

AUSTAL2000

Program Documentation of Version 2.6

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www.austal2000.de

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Changes in the program description

Changes to the program description of 2011-08-01:

- 2014-03-10 Some equation numbers in the Annexes adjusted.
- 2014-02-24 Implementation of the program update 2.6 (see the update information).

Update information of version 2.6

Major changes with respect to the last distribution 2.5:

- Substance parameters and some model parameters are placed in the external settings file `austal2000.settings`. Changes of parameters therefore do not demand recompilation of the programs. See Section B.4.
- Additional gaseous substance `hg0` (elementary mercury with the deposition velocity 0.0003 m/s).
- The log file contains the check sums of different files used in the dispersion calculation. This allows to reconstruct at a later time which programs and files have been used. This applies to:
 - Programs AUSTAL2000, TALDIA, and VDISP.
 - Depending on the project: time series, AKTerm, or AKS.
 - Applied roughness length cataster (as before).
 - Settings file `austal2000.settings`.

For DMN files, the check sum refers to the binary data part, for other files to the file contents.

- The program aborts if parameters are applied that require option `NOSTANDARD` without this option being set.
- Calm conditions should be specified in an AKTerm by both wind speed and wind direction 0. The program identifies calm conditions by wind speed 0 and gives a warning if data lines with wind speed 0 and wind direction larger 0 or vice versa are encountered.
- In the head of DMNA output files names and values are separated by blanks only (no use of tabulators).
- The definition files written into the temporary working directory `work` have the names `meteo.def` instead of `wetter.def` and `variable.def` instead of `variabel.ztr` and, as before, `param.def`.

- Problem 2013-01-11 resolved: The decimal separator in all output files is a point (drop of program option -A and input parameter 1c).
- Problem 2012-07-29 resolved: The character encoding specified in the first line of the latin1 language packages (files with extension `latin1.nls`) has been corrected.
- Problem 2003-02-14 resolved: Program VDISP was modified such that input and output is not written to the root directory but to the project directory. This avoids mixing up of these files if several program runs are carried out in parallel.

1 Overview

The program system AUSTAL2000 calculates the atmospheric dispersion of substances and odorants. AUSTAL2000 is a reference implementation of the instructions given in Annex 3 of the German Regulation on Air Quality Control (*TA Luft*).¹ The model on which AUSTAL2000 is based is described in guideline VDI 3945 Part 3.² This document describes version 2.6 of the program system.

Note: Proper use of the program system requires expert knowledge in TA Luft and immission prediction. Beside this manual, guideline VDI 3783 Part 13 provides further useful information.

The copyright holders of the program system are Janicke Consulting, 88662 Überlingen (Germany), and the Federal Environmental Agency (UBA), 06813 Dessau-Roßlau (Germany). Program and source code are provided free of charge. They are subject to the GNU PUBLIC LICENCE.

Note: Comments, suggestions, and questions should be send via email to info@austal2000.de. The analysis of an error report requires the complete set of data that have been used in the calculation, preferably in compressed form.

Executables (32-bit) are provided for Windows and Linux, including the complete source code (web site www.austal2000.de, German/English). The programs have been developed and tested under Windows (XP/Vista/7) and Linux (SUSE and Ubuntu).

The program system implements the following features:

- Calculation based on a time series
- Calculation based on a dispersion class statistics
- All substances for which limit values are given in the *TA Luft*
- Point, line, area, and volume sources
- Plume rise (explicitly or according to guidelines VDI 3782 Part 3 or VDI 3784 Part 2)
- Conversion of NO to NO₂ (according to guideline VDI 3782 Part 1)
- Dry deposition
- Gravitational settling of dust
- Calculation of odor hours according to the German guideline on odor immission (GIRL)

¹See <http://www.bmu.de/fileadmin/bmu-import/files/pdfs/allgemein/application/pdf/taluft.pdf> (link checked 2014-01-28).

²See Association of German Engineers (VDI), www.vdi.de (German/English).

- Rated odor substances
- Time-dependent emission parameters
- Situation-dependent emission parameters
- Estimate of the statistical uncertainty
- Automatic definition of the calculation grid
- Automatic derivation of the surface roughness length
- Meteorological time series (AKTerm) in the format provided by the German Weather Service (DWD)
- Extraction of the appropriate anemometer height as provided in the AKTerm
- Results for a grid of receptor points
- Time series of the additional load at given receptor points
- Characteristic immission values of the additional load
- Characteristic immission values of the total load from the time series of additional and background load
- Structured terrain
- Flow around buildings
- Automatic definition of nested calculation grids for calculations with buildings
- Verification according to guideline VDI 3945 Part 3

Note: VDI guidelines define generally agreed standards in Germany. They are bilingual (German/English) and can be ordered from the VDI (web site www.vdi.de).

The calculation of three-dimensional wind fields in case of terrain profile and/or buildings is carried out by the diagnostic wind field model *TALdia*.³

The calculation of plume rise according to guideline VDI 3784 Part 2 (*dispersion calculation for releases from cooling towers*) requires the auxiliary program *VDISP*. The program version provided within this distribution should be used.⁴

³Project *Enhancement of a diagnostic wind field model for licensing industrial facilities (TA Luft)*, Federal Environmental Agency, Project ID 203 43 256, see www.austal2000.de (German/English).

⁴A Windows version can also be obtained free of charge from the VDI, see web page www.vdi.de/vdisp. However, it applies the root directory and not the project directory for input and output.

Note: In view of the German regulations, the following naming conventions are applied: immission (Immission) as opposed to emission refers to concentration, deposition, or odor perception; limit immission value (Immissionswert) refers to the limit value of a quantity; characteristic immission value (Immissionskennwert) refers to the calculated value that is compared to the corresponding limit immission value.

The results of a dispersion calculation for odorants⁵ must be usually projected onto assessment areas according to guideline GIRL. The program A2KArea is provided for this task, see www.austal2000g.de (German). Installation (JAVA program) and usage are explained in a separate document.

⁵On behalf of: Landesanstalt für Umweltschutz (Karlsruhe; current name: Landesanstalt für Umwelt, Messungen und Naturschutz), Niedersächsisches Landesamt für Ökologie (Hildesheim; current name: Staatliches Gewerbeaufsichtsamt), Landesumweltamt NRW (Essen; current name: Landesamt für Natur, Umwelt und Verbraucherschutz). Report: JANICKE, L., JANICKE, U.: *The development of the dispersion model AUSTAL2000G* (German), Reports on Environmental Physics, No. 5, ISSN 1439-8222, Edt. Janicke Consulting, Überlingen (August 2004), see www.janicke.de.

2 Installation

A set of archives is required that can be downloaded at the web site www.austal2000.de free of charge. The following packages are provided:

<i>Base packages (see Section 2, Annexes C and B.3)</i>	
<code>a2k-vers-programs-sys_en.zip</code>	Programs AUSTAL2000, TALdia, VDISP and batch files for system <code>sys</code>
<code>a2k-vers-manual_en.zip</code>	Program documentation of AUSTAL2000
<code>a2k-vers-z0-register.zip</code>	Roughness length register for Germany (CORINE 2006) in Gauß-Krüger coordinates (3rd stripe) and UTM coordinates (zone 32)
<i>Application packages (see Section 4 and Annex A)</i>	
<code>a2k-vers-examples_en.zip</code>	Example calculations and results
<code>a2k-vers-verification.zip</code>	Verification tests and results
<code>ViewLuc-vers.zip</code>	Program and data for inspecting the registers
<i>Additional language extensions and developer packages (see Section 2.1/2.2 and Annex C)</i>	
<code>a2k-vers-nls_de.zip</code>	German language package in UTF8
<code>a2k-vers-nls_de@latin1.zip</code>	German language package in ISO-8859-1
<code>a2k-vers-nls_en.zip</code>	English language package in UTF8
<code>a2k-vers-nls_en@latin1.zip</code>	English language package in ISO-8859-1
<code>a2k-vers-programs-sys_en.zip</code>	Programs compiled with GNU-C
<code>a2k-vers-source.zip</code>	Source codes of all programs
<code>a2k-vers-source_de.zip</code>	German language files (for compilation) in UTF8
<code>a2k-vers-source_en.zip</code>	English language files (for compilation) in UTF8
<i>Other information</i>	
<code>a2k-vers-report_de.zip</code>	Project report of AUSTAL2000
<code>dmk-vers-report_en.zip</code>	Project report of TALdia
<code>a2k-vers-validation_de.zip</code>	Validation tests (see project report)
<code>dmk-vers-validation_de.zip</code>	Validation tests for TALdia (see TALdia project report)
<code>a2k-vers-test-area_de.zip</code>	Tests for a large area source (see project report)
<code>a2k-vers-test-scatter_de.zip</code>	Tests for the statistical uncertainty (see project report)
<code>a2k-vers-test-dust_de.zip</code>	Tests for the NOSTANDARD option SPECTRUM (see Annex E)
<code>a2k-vers-test-spread_de.zip</code>	Tests for the NOSTANDARD option SPREAD (see Annex F)
<code>a2k-vers-test-prfmod_de.zip</code>	Tests for the NOSTANDARD option PRFMOD (see Annex H)

Minimum requirement are the base packages. The program requires the settings file `austal2000.settings` which must be located in the same directory as the program. If the roughness length is explicitly stated, a roughness length register is not required.

Note: The settings file should not be modified. The program checks if its contents agree with the official distribution and gives a warning if this is not the case.

The current version *vers* by 2014-06-26 is 2.6.11. The executable programs are provided for the following systems:

<i>sys</i>	System	<i>K</i>
windows	Windows 7/Vista/XP, compiled with Intel-C 13.0 (optimized)	WI-x
linux	Linux, compiled with Intel-C 13.0 (optimized)	LI-x
windows-gcc	Windows 7/Vista/XP, compiled with GNU-C 4.5 (not optimized)	WG-0
linux-gcc	Linux, compiled with GNU-C 4.4 (not optimized)	LG-0

Note: A GNU version is considerably slower than an optimized Intel version and primarily serves as a reference. Annex C contains some performance comparisons.

Programs created with different compiler versions can yield in rare cases slightly different results (however, always within the given statistical uncertainty). Therefore the tag *K* that indicates the applied compiler is listed in the log file in addition to the program version.

2.1 Windows

1. Create a directory into which AUSTAL2000 is to be installed (main directory). The name is arbitrary, in the following it is referred to as *A2K*.
2. Copy the downloaded archives to *A2K*.
3. Select the archive with the desired compiler version and decompress the required archives to *A2K*, preserving the path information given in the archives. The programs *AUSTAL2000*, *TALdia*, *VDISP*, the settings file, and the language packages (*latin1*) are copied during extraction directly to *A2K*.
4. In case you require a language package different from the one installed in the previous step: Delete these packages from the program directory, decompress into it the archive with the desired language packages, and finally copy the language packages from the uncompressed subdirectory *nls\LanguagePackage* to the program directory.

This is all the installation. No changes to the system or entries into the registry are made. The archives can be deleted after installation. For deinstallation, simply delete the complete directory *A2K*.

2.2 Linux

1. Create a directory into which AUSTAL2000 is to be installed (main directory). The name is arbitrary, in the following it is referred to as *A2K*.
2. Copy the downloaded archives to *A2K*.
3. Select the archive with the desired compiler version and decompress the required archives to *A2K*, e.g.

```
lj@linde:/a2k > unzip a2k-2.6.11-programs-linux
```

The programs *AUSTAL2000*, *TALdia*, *VDISP*, the settings file, and the language packages (`utf8`) are copied during extraction directly to *A2K*.

4. In case you require a language package different from the one installed in the previous step:⁶ Delete these packages from the program directory, decompress into it the archive with the desired language packages, and finally copy the language packages from the uncompressed subdirectory `nls\LanguagePackage` to the program directory.

This is all the installation. The archives can be deleted after installation. For deinstallation, simply delete the complete directory *A2K*.

⁶Note which encoding is used by your operating system. It can be seen from the default settings of the editor or the console. It might be necessary to replace the UTF8 language packages for example by those given in ISO-8859-1.

2.3 Directory tree

The directory tree of the installed files has the following structure:

```
A2K/  
A2K/austal2000.exe  
A2K/austal2000.settings  
A2K/A2K_de@latin1.nls  
...  
A2K/nls/  
A2K/nls/de@latin1/  
A2K/nls/de@latin1/A2K_de@latin1.nls  
...  
A2K/test/  
A2K/test/anonym.aks  
A2K/test/simple/  
A2K/test/simple/austal2000.txt  
...  
A2K/verif/  
A2K/verif/verify.bat  
A2K/verif/evaluate.bat  
A2K/verif/verif00.exe  
A2K/verif/00/  
A2K/verif/00/austal2000.txt  
...
```

3 Usage

The following instructions refer to the Windows version of the program system. For the Linux version, the differences are so minor that they are not addressed.

The program *AUSTAL2000* works non-interactively. Before the calculation, all input data must be provided in the project directory (see Section 3.1). Then the program is started by the user and the calculation runs without further interaction. The results are stored to the project directory (see Section 3.2) and the calculation process is logged to a log file.

Note: Section 4.1 contains a simple example calculation.

The program is started in a DOS shell. Such a shell can be opened with the Windows menu Start/Programs/Accessories/Command Prompt

Make *A2K* the current directory. Then the program is started with the command

```
austal2000 [-D] Project [Option]
```

where *Project* is the name of the project directory that has been created before. For the directory path under Windows, either a slash (/) or a backslash (\) may be used.

