, showing a zoomed plot of vertical wind speed for flow over a single obstacle.

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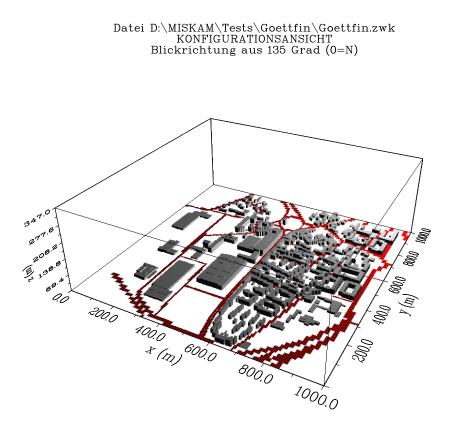
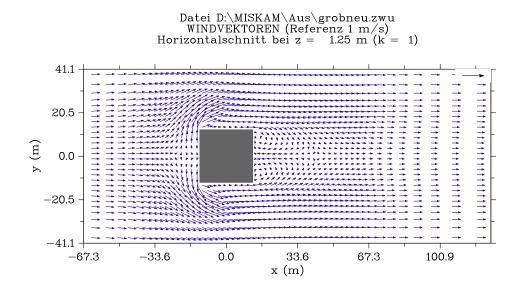


Figure 5.10: Example of MISVIS visualization: 3D-plot of a configuration file, i.e. Göttinger Straße, Hannover.

| 5.9. | Utilities | | | |
|------|-----------|--|--|--|
|------|-----------|--|--|--|

(a)



(b)

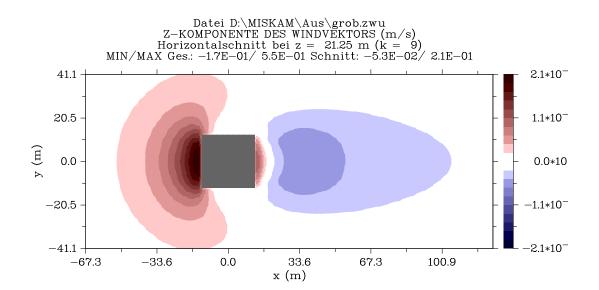


Figure 5.11: Example of MISVIS visualization: wind vectors (a) and vertical wind component (b) for flow around a single obstacle.

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|----|------------------------|
|----|------------------------|

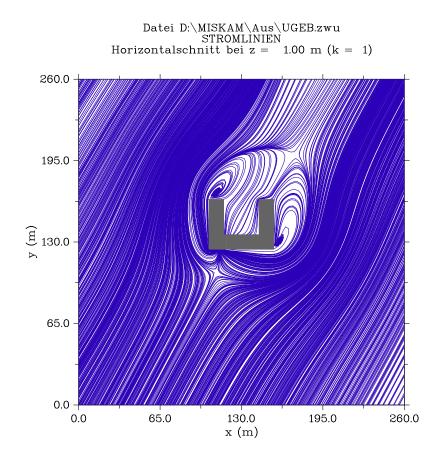


Figure 5.12: Example of MISVIS visualization: stream lines for flow around a single obstacle.

| 5.9. | 9. Utilities | |
|------|--------------|--|
|------|--------------|--|

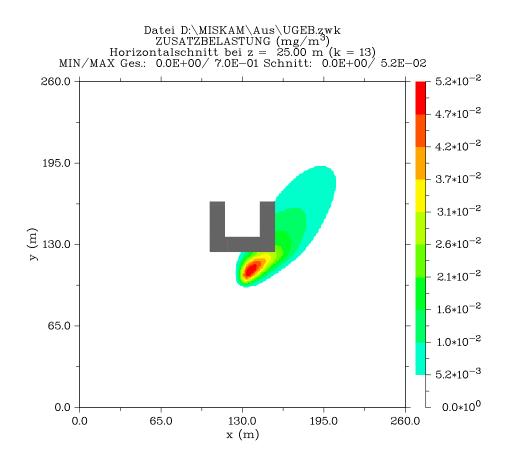


Figure 5.13: Example of MISVIS visualization: dispersal of a tracer released from a point source downwind of a single obstacle.