Without options, the program carries out a dispersion calculation. Otherwise one of the following actions is performed, depending on the selected option:

- a Re-evaluates results of a completed dispersion calculation, in particular the time series at receptor points (see Section 3.4).
- D If this option is applied as first argument in the program call: deletes contents of an existing log file before use; otherwise, log information is appended to the existing file.
- h Displays a help information with the available program options.
- help Displays all input parameters that can be set in file `austal2000.txt`.
- z If a calculation based on a time series is planned: converts a meteo file given in AKTerm format into the time series file `series.dma`. This file can then be edited in respect of further time-dependent parameters (see Section 3.4).

The following options are available in addition:⁷

--language=*lan* Forces the language package *lan* to be used.

It can be located either directly in the program directory or therein in subdirectory `nls\lan`. If *lan* is simply a minus sign (i.e. --language=-), then no language package is loaded even if one exists in the program directory.

⁷Non-documented options, that can effect the result and exist for test purposes only, are: -J, -x.

- l Creates a wind field library (see Section 3.6) in case of complex terrain or buildings. No dispersion calculation is carried out. If a wind field library already exists, it is deleted after confirmation by the user.
- p Protocols in case of a calculation for flat terrain without buildings the applied one-dimensional boundary layer profiles of each time interval to the file `austal2000.log`. For calculations with terrain or buildings, the applied base fields of the wind field library are listed.
- vLevel Sets the verbose level that controls the amount of program information being written to the log file. Default is level 3. The higher the level, the more information is written out.
- X0 Suppresses re-encoding to codepage 850. By default, screen output for language packages de@latin1 is recoded to the console default codepage 850.

3.1 Input data for the dispersion calculation

The calculation is carried out in a Cartesian coordinate system, where the x -axis runs from West to East and the y -axis from South to North. All length and coordinate specifications are in metres and refer to this coordinate system. For each project, the absolute position of the coordinate systems origin is set by the user, either in a Gauß-Krüger coordinate system (parameters `gx` and `gy`) or in a UTM coordinate system (parameters `ux` and `uy`). For practical reasons the origin should be chosen close to the centre of emissions.

Note: The parameters `gx` and `gy` respectively `ux` and `uy` are the only absolute coordinates. All other coordinate specifications may not exceed an absolute value of 200 000 (see Section 3.3).

The calculation grid is of rectangular shape with constant cell size in the horizontal and increasing cell size in the vertical (z -axis). A set of nested grids can be used with the same vertical spacing but different extents and cell sizes in the horizontal (see Section 3.8).

The following files are required:

1. text file `austal2000.txt` with the main input parameters such as emission sources and emission strengths (in the project directory).
2. A meteorological time series or a dispersion class statistics (path information provided in `austal2000.txt`).
3. For time-dependent emission parameters: time series of parameter values in file `series.dmna` (in the project directory).
4. For case-dependent parameters (in combination with a dispersion class statistics, see Section 3.5): for each parameter a DMNA file with the case-dependent values (in the project directory).

5. For an automatic calculation of the roughness length z_0 : The register of roughness lengths in the main directory of *AUSTAL2000* (file `z0-gk.dmn` for Gauß-Krüger coordinates respectively `z0-utm.dmn` for UTM coordinates).
6. For complex terrain: The terrain profile of the applied calculation area in the file `zg00.dmn` (in the project directory). It can be automatically created from a given digital elevation model (path information provided in `austal2000.txt`).

The input for *AUSTAL2000* is at minimum the text file `austal2000.txt` and either a meteorological time series (AKTerm) or a dispersion class statistics (AKS). Both are provided for example by the National Weather Service (DWD in Germany).

For test purposes, the DWD provides five time series for five subsequent years (files `anno95.akt` to `anno99.akt` and, in the new AKTerm format, files `anno95.akterm` to `anno99.akterm`) and a corresponding AKS over this period (file `anonym.aks`). These files are part of the example packages of *AUSTAL2000*.

Instead of an AKTerm, the meteorological time series may be directly provided as file `series.dmn`, optionally including the time series of other time-dependent parameters. Further details are given in Section 3.4.

For calculations with a terrain profile, file(s) `zg0l.dmn` (grid level l , $l = 0$ without nesting) with the terrain profile are required. Each file contains the terrain heights at the grid points of the calculation grid (corner points of the grid cells), see Section 3.6 (and note Section 3.8).

The text file `austal2000.txt` contains all project information. The file can be created and edited with any simple Editor.⁸ When using a word-processing program care must be taken that the file is saved as a plain text file and not for example as RTF or Word document.

The input file consists of comment lines and data lines.⁹ Comment lines start with a minus sign and may appear anywhere in the text. Data lines start with the name of a parameter and, separated by a blank or a tabulator, one or more values which are assigned to this parameter.

Values may be numbers or strings. Numbers can be specified either using a decimal point or a decimal comma (1000-separators are not allowed). Strings should be enclosed in double quotes. Comments, introduced by an apostrophe, can be appended to a data line.

Numbers are given in the units gramme, metre, and second, the heat current in MW, the temperature in degree Celsius. This implies for example that wind speed must be specified in m/s and emission strength in g/s. Odour emissions are specified in OU/s. If a parameter is not explicitly set, its default value (see below) applies.

Time specifications have the format
year-month-day.hour:minute:second.

⁸For example *Notepad*, accessible via the menu Start/Programs/Accessories/Notepad.

⁹A line may not exceed 31996 characters.

The input text terminates at the end of the file or if a line starting with a star is encountered. An example for a simple input file is:

```
-- Example for a simple input file
-----
ti "demo-1"          ' title of the project
az "../anno95.akterm" ' time series to be used
ux 706396 ' reference point (UTM, easting)
uy 5359374 ' reference point (UTM, northing)
hq      50 ' source height (m)
-----
so2  5.56 ' emission strength (g/s)
*
```

In this example, the source is located in the centre of the calculation area which is set by the program; the average surface roughness length is calculated by the program using the register `z0-utm.dma`.

3.1.1 List of parameters

A list of all presently available input parameters and their default values is given in the following (not including emission strengths).¹⁰ The parameters are alphabetically listed, in the input file they may appear in arbitrary order. Round brackets contain the number of required values, where n_q is the number of sources, n_b the number of buildings, n_n the number of calculation grids (not exceeding 6), n_p the number of receptor points (not exceeding 20), and n_z the number of vertical layers (not exceeding 100).

A parameter value that represents a string (e.g. `ti`) may not exceed 255 characters. If the string contains blanks, it must be enclosed in quotation marks.

ab (n_b) Extension of a building in x -direction before rotation (default 0).

A building is defined as a cube that may be rotated around a vertical axis. Without rotation, **xb** and **yb** refer to the lower-left (south-west) corner of its base and **cb** is its vertical extent (the base is always at the ground); **ab** and **bb** refer to its extension in x and y -direction respectively. A counterclockwise rotation around the lower left corner is defined by **wb** (in degree).

Cylindrical buildings (e.g. cooling towers) are specified by a negative value of **bb** which then defines the diameter of the cylinder. In this case, parameter **ab** must be set to 0, **xb** and **yb** define the centre of the base, and **wb** is ignored.

aq (n_q) Extension of a source in x -direction before rotation (default 0).

¹⁰Additional parameters which may influence the calculation results and are solely designed for test purposes (and require the NOSTANDARD option) are: **hm**, **ie**, **im**, **mh**, **x1**, **x2**, **x3**, **y1**, **y2**, **y3**.

A source is defined as a cube that may be rotated around a vertical axis. Without rotation, x_q and y_q refer to the lower-left (south-west) corner of its base and h_q its distance from the ground; a_q , b_q , and c_q refer to its extension in x , y , and z -direction respectively. A counterclockwise rotation around the lower left corner is defined by w_q (in degree).

as (1) Name of the dispersion class statistics (AKS).

If the AKS is not located in the project directory, then either the path relative to the project directory or the absolute path must be included. Examples:

```
as anonym.aks      ' file located in the project directory
as ../anonym.aks   ' file located in the projects parent directory
as f:/aks/anonym.aks ' file located on a different drive
```

If the project directory does not contain the time series file `series.dmna` (see Section 3.4), then either a statistics (using `as`) or a AKTerm (using `az`) must be specified.

az (1) Name of the meteorological time series (AKTerm), see `as`.

bb (n_b) Extension of a building in y -direction before rotation (default 0), see `ab`.

bq (n_q) Extension of a source in y -direction before rotation (default 0), see `aq`.

cb (n_b) Vertical extension of a building (default 0), see `ab`.

cq (n_q) Vertical extension of a source (default 0), see `aq`.

d0 (1) Displacement height d_0 of the meteorological profiles (default $6z_0$).

dd (n_n) Horizontal cell size of the calculation grid.

The default value automatically applied by the program is for calculations without buildings given by the smallest average source height $h_q + 0.5 * c_q$, with a minimum of 16 m.

The calculation grid consists of n_x cells in x -direction starting at x_0 , analogously in y -direction. If location and extent of the calculation area is not specified, it is set for calculations without buildings such that, for each source, a circle around the source with a diameter of 50 times the mean source height (minimum 1000 m) is fully inside the area. With buildings, nested grids are applied by default, here location and extent of the grids are set according to the configuration of sources and buildings (see Section 3.8).

dq (n_q) Source diameter (default 0). This parameter is only evaluated for the calculation of plume rise, see `qq`.

gh (1) Name of the file that contains the digital elevation model (usually in format Arcinfo-GRID-ASCII).

The file name is only evaluated if the terrain profile `zg0l.dmna` (grid level l , $l = 0$ without nesting) does not yet exist. Otherwise the parameter is evaluated only as an

indication of whether the calculation should be carried out for complex terrain or not. In this case a star as parameter value is sufficient (see Section 3.6).

Note: The maximum steepness of the terrain is listed in the log file (as inclination over one horizontal cell width respectively, in brackets, over two cell widths).

gx (1) *Rechts* value of the origin of the Gauß-Krüger coordinate system.

For the calculation of z_0 , the given source coordinates are internally transformed to the stripe in which the Gauß-Krüger register (file `z0-gk.dmma`) is defined (by default the 3rd stripe), see Section B.3.

gy (1) *Hoch* value of the origin of the Gauß-Krüger coordinate system, see **gx**.

ha (1) Anemometer (measurement) height h_a above ground.

If the value of the anemometer height is explicitly given, it is used. Otherwise, in case that an AKTerm containing anemometer heights for all roughness classes is provided, the value belonging to the current class is read out and used. Otherwise the standard setting $10\text{ m} + d_0$ is applied.¹¹

hh ($n_z + 1$) Vertical grid, defined by the z -coordinates of the layer boundary points as height above ground. The default setting for calculations without buildings is

hh 0 3 6 10 16 25 40 65 100 150 200 300 400 500 600 700 800 1000 1200 1500

For the case with buildings see **qb**. This parameter is only evaluated in case option **NOSTANDARD** is set, see **os**.

hp (n_p) Height of a receptor point above ground (default 1.5).

hq (n_q) Height (lower edge) of a source above ground (no default, this parameter must be set), see **aq**.

lq (n_q) Liquid water content in kg/kg used to calculate plume rise for cooling towers (default 0).

If this parameter is specified with a value larger 0, plume rise of the according source is calculated by guideline VDI 3784 Part 2. **lq** can be specified as time-dependent.

nx (n_n) Number of grid cells in x -direction, see **dd**.

ny (n_n) Number of grid cells in y -direction, see **dd**.

¹¹ For clarification: The wind speed u for neutral stability is calculated according to *TA Luft* and guideline VDI 3783 Part 8 as follows:

$$u(z) = u_a \ln \left(\frac{z - d_0}{z_0} \right) / \ln \left(\frac{h_a - d_0}{z_0} \right) \quad \text{for } z \geq d_0 + 6z_0$$

Here, u_a is the wind speed at the anemometer (read out of the AKTerm, AKS, or `series.dmma`), z is the height above ground and h_a is the height given by parameter **ha**.

According to Annex 3 of *TA Luft*, the wind speed profile below height $d_0 + 6z_0$ is interpolated to value 0 at $z = 0$ while the other profiles are kept constant at their value for height $d_0 + 6z_0$.

nz (n_z) Number of grid cells in z -direction.

Normally, this parameter should not be specified, it is automatically set by the program. It sets the value to the maximum value n_z defined by **hh**, except for nested grids with buildings, where it is set for the finest grid such that it extends up to twice the height of the highest building.

Note: The parameter is only evaluated for nested grids with buildings. Here it must be kept in mind that particles, which leave a calculation grid, enter into the next coarser grid and that particles, which leave the coarsest grid, are discarded. Thus, in particular the value for the coarsest grid should always be set to its maximum value n_z .

os (1) Option string. Several options or assignments must be defined successively and separated by a semicolon.

For standard calculations the following options are available:

NESTING Instead of a single grid a set of nested grids with different cell sizes in the horizontal are generated (see Section 3.8).

-NESTING For calculations with buildings nested grids are omitted and a single grid is used.

SCINOTAT All calculated concentration and deposition values are written out in scientific notation (exponential format with 4 significant decimal places).

Deviations from standard require the option **NOSTANDARD**. Among others, the following settings can be made in combination with this option (see also Annex A):

BS= c_{BS} For calculations with substance **odor** respectively **odor_nnn** the value c_{BS} is applied as odor assessment threshold (default is 0.25 OU/m³).

PRFMOD The boundary layer model of guideline VDI 3783 Part 13 is modified according to the proposal discussed in the Annex of *Reports on Environmental Physics* No 7 (2011). See Annex H.

SORRELAX In the SOR procedure (successive over-relaxation) for the calculation of the flow around buildings, less stringent abort criteria are applied. For example, abort of the wind field calculation due to a poorly conditioned vertical grid spacing can possibly be avoided with this option.

SPECTRUM For gravitational settling of dust, within a given PM diameter class the particle mass is distributed equally over the diameters of this class and the settling velocity is calculated separately for each particle according to its aerodynamic diameter, see Annex E.

SPREAD The minimum value of the horizontal diffusion coefficients and thereby the minimum horizontal plume width is increased in order to avoid artificial, star-like structures in the immission distribution, see Annex F.

Note: A NOSTANDARD option should only be used where really necessary and then with the required care.

- qb** (1) Quality level for the automatic generation of calculation grids and the vertical grid for calculations with buildings (default 0).

The lowest vertical layer always extends from 0 m to 3 m. Above this, the vertical grid has a constant spacing Δz up to twice the height of the highest building. Then the spacing increases up to the second-next value of the default vertical grid (see **hh**) by 50% per interval; above that the heights of the default vertical grid are applied.¹² The finest grid has the horizontal cell size Δx . The values of Δx and Δz are set as follows:

qb	-3	-2	-1	0	1
Δx	32	16	8	4	2
Δz	6	4	3	3	2

- qq** (n_q) Heat flux M_q of the exhaust in MW (default 0), used for the calculation of plume rise.

The heat flux must be calculated from the temperature T_q (in ° Celsius) and the (wet) volume flux R (in m³/s) at standard conditions¹³ as $M_q = 1.36 \cdot 10^{-3} \cdot (T_q - T_0) \cdot R$ with $T_0 = 10^\circ$ Celsius.

If only **qq** and not **vq** is specified, plume rise is calculated including only buoyancy effects according to guideline VDI 3782 Part 3. Momentum effects are only included if both **vq** and **dq** are larger 0. **qq** can be specified as time series.

If parameter **qq** is applied (preferably for plume rise calculations according to guideline VDI 3782 Part 3) then parameter **tq** should not be used or set to 0.

- qs** (1) Quality level that determines the emission rate of simulation particles (default 0).

An increase by 1 doubles the number of used simulation particles and lowers the statistical uncertainty (standard deviation) by a factor of $1/\sqrt{2}$; on the other hand, calculation time also doubles. The corresponding applies to a reduction of the quality level. By default, an AKS calculation applies at least 43 000 000 simulation particles, an AKTerm calculation at least 63 000 000.

The range of allowed values is -4 to +4; it may be exceeded when using the option NOSTANDARD.

- rb** (1) Name of the file with rasterised building shapes (DMNA format), path information as for **as**.

Such a file can be used as an alternative to explicitly defining building shapes (see **ab**). The data part is two-dimensional and contains for each cell of a grid with constant

¹²For **qb** equal 0 and a building of height 20 m for example, the automatically generated vertical grid reads 0 3 6 9 12 15 18 21 24 27 30 33 36 39 42 46 52 65 100 150 200 300 400 500 600 700 800 1000 1200 1500.

¹³Conversion formula $R = 0.25 \cdot 3.1415926 \cdot dq \cdot vq \cdot 273.15 / (273.15 + tq)$.

vertical intervals the number (integer value) of vertical intervals that are covered by a building. The vertical interval width dz , the western edge x_0 , the southern edge y_0 , and the horizontal cell size dd of the grid must be stated in the file header. It is not required for this grid to coincide with the calculation grid; before the calculation, its cells are projected to the calculation grid like it is done with explicitly defined building shapes.

rq (n_q) Relative humidity of the plume in percent for releases out of a cooling tower (default 0).

If the parameter is set to a value larger 0, plume rise for this source is calculated according to guideline VDI 3784 Part 2. **rq** can be specified as time series.

sd (1) Seed value of the random number generator (default 11111). Choosing a different number yields a different series of random numbers so that the results form a different sample set.

sq (n_q) Time scale T_U (see guideline VDI 3945 Part 3, Section D5) for the calculation of plume rise (default 0).

If this parameter is set, then plume rise is calculated according to the procedure described in guideline VDI 3945 Part 3, Section D5, where **vq** is interpreted as upward-directed excess velocity. **sq** can be specified as time series.

ti (1) Identification string of the project (default TEST). The identification is written to all result files.

tq (n_q) Exhaust exit temperature in degree Celsius (default 0) for the calculation of plume rise.

If parameter **tq** is applied (preferably for plume rise calculations according to guideline VDI 3784 Part 2) then parameter **qq** should not be used or set to 0. **tq** can be specified as time series.

ux (1) Easting of the origin using UTM coordinates.

No coordinate conversion is made when calculating z_0 , thus **ux** and **uy** must refer to the same zone as the applied register of roughness lengths (file **z0-utm.dma**), see Section B.3.

uy (1) Northing of the origin of the UTM coordinate system. See **ux**.

vq (n_q) Exhaust exit velocity (default 0), see **qq** and **sq**. **vq** can be specified as time series.

wb (n_b) Rotation angle around a vertical axis that intersects the lower-left corner of a building base (default 0), see **ab**.

wq (n_q) Rotation angle around a vertical axis that intersects the lower-left corner of a source base (default 0), see **aq**.

x0 (n_n) Left (western) edge of the calculation area, see **dd**.

- xa** (1) x -coordinate of the anemometer position (default 0). The position must be inside the calculation area.
- xb** (n_b) x -coordinate of a building (default 0), see **ab**.
- xp** (n_p) x -coordinate of a receptor point.
- xq** (n_q) x -coordinate of a source (default 0), see **aq**.
- y0** (n_n) Lower (southern) edge of the calculation area, see **dd**.
- ya** (1) y -coordinate of the anemometer position (default 0), see **xa**.
- yb** (n_b) y -coordinate of a building (default 0), see **ab**.
- yp** (n_p) y -coordinate of a receptor point.
- yq** (n_q) y -coordinate of a source (default 0), see **aq**.
- z0** (1) surface roughness length z_0 .

If this parameter is not set, the surface roughness length is automatically derived from the register of roughness lengths, see Section B.3, and rounded to one of the values according to *TA Luft*. For the derivation either **gx** and **gy** or **ux** and **uy** must be specified.

The value is not rounded if given explicitly in combination with option **NOSTANDARD**; a rounded value is then only internally used for the derivation of Monin-Obukhov lengths from a dispersion class specification and for reading an anemometer height out of the data header of a time series file.

*Note: The internal boundary layer of AUSTAL2000 is set up according to guideline VDI 3783 Part 8. It assumes a wind shear (Ekman spiral) with height typical for central Europe. This must be considered when applying AUSTAL2000 in other countries. The wind shear can be switched off with the **NOSTANDARD** option **NOSHEAR**.*

3.1.2 Emission rates and available substances

Emission rates are specified like other source parameters. The parameter name encodes the substance, the values are the emission strengths of the various sources for this substance (in g/s, or OU/s for odorants).

The substances and their properties are defined in the settings file of *AUSTAL2000* (file **austal2000.settings**). They are also listed in the table at the end of Section B.4.

The following gaseous substances are available by default:

so2	Sulphur dioxide, SO ₂
no	Nitrogen monoxide, NO
no2	Nitrogen dioxide, NO ₂
nox	Nitrogen oxides, NO _x (specified as NO ₂)
bz1	Benzene
tce	Tetrachloroethylene
f	Hydrogen fluoride (specified as F)
nh3	Ammonia, NH ₃
hg	Mercury, Hg, according to TA Luft ($v_d = 0.005$ m/s)
hg0	Elementary mercury, Hg(0) ($v_d = 0.0003$ m/s)
xx	Unspecified
odor	Unrated odorant
odor_nnn	Rated odorant with a rate factor resulting from the identifier <i>nnn</i> , see Section 3.10. Possible values for <i>nnn</i> are: 050 (in the federal state Baden-Württemberg: 040), 075 (in the federal state Baden-Württemberg: 060), 100, 150

Substance NO_x is treated by the program independently of NO and NO₂. This implies that the user has to apply here the same emissions as for NO and NO₂ (according to the rule $nox = no2 + 1.53 * no$). Substance xx can be used as place holder for a substance that is not explicitly available but for which a dispersion calculation according to *TA Luft* is required. The gaseous components of xx as well as for the odorants odor and odor_nnn are not subject to deposition.

For particulate matter (PM), different classes of the aerodynamic diameter (1 to 4 and *unknown*) can be distinguished.

- 1 smaller 2.5 µm
- 2 2.5 µm to 10 µm
- 3 10 µm to 50 µm
- 4 larger 50 µm

The parameter name consists of the name of the substance followed by a minus sign and the number of the diameter class. For PM with aerodynamic diameters larger 10 µm and unknown contributions to classes 3 and 4, the class identifier u must be used. The following PM substances are available:

pm	PM, general
as	Arsenic, As
pb	Lead, Pb
cd	Cadmium, Cd
ni	Nickel, Ni
hg	Mercury, Hg
tl	Thallium, Tl
xx	Unspecified

PM-10 is represented by the components 1 and 2 (for example pm-1 and pm-2).

3.2 Results of the dispersion calculation

The program creates on start in the project directory a log file with name `austal2000.log` (text file), to which among others the current time, the program version and the name of the project directory are logged. If this file already exists its contents is not deleted by default but the new log information is appended (deletion is forced with the option `-D`). Then the input parameters as given in input file `austal2000.txt` are listed, followed by information about the program run; finally, a short evaluation of the main results is written.

The results of the dispersion calculation are written to separate files for the different substances. The file names are of the form

Substance-TypeParameterGrid

and the file name extension is `.dmna`. The file format is specified in Annex B. The data are written out layer by layer with as many layers as required to cover all receptor heights. If no receptor positions are specified or if all receptors have their default height 1.5 m, only the near-ground layer is written out. The height values of the layer intervals are listed in the file header as parameter SK (see input parameter hh).

Note: The names for Type und Parameter depend on the language setting (see Section C.2). The English versions are used in the following.

- Result type *Type*

The types of results written out depend on the types of limit immission values for the given substance (according to EU directives and the *TA Luft*). The following table gives an overview of the applied types:

Substance	Averaging time		
	Year	Day	Hour
so2	y00	d03	h24
no2	y00		h18
nox	y00		
pm	y00 dep	d35	
nh3	y00 dep		
xx	y00 dep		
odor	y00		
odor_nnn	y00		

y00 : Annual mean of concentration / annual frequency of odor hours

dep : Annual mean of deposition

dnn : Maximum daily mean exceeded *nn* times

hnn : Maximum hourly mean exceeded *nn* times

Note: The annual mean refers, more precisely, to the mean over the time period that is covered by the meteorological time series (in integer days). This applies accordingly to the frequency of odor hours.

The calculated values are usually provided in the unit that is used by the *TA Luft* for the according limit immission value. The unit is logged in the DMNA file header as parameter `unit`.

The frequency of odor hours is always expressed as percentage of the total number of hours.¹⁴ The value range is 0 to 100, the unit is '%'.

In a calculation based on a time series, the fraction of valid hourly means in the meteorological time series must amount to at least 90% of the hours of a year (8760) according to *TA Luft*, Annex 3. If this is not the case, the number of allowed exceedances is proportionally reduced in the automatic evaluation; this modification is logged in file `austal2000.log`, the file name however is not changed. The number of exceedances that has been actually applied in the evaluation is logged in the DMNA file header as parameter `exceed`.

Note: In a calculation based on a dispersion class statistics, no characteristic immission values referring to daily means can be calculated. Hourly ones are estimated as percentiles.

¹⁴In Germany, odor assessment is based on the concept of the so-called odor hour. An hour is marked as odor hour if there is a clear odor perception in at least 10% of the time. Limit values exists for the frequency of odor hours, i.e. the fraction of odor hours in a year.

Note: Concentration of PM (applies only to pm, pb, cd, and xx) is automatically calculated as the sum of the diameter classes 1 and 2 (i.e. PM-10) and written out as such. In contrast, deposition is written out as the sum over all classes (including a gaseous contribution).

For so2 and pm, the highest daily mean (type description d00) is written out in addition, likewise for so2 and no2 the highest hourly mean (type description h00). For all other substances, which are not listed in the table, only the annual mean of concentration (type description y00) respectively deposition (type description dep) is written out.

Time series at receptor points have the type description tmp. They are written out if: 1) the calculation is carried out with a meteorological time series; 2) receptor points are defined; 3) a short-time limit immission value exists for the substance or the substance is xx or odor respectively odor_nnn. For substance odor, the probability of the presence of an odor hour is stored as percentage value, i.e. either 100 or 0.

- Parameter description *Parameter*

The parameter description consists of a single character. The character a refers to additional load. If the program is able to estimate the model-inherent statistical uncertainty of a quantity, it is stored in a separate file with the parameter description s.¹⁵

For substances for which concentration or deposition has been calculated, this file contains the estimated relative statistical uncertainty (with respect to the calculated value $\bar{c}$, i.e. $\sigma_c/\bar{c}$). The unit is '1'.