6.1 Preliminary remarks

An important aspect of the assessment of a numerical model's quality is the unambiguity and reliability of its results. The VDI guideline 3783/9 "Environmental meteorology – Prognostic microscale windfield models – Evaluation for flow around buildings and obstacles" supplies a comprehensive package of validation measures for flow models. MISKAM was subject to all checks required by the guideline and applicable to MISKAM, the model meets the given criteria for a successfull validation.

The MISKAM CD includes results of all simulations according to VDI guideline 3783/9. This section lists the resulting hit rates. The wind tunnel data are part of the copyright protected guideline and therefore cannot be published in this place. The guideline can be purchased via VDI from the publisher *Beuth-Verlag* (http://www.beuth.de).

An evaluation of the dispersal model of comparable completeness does not yet exist. Results of the comparison of MISKAM simulations and the wind tunnel data for the Mock Urban Setting Test (MUST), however, can be found in the publication by Balczo and Eichhorn (2009).

6.2 Validation according to VDI-RL 3783/9

The validation simulations are subdivided into consistency checks and comparisons to wind tunnel data. The test cases listed below are part of the guideline. The model results are located in sub-folders of the folder VALIDIERUNG on the MISKAM CD. The sub-folders are named according to the test case identifiers as given by the guideline. For a detailed description of the test cases (grid, obstacle configurations etc.) the reader is referred to the guideline.

Hit rates as achieved by MISKAM are gathered for all test cases in two tables at the end of this section.

All computations, except the homogeneity checks (B1-6) have been carried out using upstream advection as well as the combination of MacCormack and MPDATA advection, the files containing the results have been named accordingly. The hit rates listed in the tables refer to upstream advection, changes due to the refined advection schemes are insignificant (see Eichhorn, 2009).

For the simulations of flow over a beam (A1, A2, C1, C2) minor deviations from the require-

ments of the guideline have been introduced. Instead of a 3D simulation with an infinitely wide obstacle perpendicular to the flow direction, the 2D version of MISKAM has been used. By preceding test simulations it has been proven that MISKAM yields identical results for the 2D and 3D case. This justifies the use of the 2D version, resulting in far less computer time required for the test cases.

6.2.1 Consistency checks

Test case A1: Scalability Flow over a twodimensional beam is simulated for two different inflow velocities (1 m/s resp. 10 m/s in reference height). Ideally, the results should differ exactly by a factor of 10, an agreement with a maximum relative deviation of 5 % is required for at least 95 % of the grid points.

A2: Stationarity The check is based on the reference run of A1. To check if stationarity of the reference run is sufficient, the same flow is simulated with the number of timesteps doubled compared to the reference run. Again, 95 % of the grid points shall agree with a relative deviation less than 5 %.

A3: Symmetry, independence on grid resolution Two simulations of flow around a cube are carried out for different grid resolutions (2.5 m resp. 1.25 m near the obstacle). The run with coarse grid resolution serves as a check of the symmetry of results (A3-1). To examine independence on grid resolution, results of the run with fine resolution are interpolated to the coarse grid to compare the results of both runs (A3-2). For both parts of this test case the same criteria as for cases A1 and A2 are applied.

A4: Grid orientation A diagonal flow around a cube is simulated twice, first by rotating the inflow, then by rotating the grid. Results should agree to a large extent. To account for the uneven numerical diffusion depending on grid orientation, a less stringent criterion (66 % agreement with less then 25 % relative deviation) is adopted for this case.

B1 - B6: Homogeneity Wind fields over homogeneous terrain without obstacles must be stationary and independent on wind direction. To check this, simulations for a domain without obstacles are carried out for six different inflow directions. Identical results for all directions are required, the same criteria as for all previous cases except A4 are applied.

Hit rates as achieved by MISKAM are gathered in table 6.1. In addition to the allowed relative deviations already mentioned, for each case the allowed absolute deviation between reference and comparative run is listed.

| | | Hit ı | rates | | | |
|-----------|------|-------|-------|-----|-----|-------|
| Test case | D | W | u | v | w | K_m |
| B1 – B6 | 0.05 | 0.01 | 100 | 100 | ./. | 100 |
| A1 | 0.05 | 0.01 | 100 | ./. | 100 | ./. |
| A2 | 0.05 | 0.01 | 100 | ./. | 100 | ./. |
| A3-1 | 0.05 | 0.01 | 100 | ./. | 100 | ./. |
| A3-2 | 0.05 | 0.05 | 99 | 100 | 99 | ./. |
| A4 | 0.25 | 0.06 | 82 | 79 | 87 | ./. |

Table 6.1: Hit rates (%) for consistency checks. D ist the allowed relative deviation, W the allowed absolute deviation between reference and comparative values. Required hit rate is 66 % for case A4, 95 % for all other cases.