For the substances odor and odor_nnn, the file contains the absolute uncertainty of the calculated frequency of odor hours $\bar{h}$, i.e. σ_h (both given as percent of the total number of hours). The value range is 0 to 100, the unit is '%'.

For values that correspond to daily averages an additional file is created which contains the index of the day at which the given characteristic immission value occurred. The parameter description is i. Indexing starts with 1 for the first day of the time series.

- Grid specification *Grid*

The grid specification is omitted if only a single grid is applied. For nested grids, *Grid* contains the grid number in form of a two-digit number with leading zero and starting with 1 for the finest grid.

For example, if a dispersion calculation was carried out for SO₂ using nested grids and specifying receptor points, the following result files are created:

¹⁵For PM-10 it is possible that the given statistical uncertainty is somewhat too high. This is because the results of the components x-1 and x-2 are added and the program assumes that the corresponding statistical uncertainties are correlated with each other. However, this is only true if they originate from the same source.

Using a meteorological time series:

- so2-y00a.dmna
- so2-y00s.dmna
- so2-d03a.dmna
- so2-d03s.dmna
- so2-d03i.dmna
- so2-d00a.dmna
- so2-d00s.dmna
- so2-d00i.dmna
- so2-h24a.dmna
- so2-h24s.dmna
- so2-h00a.dmna
- so2-h00s.dmna
- so2-tmpa.dmna
- so2-tmps.dmna

Using a dispersion class statistics:

- so2-y00a.dmna
- so2-y00s.dmna
- so2-h24a.dmna
- so2-h00a.dmna

The concentration fields are stored as three-dimensional tables (grid indices i , j , and k). Index i runs in x -direction, index j in y -direction, and index k in z -direction. All indices start with 1. Concentration is usually provided for the near-ground layer so that k takes only the value 1. If elevated receptor points have been specified, as many layers are provided as are necessary to cover the upper-most receptor point.

The table is written out such that the numbers for a given horizontal layer have the same spatial arrangement as the corresponding centre points of the grid cells in a map presentation. Numbers have the unit of the corresponding limit immission value. Odour hour frequencies are given as percentage of the total number of hours.

Deposition fields are two-dimensional tables but beside this structured like concentration fields.

The time series of hourly concentration values at the receptor points are two-dimensional tables. The row index i runs over the hours of the given time period, the column index j runs over the receptor points. Both indices start at 1. Invalid entries are marked by a negative value. Numbers have the unit of the corresponding limit immission value.

The exact structure of the files is specified in Annex B.

The names of all created files are listed in the log file. In addition, the characteristic immission values deduced from these files are given. Each characteristic value is given in a line of

the following structure:

Substance Type : *Value* (+/- *Spread*%) at *x*= *x* m, *y*= *y* m (*Grid* : *i*, *j*)

where *Substance* substance,

Type averaging time and number of exceedances,

Value calculated maximum characteristic value in the lowest layer,

Spread its statistical uncertainty,

x, y its coordinates,

i, j the indices of the corresponding grid cell,

Grid the number of the corresponding grid (for nested grids).

Example:

S02 S24 : 159 $\mu\text{g}/\text{m}^3$ (+/- 15.0%) at *x*= -125 m, *y*= 325 m (1: 18, 27)

The hourly mean near ground that has been exceeded 24 times during the year is at the most 159 $\mu\text{g}/\text{m}^3$ and occurred in the finest grid in the grid cell with indices *i* = 18, *j* = 27, corresponding to the coordinates *x* = -125 m, *y* = 325 m, *z* = 1.5 m. The value has an estimated statistical uncertainty of 15% which means that the true model value can be expected to be found with a probability of 68% in the range $\pm 15\%$ ($\pm 24 \mu\text{g}/\text{m}^3$) and with a probability of 95% in the range $\pm 30\%$ ($\pm 48 \mu\text{g}/\text{m}^3$) around the listed value.¹⁶

3.3 Coordinates and coordinate system

Coordinate specifications for sources, buildings, anemometer position, and receptor points may not exceed the absolute value 200 000 (metres) in AUSTAL2000. It is therefore in most cases required to use relative coordinates with respect to an absolute reference point. This can also be helpful to avoid lengthy absolute coordinate specifications.

The reference point can be defined in the Gauß-Krüger coordinate system¹⁷ (parameters *gx* and *gy*) or in the UTM coordinate system¹⁸ (parameters *ux* and *uy*). All absolute coordinate specifications must refer to the same coordinate system, likewise all relative coordinate specifications must refer to the same reference point.

If *gx/gy* or *ux/uy* is specified, the applied coordinate system (GK and UTM, respectively) is documented as parameter *gccs* in the file headers of the DMNA output files.

If the register of roughness lengths (see Section B.3) that is given in the Gauß-Krüger coordinate system is applied, the program tries to transform the source coordinates (reference

¹⁶In the evaluation written to the log file, the two outmost rows of grid cells in inner grids in case of nested grids are not considered (see Section 3.8).

¹⁷Bessel ellipsoid, Potsdam date.

¹⁸WGS84 ellipsoid.

point plus relative coordinate) to the Gauß-Krüger stripe used by the register (by default the 3rd stripe). When using UTM coordinates, the source coordinates must refer to the same zone as the register (by default zone 32).

A file with the terrain profile (see Section 3.6.1) may contain in its header (format DMNA or GRIDASCII) a reference point different from `gx` and `gy` respectively `ux` and `uy`; but it must refer to the same stripe respectively zone.

If neither a register of roughness lengths nor a terrain profile is applied, specification of a reference point is optional and not required by the program.

3.4 Calculations based on a time series

Meteorological data are usually provided in form of an AKTerm (meteorological time series in the format used by the German Weather Service, DWD), which is specified by parameter `az`. An AKTerm is a text file with one line of data for each successive hour of the year. In addition to meteorological input, it may be necessary to specify emission parameters in form of a time series.

Note: The internal boundary layer of AUSTAL2000 is set up according to guideline VDI 3783 Part 8. It assumes a wind shear (Ekman spiral) with height typical for central Europe. This must be considered when applying AUSTAL2000 in other countries. The wind shear can be switched off with the NOSTANDARD option NOSHEAR.

Klug/Manier is the default German classification scheme for the atmospheric stability.

The Klug/Manier class ID is specified as: 1: Klug/Manier I (very stable), 2: Klug/Manier II (stable), 3: Klug/Manier III/1 (stable to neutral), 4: Klug/Manier III/2 (neutral to unstable), 5: Klug/Manier IV (unstable), 6: Klug/Manier V (very unstable). The Klug/Manier stability classes 1 to 6 correspond approximately to the Pasquill/Gifford classes F to A.

In the time series file `series.dmna`, the Monin-Obukhov length is specified as a more direct and detailed measure of the stability. The conversion of Klug/Manier class to Monin-Obukhov length and vice versa is implemented in AUSTAL2000 according to TA Luft, Annex 3:

Klug/ Manier	Roughness length z_0 in m								
	0.01	0.02	0.05	0.10	0.20	0.50	1.00	1.50	2.00
I	7	9	13	17	24	40	65	90	118
II	25	31	44	60	83	139	223	310	406
III/1	99999	99999	99999	99999	99999	99999	99999	99999	99999
III/2	-25	-32	-45	-60	-81	-130	-196	-260	-326
IV	-10	-13	-19	-25	-34	-55	-83	-110	-137
V	-4	-5	-7	-10	-14	-22	-34	-45	-56

For intermediate values, a logarithmic interpolation with respect to z_0 and a reciprocal one for L_M apply. For values of z_0 less than 0.01 m or greater than 2 m the respective boundary values are used.

3.4.1 Deprecated AKTerm format

Each line contains 24 characters representing a data record valid for one hour. The structure of a record is:

Parameter	Position
Station ID (*)	1 to 5
Date (YYYYMMDDHH)	6 to 15
Interpolation ID (*)	16
Wind direction (10 degrees)	17 to 18
Wind speed (knots)	19 to 20
Klug/Manier stability class (1..6)	21
Turner class (*)	22
WW key ID (*)	23 to 24

(*) Value required but not evaluated

The station ID must be a 5-digit number. For missing or invalid records, only station number and date are required and the other parameter values must be replaced by blanks. Records with Klug/Manier class 0 or larger 7 are interpreted by *AUSTAL2000* also as invalid.

If the stability class could not be determined (value 7), value 3 is substituted. Wind directions larger 360 are replaced by a random direction.

3.4.2 Current AKTerm format

The file consists of a header and a data part. The header is at the beginning of the file and consists of at most 5 comment lines, each introduced by a star (*) as the first character. The

comment lines are followed by a line with the formal anemometer heights that correspond to the 9 roughness length classes of the *TA Luft*. This line starts with a plus sign and the 9 height values are expected after the first colon; the line could e.g. start as

+ anemometer heights (0.1m):

followed by 9 integer heights in units of 0.1 m (4 digits each without leading zeros, separated by a blank) for the roughness lengths 0.01 m to 2 m of Annex 3 of the *TA Luft*.

Note: The measured data are influenced by the local surface roughness. If they are applied at a different site which is characterized by a different surface roughness length, the data need to be transformed. The simplest transformation consists of an adjustment of the applied anemometer height. The DWD provides an according methodology (see www.dwd.de). It is based on the assumption that the logarithmic wind profile at larger altitude (reference height 60 m) should not depend on the local roughness length.

The data part consists of lines each with 16 entries that are separated by exactly one blank. The entries are:

Entry	Meaning	Position	Value range
KENN	Data set ID (*)	1 bis 2	AK
STA	Station ID (*)	4 bis 8	00001-99999
JAHR	Year	10 bis 13	1800-2...
MON	Month	15 bis 16	1-12
TAG	Day	18 bis 19	1-31
STUN	Hour	21 bis 22	0-23
NULL	Zeros	24 bis 25	0
QDD	Quality byte (wind direction)	27	0,1,2,9
QFF	Quality byte (wind speed)	29	0,1,2,3,9
DD	Wind direction	31 bis 33	0-360,999
FF	Wind Speed	35 bis 37	0-999
QB	Quality byte (value status) (*)	39	0-5,9
KM	Klug/Manier stability class	41	1-7,9
QB	Quality byte (value status) (*)	43	0,1,9
HM	Mixing layer height (m) (*)	45 bis 48	0-9999
QB	Quality byte (value status) (*)	50	0-5,9

(*) Value required but not evaluated

Example:

```

* AKTERM, German Weather Service, Offenbach (KB1A)
* Period 01/1995 to 12/1995
* Anonymized data, date: 11.04.2002
+ anemometer heights (0.1 m):  32   41   57   74   98  144  200  244  283
AK 10999 1995 01 01 00 00 1 1 210  56 1 3 1 -999 9
AK 10999 1995 01 01 01 00 1 1 220  64 1 3 1 -999 9
AK 10999 1995 01 01 02 00 1 1 260  68 1 3 1 -999 9
AK 10999 1995 01 01 03 00 1 1 270  65 1 3 1 -999 9
AK 10999 1995 01 01 04 00 1 1 250  64 1 3 1 -999 9
AK 10999 1995 01 01 05 00 1 1 250  64 1 3 1 -999 9
...

```

The quality byte for the wind direction can take the following values:

QDD	Meaning
0	Wind direction in 10 degrees
1	Wind direction in degree, original value in 10 degrees
2	Wind direction in degree, original value in degree
9	Wind direction missing

The quality byte for the wind speed can take the following values:

QFF	Meaning
0	Wind speed in knots
1	Wind speed in 0.1 m/s, original value in 0.1 m/s
2	Wind speed in 0.1 m/s, original value in knots (0.514 m/s)
3	Wind speed in 0.1 m/s, original value in m/s
9	Wind speed missing

KM is 7 if the stability could not be determined, *AUSTAL2000* applies 3 (III/1) in this case. KM is 9 if an information on stability is missing; *AUSTAL2000* applies 0 in this case, i.e. treats this time interval as a measurement gap.

Time must be specified in UTC (GMT). The data are regarded as being representative for the time period of one hour and the specified time is interpreted as the end of this period. The DWD provides for test purposes five time series for five subsequent calendar years (anno95.akt to anno99.akt in the old format and anno95.akterm to anno99.akterm in the new format).

Transformation

First, the AKTerm is transformed by *AUSTAL2000* into time series of wind direction r_a , wind speed u_a , and Monin-Obukhov length L_M . The directives of Annex 3 of the *TA Luft*

are accounted for (filling of gaps, minimum wind speed, redistribution of wind directions for small wind speed, elimination of steps).

The DWD explicitly states and applies the conversion $1 \text{ kn} = 0.514 \text{ m/s}$. Therefore, this conversion is applied in case the wind speed is provided in knots. Likewise wind speeds that are given in units of 0.1 m/s but based on original values in knots are first converted to integer knots and then to m/s . Afterwards the values are distributed equally over the step range. If the wind direction is given in integer degrees the values are formally spread over a range of 1 degree width and then rounded again to integer values in order to have a more consistent distribution over the one-degree sectors. The transformation consists of the following steps:

- Read AKTerm and mark hours with invalid data by a Klug/Manier class 0.
- Convert wind direction to degree and wind speed to m/s and distribute values equally over the step ranges (random selection).
- Choose random wind direction in case $DD > 360$.
- Determine distribution of wind direction for small wind speeds.
- Close measurement gaps of one or two hours duration by interpolation.
- Set wind direction for short-time calms by interpolation.¹⁹
- Set wind direction for longer calms according to the distribution of wind direction for small wind speeds (weighted random selection).
- Set minimum values of wind speed (according to *TA Luft* 0.7 m/s).
- Round wind speed to integers of 0.1 m/s and wind direction to integer degrees.
- Determine the average wind speed for each stability class (required by *TALdia*).

If *AUSTAL2000* is called with option *-z*, for example

```
austal2000 test/h50a95 -z
```

then only this transformation is performed and the time series are written out to the text file *series.dmn*a (format specification given in Section B). For invalid or missing data sets the Monin-Obukhov length L_M has value 0. Thus,

¹⁹Calm conditions should be specified in a AKTerm by both wind speed and wind direction 0. The program identifies calm conditions by wind speed 0 and gives a warning if data lines with wind speed 0 and wind direction larger 0 or vice versa are encountered.

AKTerm anno95.akterm

```

* AKTERM, German Weather Service, Offenbach (KB1A)
* Period 01/1995 to 12/1995
* Anonymized data, date: 11.04.2002
+ anemometer heights (0.1 m): 32 41 57 74 98 144 200 244 283
AK 10999 1995 01 01 00 00 1 1 210 56 1 3 1 -999 9
AK 10999 1995 01 01 01 00 1 1 220 64 1 3 1 -999 9
AK 10999 1995 01 01 02 00 1 1 260 68 1 3 1 -999 9
AK 10999 1995 01 01 03 00 1 1 270 65 1 3 1 -999 9
AK 10999 1995 01 01 04 00 1 1 250 64 1 3 1 -999 9
AK 10999 1995 01 01 05 00 1 1 250 64 1 3 1 -999 9
AK 10999 1995 01 01 06 00 1 1 250 70 1 3 1 -999 9
...
```

Time series series.dma

```

form "te%20lt" "ra%5.0f" "ua%5.1f" "lm%7.1f"
locl "C"
mode "text"
ha 3.2 4.1 5.7 7.4 9.8 14.4 20.0 24.4 28.3
z0 0.50
d0 3.00
sequ "i"
dims 1
size 24
lowb 1
hghb 8760
*
1995-01-01.01:00:00 206 5.6 99999.0
1995-01-01.02:00:00 216 6.4 99999.0
1995-01-01.03:00:00 255 6.8 99999.0
1995-01-01.04:00:00 271 6.5 99999.0
1995-01-01.05:00:00 251 6.4 99999.0
1995-01-01.06:00:00 250 6.4 99999.0
1995-01-01.07:00:00 247 7.0 99999.0
...
```

The time series contains 4 columns: in the first column time t_e (end of the hour) in GMT+1, in the following ones r_a , u_a , and L_M are listed. The column names and the data formats are specified by parameter `form` in the file header.

3.4.3 Explicit time series

As an alternative to a AKTerm, a time series can be directly specified. If *AUSTAL2000* encounters the file `series.dma`²⁰ in the project directory, it uses it and interprets its contents as being a transformed AKTerm. In this case a specification of `as` (AKS) or `az` (AKTerm) in the input file is ignored. In this way it is possible to apply specific meteorological measurements in the dispersion calculation.

The time series must start with the first hour of a day. It must consist of an integer number of days and should cover a complete calendar year. The first 4 columns of the data part must contain the end of the 1-hour interval (`te`), the wind direction (`ra`, in deg), the wind speed (`ua`, in m/s), and the Monin-Obukhov length (`lm`, in m) – in exactly this order.

The time series may contain additional columns for time-dependent emission parameters. Emission strengths and parameters `vq`, `qq`, `sq`, `tq`, `rq`, and `lq` can be defined in a time series. The time dependence is stated to the program by a question mark instead of a value in the input file. The time series file must contain for each time-dependent parameter a column with the name *Source.Parameter*. Here, *Source* is the number of the source to which the parameter applies (2-digit value with leading zeros, starting with 01).

To facilitate the creation of such a time series, *AUSTAL2000* when invoked with option `-z` writes out the time series that already includes a column for each parameter that has been specified as being time-dependent. The columns contain zero values which can then be

²⁰English language package (German one: `zeitreihe.dma`).

replaced by the actual ones.

As an example, the time series for a facility with a 2-fold shift operation, where emissions of SO₂ only occur between 6 a.m. and 10 p.m., may read as follows:²¹

```
form    "te%20lt" "ra%5.0f" "ua%5.1f" "lm%7.1f" "01.so2%10.3e"
mode    "text"
sequ    "i"
dims    1
size    24
lowb    1
hghb    8760
*
```

```
1995-01-01.01:00:00    206    5.6 99999.0 0.000e+000
1995-01-01.02:00:00    216    6.4 99999.0 0.000e+000
1995-01-01.03:00:00    255    6.8 99999.0 0.000e+000
1995-01-01.04:00:00    271    6.5 99999.0 0.000e+000
1995-01-01.05:00:00    251    6.4 99999.0 0.000e+000
1995-01-01.06:00:00    250    6.4 99999.0 0.000e+000
1995-01-01.07:00:00    247    7.0 99999.0 1.168e+001
1995-01-01.08:00:00    252    6.4 99999.0 1.168e+001
1995-01-01.09:00:00    264    6.9 99999.0 1.168e+001
1995-01-01.10:00:00    264    7.4 99999.0 1.168e+001
1995-01-01.11:00:00    261    7.4 99999.0 1.168e+001
1995-01-01.12:00:00    264    8.4 99999.0 1.168e+001
1995-01-01.13:00:00    270    8.9 99999.0 1.168e+001
1995-01-01.14:00:00    271    8.9 99999.0 1.168e+001
1995-01-01.15:00:00    265    9.0 99999.0 1.168e+001
1995-01-01.16:00:00    250    8.6 99999.0 1.168e+001
1995-01-01.17:00:00    252    9.5 99999.0 1.168e+001
1995-01-01.18:00:00    260    8.7 99999.0 1.168e+001
1995-01-01.19:00:00    251    7.9 99999.0 1.168e+001
1995-01-01.20:00:00    253    7.8 99999.0 1.168e+001
1995-01-01.21:00:00    243    6.9 99999.0 1.168e+001
1995-01-01.22:00:00    236    7.1 99999.0 1.168e+001
1995-01-01.23:00:00    251    7.0 99999.0 0.000e+000
1995-01-02.00:00:00    243    7.4 99999.0 0.000e+000
```

...

3.4.4 Results

As a result of a time series calculation for a substance for which a short-time limit immission value exists, the time series of concentration at the receptor points are written out, one column for each receptor point. The absolute time reference is given in form of a comment at the end of each data line. Negative concentration values (value -1) indicate that the concentration could not be determined due to missing input data.

The following example lists such a time series for a short period of time.

²¹Note that the year 1995 started with a Sunday. In a real case, emission would probably be zero for the first day and shift operation would start the second day.

```

idnt  "Test H50A95"
mntn  "01"  "02"
mntx   375.0  -375.0
mnty   -25.0   125.0
mntz    1.5    1.5
T1  "1995-04-01.00:00:00"
T2  "1995-04-02.00:00:00"
interval  "01:00:00"
axes  "ti"
name  "so2"
file  "so2-zbpz"
unit  "ug/m3"
form  "con%5.1f"
refv   50.0
undf  -1
...
dims  2
sequ  "i,j"
lowb   1    1
hghb  24    2
*
      0.0    0.0 ' 1995-04-01.01:00:00
      0.0    0.0 ' 1995-04-01.02:00:00
      0.0    0.0 ' 1995-04-01.03:00:00
      0.0    0.0 ' 1995-04-01.04:00:00
      0.8    0.0 ' 1995-04-01.05:00:00
      3.1    0.0 ' 1995-04-01.06:00:00
      0.0    0.0 ' 1995-04-01.07:00:00
...

```

The file header lists, among others, the parameters that define the receptor points: name `mntn`, x -coordinate `mntx`, y -coordinate `mnty`, and height above ground `mntz`.

If background concentration is likewise provided as a time series, *AUSTAL2000* can calculate the characteristic immission values of the total load. For this purpose, background concentration must be provided as file *Substance-tmpp.dma*²² in the project directory. The structure of the data part (start time, number of intervals, sequence of receptor points) must be identical to the time series file with the additional load.

The log file `austal2000.log` contains in this case an additional section with the characteristic immission values of the total load at the receptor points.

The evaluation can be carried out also at a later time after the dispersion calculation: Calling *AUSTAL2000* with option `-a` omits the dispersion calculation and evaluates the existing results with respect to the characteristic immission values.

²²English language package (German one: *Substance-zbpv.dma*).

3.5 Situation-dependent parameters

Time-dependent emission conditions should be handled in form of a time-series calculation (see Section 3.4). In a calculation based on a dispersion class statistics, such a temporal assignment cannot be made. However, there are situations where the temporal variation is solely caused by a change in meteorological conditions, like it is the case for example for wind-induced emissions. Here, the emission strength is a function of wind velocity (example: emission of NH_3 by open stables). Likewise the distance and rise of a thermal plume is a function of wind speed and atmospheric stability; here, the calculation of plume rise is carried out internally by the program so the user has not to take special care for this.

Although wind-induced emissions or a different modelling of plume rise can be handled in a time-series calculation, devotees of a dispersion class statistics (AKS) is offered the possibility to do the same.

By definition, the value of a situation-dependent parameter depends on wind speed and stability class. It is the set of parameters that can be defined as time-dependent that can also be defined as situation-dependent: vq , qq , sq , tq , rq , lq , and the emission strengths of the different substances. Like for time-dependent parameters, a question mark is assigned to the parameter instead of a value.

The values v must be provided as a two-dimensional table $v_{i,j}$ in form of a DMNA file (see Section B), where $i = 1, 2, \dots, 6$ denotes the stability classes and $j = 1, 2, \dots, 9$ the velocity classes of the AKS. The file name must have the form *Source.Parameter.dmn*a, where *Source* is the number of the source and *Parameter* the name of the parameter, e.g. `01.nh3.dmna for the emission of  $\text{NH}_3$  of the first source or 143.vq.dmna for the exit velocity of the 143rd source.`

File 01.nh3.dmn in example test\h00aks-nh3 contains emission strengths that are proportional to $\sqrt{u_a}$ with the value 0.04 g/s for $u_a=1$ m/s:

```

dims      2
lowb      1   1
hghb      6   9
size      4
form      "%6.3f"
sequ      "i,j"
mode      "text"
unit      "g/s"
fact      25
*
1.000 1.225 1.414 1.732 2.121 2.449 2.739 3.000 3.464
1.000 1.225 1.414 1.732 2.121 2.449 2.739 3.000 3.464
1.000 1.225 1.414 1.732 2.121 2.449 2.739 3.000 3.464
1.000 1.225 1.414 1.732 2.121 2.449 2.739 3.000 3.464
1.000 1.225 1.414 1.732 2.121 2.449 2.739 3.000 3.464
1.000 1.225 1.414 1.732 2.121 2.449 2.739 3.000 3.464
***

```

3.6 Calculation for complex terrain

Terrain profile and buildings are accounted for in the dispersion calculation with the help of the diagnostic wind field model *TALdia*. Its use is triggered by the parameter setting *gh* or by the definition of buildings in the input file *austal2000.txt*.

The value of parameter *gh* is the name of the file with the digital elevation model that contains the terrain heights within the calculation area. Buildings are defined by parameters *xb*, *yb*, *ab*, *bb*, *cb*, *wb* or in form of a raster file specified by parameter *rb*. Terrain profile and buildings can be simultaneously defined.

Note: Calculations for complex terrain demand considerably more effort and computation time as compared to ones for plain terrain! In addition, they offer significantly more possibilities for making mistakes.

3.6.1 Definition of the terrain profile

The digital elevation model (DEM) can usually be ordered from a regional or national land surveying office. The following formats are supported by *AUSTAL2000* (all of them are simple text files that can be inspected or edited with any text editor):

1. Arcinfo-GRIDASCII. The file has the following structure:

- The terrain heights are defined on a regular grid with a cell size of typically 20, 40, 50, or 100 m. The values are interpreted as the terrain height in the centre of a grid cell.
- The first 6 lines contain general information, each line containing the name of a parameter and its value:

<code>ncols</code>	Number of columns of the grid
<code>nrows</code>	Number of rows of the grid
<code>xllcorner</code>	Absolute x -coordinate of the lower-left corner of the lower-left grid cell
<code>yllcorner</code>	Absolute y -coordinate of the lower-left corner of the lower-left grid cell
<code>cellsize</code>	Cell size (m)
<code>NODATA_value</code>	Value indicating missing data (no missing data allowed!)

- Then a two-dimensional table of the height values follows, the values being ordered like the grid cells in a map. Thus, the first value in the first data line is the terrain height at the point with x -coordinate

`xllcorner+0.5*cellsize`

and y -coordinate

`yllcorner+(nrows-0.5)*cellsize`.