Comparison to wind tunnel data 6.2.2

The comparisons to wind tunnel data are based, in part, on simulations already carried out for the consistency checks. For all comparisons, a hit rate of 66 % with a maximum relative deviation of 25 % is required. The allowed absolute deviation is given as the repeatability of the wind tunnel data as specified in the corresponding data set, values are given in table 6.2.

The wind tunnel data supplied with the guideline are based on the freely available CEDVAL¹ data published by the Meteorological Institute of the University of Hamburg.

C1: Flow over a beam 1 For this case, the reference run of case A1 / A2 is used and compared point by point with wind tunnel data.

C2: Flow over a beam 2 Since the available wind tunnel data set proved unsuitable, the test case was reduced to a comparison of the extent of the flow separation zone. For case C2 with a reduced surface roughness compared to C1, a larger lee vortex must be simulated.

C3: Flow around a cube, 270° For this case, the simulation for A3 (coarse grid) is used.

C4: Flow around a cube, 225° This case adopts the results of case A4.

C5: Flow around a cuboid, 270° New simulation, not included in consistency checks.

C6: Array of 21 obstacles, 270° New simulation with modified set-up. The simulations for single obstacles had been carried out with open lateral boundaries. For this case, to ensure analogy to the wind tunnel set-up, closed lateral boundaries have been implemented.

For all cases except C6 additionally hit rates for the near field immediately surrounding the obstacle are given, for details see the guideline.

¹http://www.mi.uni-hamburg.de/CEDVAL-Val.427.0.html

For case C4 the comparatively low near field hit rate of the lateral wind component is noticed. A thorough examination of the wind tunnel data revealed that the flow was not oriented exactly diagonally. For both, a rotation of the inflow profile and a rotation of the measured vectors, an improvement of the hit rate resulting in fulfillment of the guideline is achieved.

| | | | | Hit rates | |
|-----------|------|------|---------|-----------|---------|
| Test case | D | W | u | v | w |
| C1 | 0.25 | 0.06 | 87 (71) | ./. | 95 (90) |
| C3 | 0.25 | 0.06 | 93 (90) | 97 (95) | 93 (89) |
| C4 | 0.25 | 0.07 | 84 (74) | 76 (63) | 80 (66) |
| C4-1 | 0.25 | 0.07 | 84 (74) | 79 (66) | 81 (66) |
| C4-2 | 0.25 | 0.07 | 84 (76) | 81 (68) | 81 (67) |
| C5 | 0.25 | 0.07 | 77 (74) | 90 (86) | 87 (79) |
| C6 | 0.25 | 0.10 | 93 | 66 | 81 |

Table 6.2: Hit rates (%) for comparisons with wind tunnel data. Required hit rate: 66 % for all test cases. Values for near field (except case C6) in brackets. C4-1: measured wind vectors rotated by 2°; C4-2: simulated inflow direction 223°.