Example (partial):²³

<code>ncols</code>	261
<code>nrows</code>	241
<code>xllcorner</code>	4597475.0000
<code>yllcorner</code>	5396475.0000
<code>cellsize</code>	50.0000
<code>NODATA_value</code>	-9999
542.9	532.4 517.1 503.5 497.3 497.7 501.7
549.5	539.3 526.0 511.8 499.0 491.0 490.1
544.0	536.0 527.3 518.2 507.3 495.9 487.6
532.3	525.2 518.1 512.9 507.5 499.0 488.3
523.5	515.8 509.0 505.0 502.1 497.4 489.4

2. DMNA. The file has the following structure:

- The file header contains the usual specifications of format and dimension (see Section B.1).
- The data part is very similar to the format GRIDASCII, if the values are written North-oriented (`sequ` has the value `j-,i+`). The difference is that the height values refer to the corners of the grid cells instead of the centre.
- The lower-left corner of the lower left cell (if North-oriented) has the coordinates `xmin` and `ymin` (m). These can be relative coordinates that refer to a reference point given by `refx` and `refy` (alternatively `gakrx` and `gakry`).

²³The data (file `tittling.dmn`) have been created from the free test data provided by the land surveying office of the federal state Bavaria (web page www.bayern.de/vermessung); they cover an area of 13×12 km² near Tittling (Germany).

- The cell size is specified as parameter `delta` (m).

Example (as above):

```
xmin 4597500.0
ymin 5396500.0
form "Z%6.1f"
delta 50.0
sequ "j-,i+"
dims 2
lowb 0 0
hghb 260 240
*
542.9 532.4 517.1 503.5 497.3 497.7 501.7
549.5 539.3 526.0 511.8 499.0 491.0 490.1
544.0 536.0 527.3 518.2 507.3 495.9 487.6
532.3 525.2 518.1 512.9 507.5 499.0 488.3
523.5 515.8 509.0 505.0 502.1 497.4 489.4
```

3. XYZ. Each line of the text file contains the triplet x , y , and z (m), where x and y are the absolute coordinates at which the terrain height z applies. The list must contain values for all grid points of a rectangular grid with constant grid width.

Note: The program expects that valid height values are provided at all grid points of the DEM. If this is not the case, implausible results may be the consequence.

The program determines from the DEM the height values at the grid points of the calculation grid and stores them as file `zg0l.dma` (grid level l , $l = 0$ without grid nesting) in the project directory. The cell size of the DEM may be different to the one of the calculation grid, but the calculation area must be completely included in the area covered by the DEM.

Note: The absolute coordinates used in the definition of the calculation grid must refer to the same Meridian stripe respectively UTM zone as the coordinate specifications applied in the DEM. In contrast to the reference point specified in the input file of AUSTAL2000 (gx or ux) and the reference point in the roughness class register, a missing UTM zone is not completed on reading the DEM file.

If the project directory already contains files `zg0l.dma` with proper dimensions, the file name specified in `gh` is ignored and the terrain profile is not re-calculated.

The log file contains information about the maximum steepness of the terrain. Terrain heights at neighbouring grid points are compared and the steepness is logged for example in the following form:

The maximum steepness of the surface is 0.52 (0.47)

The first number is the steepness resulting from a comparison of adjacent grid points, the second number in brackets is the one resulting from a comparison of second-next grid points. In the latter case, grid points have usually a distance of twice the stack height. The value 0.2 implies a steepness of 1:5.

3.6.2 Definition of buildings

Buildings are like sources specified in form of cuboids; in contrast to sources the base is always at the ground. Buildings can be defined as well with a circular base by specification of a negative value for parameter `bb`, the absolute value of which defines the radius of the circle. An alternative definition of buildings is a raster file which is specified by parameter `rb`.

Buildings are internally rastered on the calculation grid, i.e. those grid cells are interpreted as a building cell which are fully or to their major part occupied by a building.²⁴ This procedure has, among others, the advantage that it is not required for the user to avoid an overlap of buildings or small gaps between them as these are automatically eliminated in the rasterization process.

Note: The rastered buildings may not overlap with sources. To avoid a program abort for small overlaps, AUSTAL2000 tries to move particles, which are created inside a building cell, out of this cell; the maximum displacement is one horizontal cell width; if the procedure does not succeed, the program aborts with an error message.

At the beginning of a wind field calculation, the rastered buildings are written to file `volout00.dmn` in the project directory (for nested grids file `volout01.dmn` and possibly as well file `volout02.dmn`). The data part contains for each cell of the calculation grid an integer value which is 1 if the cell is a building cell and 0 otherwise. The user should check by an inspection of this file whether the buildings are sufficiently resolved within the chosen cells.

3.6.3 Calculation of the wind field

The wind field is calculated by the diagnostic wind field model *TALdia* described in Annex D. It is not required to calculate the full wind field for each individual meteorological situation; the program takes advantage of the fact that the linear combination of two wind fields again yields a valid wind field for a given atmospheric stability. For building effects this procedure is not thoroughly correct but the error is small if the two wind fields are not too different.

For the case without buildings, *TALdia* calculates for each of the 6 stability classes two wind fields, one for an incoming flow from South and one for an incoming flow from West; these 12 base fields are stored in a wind field library. In case of buildings 36 wind fields are created

²⁴For a cubic cell with centre point (x_m, y_m, z_m) , horizontal width Δx , and vertical width Δz , it is checked whether the centre point and the points $(x_m \pm \Delta x/4, y_m \pm \Delta x/4, z_m \pm \Delta z/4)$ are located inside a building or on a building face. If this is the case for at least 6 points, the centre point counting twice, then the grid cell is interpreted as a building cell.

for each stability class, corresponding to incoming flows for an isotropic wind rose in steps of 10 degree.

In the dispersion calculation, for each dispersion situation those two wind fields are selected out of the base fields belonging to the current stability that show a wind direction at the anemometer position which is closest to the specified one, preferably inclosing it. The two fields are linearly combined (superposition) such that the resulting field shows at the anemometer position exactly the required wind speed and wind direction.

In case of nested grids the wind vector at the anemometer position is determined by the program at hand of the finest grid that contains the anemometer position. The resulting superposition factors are then applied to all grids.

If a terrain profile and buildings are defined, the program *TALdia* first calculates a divergence-free wind field without building effects. These are introduced in a second step.²⁵ The result is a divergence-free wind field with boundary conditions adjusted to terrain and buildings. In case of buildings, fields with additional velocity fluctuations and diffusion coefficients are calculated and written out together with the wind fields.

Each of the wind fields of the library is calculated in an iterative procedure. The program starts with a wind field that is not divergence-free and tries to iteratively remove the divergence. To which degree the program succeeds should be checked at hand of the log file `taldia.log`. It lists as a scaled divergence the maximum absolute value of the encountered divergences multiplied by Δ/u_a (Δ : horizontal cell size, u_a : wind speed at the anemometer).

Note: The scaled divergence listed by the program should be below 0.05.

In principle it can happen that the iterative procedure does not converge. In this case the program aborts with an error message. However, if all of the limitations are considered that the *TA Luft* states with regard to the steepness of the terrain, this case should not happen in practice.

For calculations in complex terrain or generally when applying externally created wind fields it is important to guarantee that the anemometer is subject to a free incoming flow. If it is located close to obstacles, the meteorological models which are applied here are not suited to deduce the incoming flow with a sufficient precision.²⁶ To prevent a selection of such inappropriate anemometer positions the following checks are performed which may cause a program abort:

1. For each of the wind fields in the wind field library, the wind speed at the anemometer position must exceed 0.5 m/s.

²⁵This part is carried out by the microscale wind field model DMK which is described in the final report `taldmk.pdf` on web site www.austal2000.de.

²⁶In practice such a situation only occurs if meteorological data are translated from the real measurement position to an auxiliary position inside the calculation area and if the latter is not selected with sufficient care.

2. The final wind field used for the dispersion calculation may nowhere take a vertical component that exceeds an absolute value of 50 m/s.²⁷
3. The sum of squares of the superposition factors for the two base fields must be smaller than 100 and larger than 1/400.

3.6.4 Practical procedure

Only three steps are necessary to account for terrain profile and buildings in a dispersion calculation:

1. The digital elevation model is provided in form of a text file (e.g. in the format Arcinfo-GRIDASCII). It must cover the calculation area.
2. The name of the file is specified in the input file `austal2000.txt` by parameter `gh`.
3. Buildings are specified in the input file `austal2000.txt`, either explicitly by parameters `xb`, `yb`, `hb`, `cb`, and `wb` or in form of a raster file, the name of which is specified by parameter `rb`.

The program *AUSTAL2000* then automatically invokes program *TALdia*. It creates the terrain profile `zg0l.dma` (grid level *l*, *l* = 0 without nesting) in the project directory and the wind field library in subdirectory `lib`. For further information on *TALdia* see Annex D. The fields are then used in the subsequent dispersion calculation carried out by *AUSTAL2000*. The turbulence fields are calculated locally like for flat terrain as a function of height above ground.

Calculation time increases because of the following reasons:

1. The wind fields of the wind field library must be created.
2. For each hour of the year (in case of a time series calculation) three-dimensional wind and turbulence fields must be calculated.
3. The determination of the particle trajectories is more elaborate for a three-dimensional meteorology than it is for a one-dimensional one.

Note: This can lead to an overall increase of calculation time by a factor 5 to 10.

The following issues need to be considered in addition to the standard procedure described above:

²⁷The checked vertical component is the one of the terrain-adjusted coordinate system and it is therefore also a function of terrain steepness and the horizontal components.

- If the project directory already contains file `zg01.dmma`, this file is applied and the specified DTM is not evaluated.
- If the project directory contains a subdirectory `lib`, *AUSTAL2000* expects it to contain a valid and complete library and skips the creation of a new one.
- If *AUSTAL2000* is called with option `-1`, only the wind field library is created and the dispersion calculation is omitted. In this case, wind fields that already exist in the library are deleted after confirmation by the user.
- Instead of calling *AUSTAL2000* with option `-1`, the wind field model can be directly invoked:

`taldia ProjectDirectory`

3.7 Using externally created wind fields

As discussed in Section 3.6, *AUSTAL2000* applies for calculations in complex terrain the wind fields in subdirectory `lib`. It is not required that these fields have been created by *TALdia*, they may also result from another meteorological pre-processor like a prognostic model. In addition to a wind field, turbulent velocity fluctuations and exchange coefficients can be provided.

The following conditions must be met to enable *AUSTAL2000* to correctly identify and apply these fields:

1. The files must have a structure as described in Annex B. Numbers must be provided as floats, either in text format or in binary format (4 bytes per number).
2. The file name specifies the type of data. The following names apply:

w????a00.dmna	Wind vector with the components z_p (height above sea level), v_x (x -component of the wind vector), v_y (y -component of the wind vector), $\tilde{v}_s$ (s -component of the wind vector, see Section D.1.1). <i>AUSTAL2000</i> does not directly use the given value $\tilde{v}_s$ but recalculates the value by the condition of vanishing divergence in each grid cell. The numbers have the units m respectively m/s.
v????a00.dmna	Turbulent velocity fluctuations (turbulence field) with the components σ_u , σ_v , σ_w , and ϑ (potential temperature in degree Celsius). They replace the values of the boundary layer model of <i>AUSTAL2000</i> . The numbers have the unit m/s.
v????d00.dmna	Turbulent velocity fluctuations that are added (quadratically) to the ones of the boundary layer model of <i>AUSTAL2000</i> . The numbers have the unit m/s.
k????a00.dmna	Exchange field (K field) with the components K_H (horizontal diffusion coefficient) and K_V (vertical diffusion coefficient). They replace the values of the boundary layer model of <i>AUSTAL2000</i> . The numbers have the unit m^2/s .
k????d00.dmna	Exchange coefficients that are added to the ones of the boundary layer model of <i>AUSTAL2000</i> . The numbers have the unit m^2/s .
zp00.dmna	z -coordinate of the grid points (in m above sea level).
zg00.dmna	Terrain profile (lowest layer of zp00.dmna).

The 4 question marks correspond to 4 digits which specify the dispersion situation; for example, 2019 may be used for "stable stratification (Klug/Manier II), wind direction 190 degree". The choice of encoding is quite arbitrary (but see below) as long as it results in a valid file name.

Wind fields should be provided for at least those situations for which *AUSTAL2000* would create base fields. Files of type 'v' or 'k' must be given either for none or for all situations.

- It must be specified to which stability class a file refers to: either by the dispersion class index ak1 in the file header with a value between 1 (corresponding to Klug/Manier I) and 6 (corresponding to Klug/Manier V), or by the 4-digit specifier in the file name, where the first digit is interpreted as dispersion class index.
- The files contain three-dimensional data tables (with the exception of zg00.dmna), the index ranges are $0..n_x$, $0..n_y$, and $0..n_z$. n_x and n_y correspond to the parameters nx (number of cells in x -direction) and ny (number of cells in y -direction) of the input file. The number of vertical cells results from the vertical grid which can be explicitly specified by parameter hh (height above ground). The default in the absence of buildings is

hh 0 3 6 10 16 25 40 65 100 150 200 300 400 500 600 700 800 1000 1200 1500

i.e. $n_z = 19$.

5. The velocity components are defined on the Arakawa-C grid, for example v_x as surface average over a cell side perpendicular to the x -direction at the grid points ($0 \leq i \leq n_x$) in x -direction and in y - and z -direction on the centre points of the intervals ($1 \leq j \leq n_y, 1 \leq k \leq n_z$). According definitions apply to v_y and v_z . All other quantities are defined on the grid points (corners of the grid cells).