7 Literature

- Balczó, M. und J. Eichhorn, 2009: Refined MISKAM simulations of the Mock Urban Setting Test. Proceedings of the XXIII. MicroCAD International Scientific Conference, Miskolc / Hungary, pp. 7-12; ISBN 978-963-661-866-7.
- **Douglas, J. und H. Rachford, 1956:** On the numerical solution of heat conduction problems in two and three space variables. *Trans. Amer. Math. Soc.*, **82**, 421–439.
- **Eichhorn, J., 1989:** Entwicklung und Anwendung eines dreidimensionalen mikroskaligen Stadtklima-Modells. Dissertation, Universität Mainz.
- **Eichhorn, J., 1996:** Validation of a microscale pollution dispersal model. In: *Air Pollution Modeling and its Application IX*, Plenum PRess, New York.
- Eichhorn, J., K. Cui, M. Flender, T. Kandlbinder, W.-G. Panhans, R. Ries, J. Siebert, T. Trautmann, N. Wedi und W.G. Zdunkowski, 1997: A three-dimensional viscous topography mesoscale model. *Beitr. Phys. Atmosph.*, 70/4, 301–317.
- **Eichhorn, J., 2003:** Numerical Simulation of Effects of Roof Shape on Microscale Flow: Extension of the Numerical Model MISCAM. 4th International Conference on Urban Air Quality, Prague/Czech Republic).
- **Eichhorn, J., 2009:** Modell-Evaluierung nach VDI-RL 3783/9 und COST 732 Erfahrungen mit MISKAM, METTOOLS VII, Hamburg/Germany.
- **Eichhorn, J. und A. Kniffka, 2010:** The Numerical Flow Model MISKAM: State of Development and Evaluation of the Basic Version. *Meteorol. Zeitschrift*, **19/1**, 81–90.
- **Green, S.R., 1992:** Modeling turbulent air flow in a stand of widely-spaced trees. The PHOENICS Journal of Computational Fluid Dynamics and its Application 5, 294–312, Wimbledon.
- **Groß, G., 1993:** Numerical Simulation of Canopy Flows (Springer Series in Physical Environment), Springer-Verlag, Heidelberg.
- Kato, M. und B.E. Launder, 1993: The modelling of turbulent flow around stationary and vibrating square cylinders. Proceedings of the 9th Symposium on Turbulent Shear Flows, Kyoto, August 1993, pp. 10.4.1-10.4.6.

- Lauerbach, H. und J. Eichhorn, 2004: Flow Through Decidious Tree Crowns Comparison of Measurements and High Resolution Numerical Modelling. NATO Advanced Study Institute "'Flow and Transport Processes in Complex Obstructed Geometries"', 4–15 Mai 2004, Kiew, Ukraine.
- Lopez, S.D., Lüpkes, C. und K.H. Schlünzen, 2005: The effect of different $k \varepsilon$ closures on the results of a microscale model for the flow in the obstacle layer. *Meteorol. Zeitschrift*, 14, 839–848.
- Panhans, W. G. und R. Schrodin, 1980: A one-dimensional circulation and climate model and its application to the lower atmosphere. *Beitr. Phys. Atmosph.*, **53**, 264–294.
- Paterson, D. A. und C. J. Apelt, 1986: Computation of wind flows over three-dimensio"nal buildings. J. of Wind Engineering and Industrial Aerodynamics, 24, 193–213.
- Paterson, D. A. und C. J. Apelt, 1986: Simulation of wind flow around three-dimensio"nal buildings. *Building and Environment*, 24, 39–50.
- Patrinos, A. N. A. und A. L. Kistler, 1977: A numerical study of the Chicago lake breeze. Boundary Layer Meteor., 12, 93–123.
- Ramanathan, N., K. Srinivasan und B. V. Seshasayee, 1995: Numerical simulation of boundary layer variables using *e*-*ε* closure scheme. *J. Appl. Meteor.*, **34**, 542–548.
- Röckle, R. und C. J. Richter, 1995: Ermittlung des Strömungs- und Konzentrationsfeldes im Nahfeld typischer Gebäudekonfigurationen - Modellrechnungen. Abschlussbericht PEF 92/007/02, Forschungszentrum Karlsruhe.
- **Rodi, W., 1980:** Turbulence Models and Their Application in Hydraulics A State of the Art Review. Iahr Monograph Series, A. A. Balkema, Delft.
- Smolarkiewicz, P. K. und W. W. Grabowski, 1989: The multidimensional positive definite advection transport algorithm: Nonoscillatory option. J. Compu. Physics, 86, 355–375.
- VDI, 2005: Umweltmeteorologie Prognostische mikroskalige Windfeldmodelle Evaluierung für Gebäude- und Hindernisumströmung. – VDI-Richtlinie 3783, Blatt 9; Beuth-Verlag, Berlin, 53 pp.
- Yee, E., Biltoft, C.A., 2004: Concentration fluctuation measurements in a plume dispersing through a regular array of obstacles. – *Boundary-Layer Meteorol.*, **111**, 363–415.