The type of definition (Arakawa-C, point value) must be stated in the file header by parameter `vldf`; it specifies by one character for each component the type of definition:

```

vldf PXYS   for wind fields
vldf PPPP   for velocity fluctuations
vldf PP     for exchange coefficients
vldf P      for grid definitions

```

The file header must contain the grid parameters `dd`, `x0`, `y0`, and `hh` and in addition the following parameters:²⁸

```

axes   xyz
lsbf   1
sscl   0
zscl   0

```

6. Wind fields describing the flow around buildings are not defined inside the cells that are assigned as being part of a building. The program identifies these building cells by the value -99 for v_s at the bottom of the cell. This encoding must be used in the provided wind fields. Overhanging buildings or bridges for which a building cell would appear on top of a non-building cell are not allowed.

If *AUSTAL2000* detects a library (i.e. subdirectory `lib` in the project directory), it indexes the encountered fields and checks for completeness. Then the stability class and the wind vector at the anemometer position are inserted in the catalogue for each wind field.

Note: Subdirectory `lib` may not contain other than the library files.

During the dispersion calculation, a wind field for a given stability class, wind speed, and wind direction is required; the catalogue is checked for two base fields of the given stability with a wind direction as close as possible to the given one;²⁹ these fields are superposed so that the resulting field takes the desired wind speed and wind direction at the anemometer position. The same superposition factors are applied to combine the according turbulence and exchange fields (if they exist).

This procedure is also applied for nested grids (see Section 3.8). Here, the fields must be provided for each grid. The grid number n ($1 \leq n \leq n_n$) must be specified in the file name, it replaces the string `00` at the end of the name in the form `i1` with $i = n_n + 1 - n$. For

²⁸The setting "lsbf 1" states that the least significant byte comes first in binary encoding of the data part. This is the default for processors of Intel and AMD.

²⁹This implies that at least two wind fields must be provided for each stability class.

example, for three nested grids the wind fields defined in the finest grid are stored in files `w????a31.dma`.

Note: With nested grids in complex terrain the terrain profiles must be tuned at the grid edges: the two outermost stripes of a finer grid must contain the height values of the next coarser grid, either directly or derived by means of linear interpolation. It is therefore recommended to first create the terrain profiles `lib\zgi1.dma` with `TALdia` and then to apply these data in the external wind field calculation (note that the files `zg01.dma` in the project directory are not suited). This can be done by calling `TALdia` with option `-oGRIDONLY` so that it stops after the profiles are written out. Note that the program checks whether the internally tuned profiles coincide with the ones given in the wind field files and aborts if larger differences (> 0.2 m) are encountered.

Example:

Directory `house-01` contains an example with an externally created wind field library. The wind fields describe the flow around an u-shaped building for a cell size of 4 m and 40 times 50 cells in the horizontal. The vertical cell size is also 4 m and the grid extends up to a height of 60 m above ground. For a better illustration of the buildings effects, the source is placed inside the patio of the building at a height of 2 m. SO_2 is emitted with a source strength that corresponds to 10% of the bagatelle mass flow according to *TA Luft*.

The library contains wind fields, fields of additional turbulence, and fields of additional exchange coefficients for neutral stability and wind directions between 200 deg and 280 deg in steps of 10 deg. This is sufficient to run the first day of `AKTerm anno95.akterm`.

3.8 Choice of calculation grids

Usually only a single grid is applied if no buildings are defined. The grid is set by the user or automatically generated by the program. The program applies settings such that the cell size is sufficiently small for the lowest source and the distance to the edge of the calculation grid sufficiently large for all sources. This implies according to *TA Luft* that the horizontal cell size is set equal to the construction height of the lowest source (but without buildings at least 16 m) and that for all sources a circle with a radius of 50 times the construction height with the source in its centre is fully contained in the calculation area. Here, the construction height is the average height defined by the real construction height `hq` plus half the vertical extension `cq`.

*Note: If the calculation area is explicitly set in the input file, all parameters must be defined, i.e. `dd`, `x0`, `nx`, `y0`, and `ny`. The parameters `dd`, `x0`, and `y0` should be integer numbers as internal rounding errors may cause problems otherwise (for example, $3*0.1$ is not exactly 0.3 in the internal handling of the computer).*

For calculations with buildings or for source configurations with strongly varying construction heights this procedure is not straightforward: buildings and low sources require a small horizontal cell size and at the same time a large area must be covered because of the high sources; in addition, at large distances an unnecessarily small horizontal cell size is applied which causes large statistical uncertainties in the modelled concentrations.

This can be avoided by the use of nested grids: In the surrounding of buildings and low sources a grid with a small cell size and further outside a grid with a larger cell size is applied. There are several restrictions such a set of nested grids must obey in order to minimize artifacts in the calculated concentration fields:

- The horizontal cell size must increase from a finer to the next coarser grid by exactly a factor of 2.
- The edges of a finer grid must coincide with grid lines of the next coarser grid.
- A coarser grid must have at least the extension of the next finer grid. It is recommended to keep a distance between the edge of a coarser grid and the one of the next finer grid of at least 4 cell sizes of the coarser grid.
- The finer grids must have an extension in each coordinate direction that is 2 cells larger than required according to *TA Luft* because the values in the two outermost rows respectively columns may not be used for evaluation.³⁰

A single grid is set up by the program if no buildings are defined. Nested grids are enforced by specifying the string `NESTING` in the option parameter `os`. The applied grid parameters are listed in the log file. They may be copied for explicit use directly into the input file.

If nested grid are defined by the user in the input file, the grids must be specified in increasing order of the horizontal cell size.³¹ A valid grid specification for a point source at 50 m height and located in the origin of the coordinate system is for example:

dd	50	100	200
x0	-1100	-2200	-2800
nx	44	44	28
y0	-1100	-2200	-2800
ny	44	44	28

Additional features must be accounted for in case buildings are defined:

1. Buildings are rasterized on the calculation grid. Horizontal cell size and vertical intervals must be chosen such that the buildings are sufficiently well resolved in the calculation grid. The rasterization can be checked at hand of the files `volout01.dmn` that are written out by *TALdia*.

³⁰The values may be distorted due to the mapping of the grids.

³¹Option `NESTING` is not required in this case.

2. For nested grids, buildings are accounted for in the wind field calculation only in the finest grid (the one with the smallest horizontal cell size). A building influences the downstream wind up to a distance of typically 5 times the building height. The extension of the finest grid should be chosen accordingly. The boundary stripes of the grid may not contain buildings.
3. To guarantee good convergence of the iterative calculation of the wind field in the finest grid, its vertical intervals should be as far as possible constant. The finest grid should extent vertically up to twice the height of the highest building. Both conditions can be met by an appropriate setting of the vertical grid (hh) and the upper edge of the finest grid (nz).
4. The influence of buildings on the turbulence properties of the flow downstream extends up to typically 10 times the building height. If the finest grid has a smaller extension, then the additional turbulence fields are created also for the next coarser grid; in this case the horizontal cell size of that grid should also be sufficiently small to resolve the buildings. This condition on grid extension must be met as well if only a single grid is applied.

If no user-defined grids are provided the program tries to meet all of these conditions when automatically setting up the grids. For calculations with buildings, nested grids are applied by default. This can be suppressed with the string -NESTING in the option parameter os. Both the building and the source configuration are accounted for in the automatic setting of the grids. The maximum building height and the parameters of the nested grids are listed in the log file.

The program calculates the concentration and deposition for each of the grids. To distinguish the different results, the grid number is appended to the name of a result file (starting with 1 for the finest grid). For the set of nested grids stated in the example above, the files so2-j00z01.dmna, so2-j00z02.dmna, and so2-j00z03.dmna are created instead of file so2-j00z.dmna.

The maximum of the characteristic immission values which are listed in the log file are the absolute maxima across the grids. This means for example for the result type h24 (hourly mean exceeded 24 times) that first the value H24 is calculated for each grid cell in each grid and then the absolute maximum is selected and written to the log file, together with the information in which grid this value occurs.

Note: For nested grids and terrain profile the applied digital terrain profile must cover the coarsest grid.

For nested grids, the surface files derived by the digital terrain profile include in their name instead of 00 the grid number, for example zg03.dmna.

3.9 Discharge of exhaust by stacks and cooling towers

Plume rise in connection with the discharge of exhaust by stacks is parametrically calculated according to guideline VDI 3782 Part 3. The plume rise formulae of the guideline are applicable for wind speeds at construction height $u_q > 1$ m/s. To allow an application in practice for arbitrary AKTerm time series, plume rise for $u_q < 1$ m/s is calculated with the value 1 m/s.

The plume rise of exhaust released by cooling towers is parametrically calculated according to guideline VDI 3784 Part 2.

Note: A source is interpreted as cooling tower if parameter lq (liquid water content) or rq (relative humidity) has a value larger 0.

A recent study on modelling the discharge by cooling towers with the model combination AUSTAL2000/TALdia points out the following aspects:³²

- The cooling tower should be explicitly modelled as a building (tower).
- The mean diameter should be used for the diameter of the tower.
- The vertical grid should be chosen such that the upper edge of the cooling tower (and other buildings) is close to a grid surface.
- The cooling tower as an emitter should be specified in form of an area source (square in the centre of the outlet). The source height should be slightly above the height of the rastered cooling tower.
- Nested grids should be used.

The calculation is carried out internally with the help of the program *VDISP* which is made available by the VDI. AUSTAL2000 creates the required input file *VDIIN.DAT* in the project directory, invokes the program *vdisp.exe* and reads in the results out of file *VDIOUT.DAT* located in the project directory. The slope of plume rise as calculated by *VDISP* is analysed and the parameters vq and sq are internally set such that in the dispersion calculation the same final rise (effective source height) and at the same distance half the final rise is achieved (see verification 51c). Hence the program even goes beyond the demand of guideline VDI 3784 Part 2 which states that just the effective source height needs to be adopted by the dispersion model.

³²Bahmann, W., Schmonsees, N., Janicke, L. (2006): *Studie zur Anwendbarkeit des Ausbreitungsmodells AUSTAL2000 mit Windfeldmodell TALdia im Hinblick auf die Gebäudeeffekte bei Ableitung von Rauchgasen über Kühltürme und Schornsteine* (study on the applicability of the dispersion model AUSTAL2000 with wind field model TALdia in view of building effects for the discharge of exhaust gases by cooling towers and stacks), VGB research project Nr. 262, see Internet www.vgb.org/data/vgborg_/Forschung/FE262.pdf.

To avoid making this analysis for each individual simulation particle, *AUSTAL2000* creates an internal table of the situations that have been already calculated by *VDISP* and the resulting values for v_q and s_q . If plume rise has to be calculated for a simulation particle, this table is checked first to see whether the required values are already available. Here, a deviation of the wind speed of up to 10% is tolerated.

In case that the program *VDISP* aborts without having calculated the plume rise (for example because of a Froude number that is too small), the calculation for this situation is carried out without plume rise and at the end of the dispersion calculation an according warning message is written to the log file.

With regard to the application of *VDISP* in the context of *TA Luft*, the co-author of the model, guideline and program *VDISP*, Prof. Schatzmann, makes the following statement:

Die Ableitung der Rauchgase zusammen mit dem Wasserdampfschwaden über einen Naturzugnasskühlturm ist attraktiv, weil Kühlturmschwaden verglichen mit Schornsteinfahnen einen wesentlich größeren Wärmeinhalt besitzen. Die das Verhältnis von Impuls- zu Auftriebskräften am Einleitungsort kennzeichnende hydrodynamische Ähnlichkeitskennzahl, die densimetrische Froudezahl, unterscheidet sich bei Schornsteinfahnen und Kühlturmschwaden um etwa eine Größenordnung. Die relative Bedeutung der Auftriebskräfte ist bei Kühlturmschwaden somit etwa 10 mal größer als bei Rauchgasfahnen aus Schornsteinen. Dies führt vor allem bei geringen Windgeschwindigkeiten zu größeren effektiven Quellhöhen. Da sich das zu erwartende Bodenkonzentrationsmaximum in etwa invers proportional zum Quadrat der effektiven Quellhöhe verhält, wird in diesem Geschwindigkeitsbereich der Kühlturm zu geringeren Immissionen führen als der Schornstein.

Bei Starkwind kehren sich die Verhältnisse dagegen um. Kühlturmschwaden treten im Vergleich zu Schornsteinfahnen mit einer viel geringeren Vertikalgeschwindigkeit in die Atmosphäre ein. Bei Starkwind übersteigt in Kühlturmkronehöhe die Windgeschwindigkeit die Schwadenaustrittsgeschwindigkeit, mit der Folge, dass Teile des Schwadens in den Kühlturmnachlauf gezogen und zum Boden

gemischt werden. Zusätzliche "down-wash"-Effekte gehen von anderen hohen Bauwerken des Kraftwerks und seiner Umgebung aus. Da hohe Windgeschwindigkeiten seltener vorkommen als geringe, bleibt – betrachtet über repräsentative Zeiträume – die Ableitung der Abgase zusammen mit dem Kühlturmschwaden die günstigere Ableitungsvariante. Da die Intensität der "down-wash"-Erscheinungen von der speziellen Geometrie des Kraftwerkskomplexes und seiner Umgebung abhängt, ist allerdings jeweils zu prüfen, ob diese generelle Aussage auch im Einzelfall zutrifft und die in der TA-Luft festgeschriebenen Immissionswerte eingehalten werden.

Die komplexen Schwaden/Bauwerks-Wechselwirkungen lassen sich mit numerischen Modellen derzeit noch nicht simulieren. Deshalb werden üblicherweise in Grenzschicht-Windkanälen Experimente durchgeführt, mit dem Ziel, sogenannte Verstärkungsfaktoren zu bestimmen. Diese Faktoren dienen dazu, Rechenergebnisse zu korrigieren, wie sie mit den im Genehmigungsverfahren üblicherweise verwendeten Standardmodellen für die Bestimmung von Immissionskennwerten nach TA-Luft ermittelt werden. Diese Standardmodelle setzen die freie Abströmung der Abgase in eine ungestörte Windströmung voraus. Bauwerkseinflüsse können sie nicht berücksichtigen.

The examples **tower-01** and **tower-02** apply the cooling tower which is described as an

example in guideline VDI 3784 Part 2. The example `tower-01` uses standard settings; it reveals 1) the maximum concentration is far away because of the strong plume rise, 2) the required statistical uncertainty is hard to meet. Therefore example `tower-02` applies a larger calculation area and an appropriate horizontal cell size that has been increased from 130 m to 500 m.

The verification test 51c compares the slope of plume rise as calculated with *VDISP* with the one obtained by *AUSTAL2000*.

Beside the parameterization of plume rise either according to VDI 3782 Part 3 or according to VDI 3784 Part 2, plume rise can be explicitly defined by means of the parameters `vq` and `sq`, also in form of a time series.

3.10 Rated frequency of odor hours

In a simple dispersion calculation for the derivation of odor hour frequencies, no distinction is made between different odorant types. All odorants are merged into the single substance odor and for this substance the frequency of odor hours r is determined.

In contrast, the new Guideline on Odour Immissions³³ prescribes a more sophisticated procedure for odor emissions in the context of animal husbandry. It accounts for the fact that for example odor of chicken farms is more annoying than odor of cowsheds; the frequencies of odor hours are separately determined for each animal type and then, together with type-specific rating factors, used to derive an overall rating factor:

First, all odor emissions are merged into a single substance S and the (unrated) frequency of odor hours r is calculated.

Second, four odorant classes S_i ($i=1, \dots, 4$) are defined, where each class contains all odorant species to which a common rating factor f_i is assigned. The classes are sorted by descending rating factor, i.e. $f_i > f_{i+1}$ must hold. The frequencies of odor hours r_i are separately calculated for each class.

The calculated values obey the relation

$$0 \leq r_i \leq r \leq 1 \quad (1)$$

The rated frequency of odor hours r_b should satisfy the following conditions:

1. If there is only one odorant class S_i , $r_b = f_i r_i$ and also $r_i = r$.
2. If there are mixtures of odorant classes, r_b is a continuous function of the values r_i and an increase of a value r_i does not cause a decrease of r_b .

³³Guideline on Odour Immissions (*Geruchsimmissions-Richtlinie*, GIRL), version of February 29, 2008, with extensions of September 10, 2008.

The algorithm described in the following guarantees this for the case $\sum r_i \geq r$.

The following auxiliary quantities h_i are formed:

$$h_1 = r_1, \quad (2)$$

$$h_2 = \min(r_2, r - h_1), \quad (3)$$

$$h_3 = \min(r_3, r - h_1 - h_2), \quad (4)$$

$$h_4 = \min(r_4, r - h_1 - h_2 - h_3) \quad (5)$$

For all h_i it holds that

$$0 \leq h_i \leq r_i \quad (6)$$

The rated frequency of odor hours r_b is then calculated from the unrated frequency r and the rating factor f_{total} :

$$r_b = f_{\text{total}} r \quad \text{with} \quad f_{\text{total}} = \frac{1}{\sum_i h_i} \sum_i f_i h_i \quad (7)$$

This quantity determines the characteristic value IG_b (given in percent) according to GIRL.

The rating factor f_{total} can be larger than 1 and thus the calculation may yield frequencies of odor hours exceeding the value 100%. This is prevented by setting an upper limit for IG_b (given as percent of the total hours):

$$\text{IG}_b = 100 \min(r_b, 1) \quad (8)$$

Working with type-specific emissions

The prescribed calculation steps are automatically carried out by *AUSTAL2000* if the user specifies rated odorant classes. They have names of the form `odor_nnn`, where *nnn* is an integer number that points to the rating factor. The following odorant classes are recognized by *AUSTAL2000*:

Class name	Rating factor
<code>odor_040</code>	0.40
<code>odor_050</code>	0.50
<code>odor_060</code>	0.60
<code>odor_075</code>	0.75
<code>odor_100</code>	1.00
<code>odor_150</code>	1.50

Note: The GIRL regulates the assignment of odorant types respectively animal types to the odorant classes. To present knowledge, the rating factors 0.4 (instead of 0.5) and 0.6 (instead of 0.75) are only applied in the federal state Baden-Württemberg.

If in the input file emissions are specified for rated odorant classes, *AUSTAL2000* ignores any setting of `odor` and sets the emission for this substance according to the sum over all odorant classes. Therefore, in this case the user should not explicitly specify `odor`.

As result, the unrated frequency of odor hours both for the merged substance `odor` (r) and the applied odorant classes (r_i) and the rated frequency of odor hours under the name `odor_mod` (IG_b) are written out.

A simple and instructive application of rated odorant classes is given in the verification test 02 (Section A). A more practical application is the example `odor\h20rated`.

4 Examples

The distribution of *AUSTAL2000* includes several example calculations which are installed to the subdirectory *test*. One of these examples is used in the following to give a brief introduction into running *AUSTAL2000*. The section ends with a listing of all examples.

4.1 Example calculation

It is assumed that *AUSTAL2000* and the examples have been installed on a Windows system according to the specifications of Section 2.

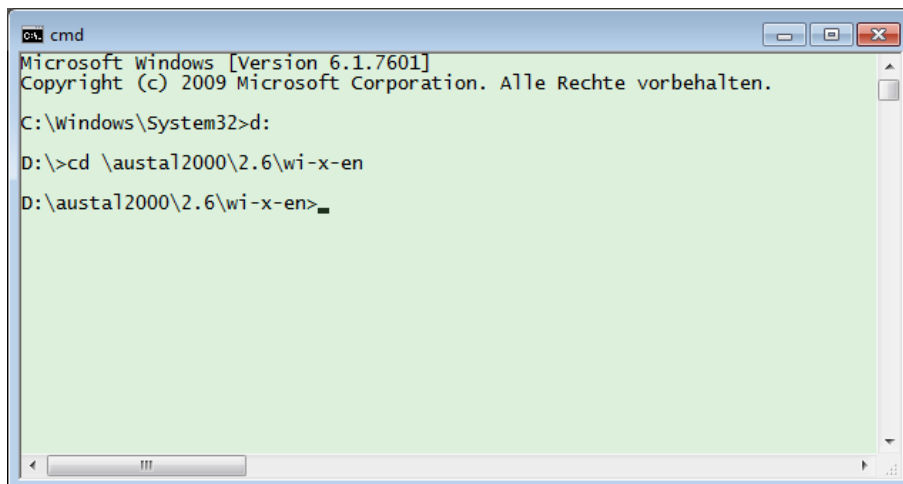
First a DOS shell must be opened in order to execute the program. Proceed to menu

Start → Programs → Accessories

and select the menu *Command Prompt*. A new windows opens into which commands can be written.

Left to the command prompt ('>') the current drive (e.g. C:) and the current directory is listed. Change to the drive and directory, where *AUSTAL2000* has been installed, i.e. where the executable program *austal2000.exe* is located.

Typing the drive letter followed by a colon and then pressing the RETURN key changes the current drive. The command *cd* (change directory) can be used to change to the desired directory. The following figure shows an example. The command *dir* can be used to list the files of the current directory.



```
cmd
Microsoft Windows [Version 6.1.7601]
Copyright (c) 2009 Microsoft Corporation. Alle Rechte vorbehalten.

C:\Windows\System32>d:
D:\>cd \austal2000\2.6\wi-x-en
D:\austal2000\2.6\wi-x-en>
```

The example project *simple* is run which is located in a subdirectory (project directory) of directory *test*. All input data are specified in file *austal2000.txt* which has the following content:

```
ti "Test Simple"
az "../anno95.akterm"
z0      0.5
hq      20
so2     2.78 ' 10 kg/h
qs      -4
```

The first line contains the project title, the second line the file name of the AKTerm to be applied. The path is given relative to the project directory, thus the statement refers to the AKTerm with name `anno95.akterm` in directory `test`. The following line specifies the average surface roughness length.

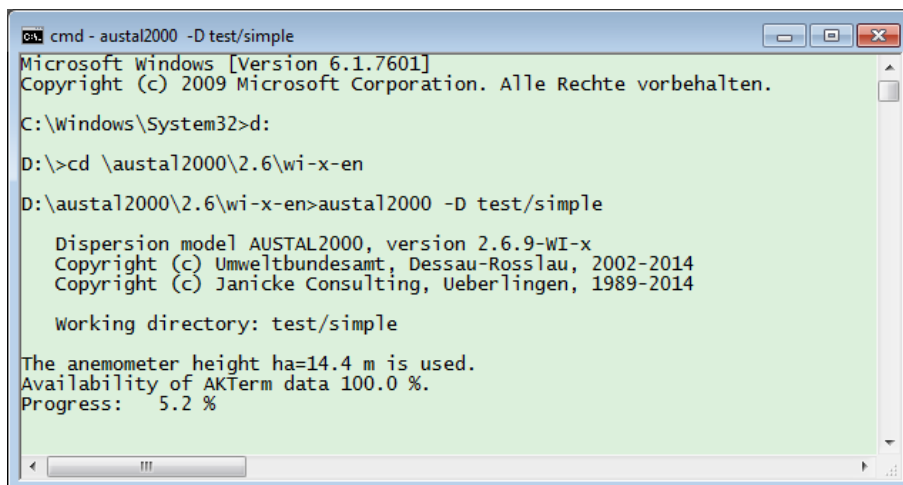
The source position `xq` and `yq` is not explicitly stated, thus the default values 0 are applied. The source height is 20 m and SO₂ is emitted with a constant emission strength of 2.78 g/s.

The calculation grid is automatically generated by the program. The quality level -4 is pretty low in order to minimize calculation time for this test example. The dispersion calculation is started with the command

```
austal2000 -D test/simple
```

Option `-D` deletes an existing log file `austal2000.log` in directory `simple` before the calculation, otherwise log information is appended to the file.

Several information is written to the DOS window (program version, calculation progress), see the following figure. A final message is prompted when the dispersion calculation and the subsequent result evaluation have finished.



```
cmd - austal2000 -D test/simple
Microsoft Windows [Version 6.1.7601]
Copyright (c) 2009 Microsoft Corporation. Alle Rechte vorbehalten.

C:\Windows\System32>d:
D:\>cd \austal2000\2.6\wi-x-en
D:\austal2000\2.6\wi-x-en>austal2000 -D test/simple

Dispersion model AUSTAL2000, version 2.6.9-WI-x
Copyright (c) Umweltbundesamt, Dessau-Rosslau, 2002-2014
Copyright (c) Janicke Consulting, Ueberlingen, 1989-2014

Working directory: test/simple

The anemometer height ha=14.4 m is used.
Availability of AKTerm data 100.0 %.
Progress: 5.2 %
```

The project directory `simple` now contains the log file `austal2000.log` with information on the program, the program run, the applied input data of file `austal2000.txt`, and a list with the main results of the dispersion calculation.

Note: Input file and log file are simple text files that can be inspected and edited with any text editor (e.g. by double-clicking the file name in an Explorer window).

The project directory `simple` contains as well DMNA files with the concentration distributions near ground for the various characteristic immission values (annual mean, short-time values). These files are also simple text files (see Section B.1). Their contents can be processed further with suitable programs (e.g. OpenOffice or Excel).

4.2 Examples

The following contains a brief description of the examples that are part of the *AUSTAL2000* distribution. All examples are located in subdirectory `test` and can be individually run with the command

```
austal2000 -D test/Example
```

The applied meteorological data and terrain profile are located in directory `test`.

The examples `h50aks` and `h50a95` to `h50a99` are discussed in more detail in the final report of the AUSTAL2000 project.

Note: To rerun from scratch examples with buildings or terrain profile, the subdirectory `lib` with the wind field library and the files `zgj.j.dmn` must be deleted, otherwise AUSTAL2000 takes these data instead of recalculating them.

`h50aks`

Calculation with the dispersion class statistics `anonym.aks` for a stack of 50 m height; no plume rise; substances SO_2 , NO, NO_2 , and PM-10.

`h50a95` bis `h50a99`

Calculations with AKTerm `anno95.akterm` to `anno99.akterm` for a stack of 50 m height; no plume rise; substances SO_2 , NO, NO_2 , and PM-10 (`h50a95` also including substance `xx`).

`2h50a95`

Calculation with AKTerm `anno95.akt` for two stacks of 50 m height separated by 750 m; no plume rise, substances SO_2 , NO, and NO_2 .

`h50a95-2`

Calculation with AKTerm `anno95.akterm` for two stacks of 50 m height separated by 750 m; time-dependent emission of SO_2 ; additionally a diffusive source with constant emission of plumbiferous dust; no plume rise.

h50a95g

Like example h50a95. In addition, a time series with background concentrations is processed and the surface roughness length z_0 is automatically set.

h50a95gaps

Like example h50a95gaps, but the applied meteorological time series contains about 10% measurement gaps that are internally handled by the program.

h00aks-nh3

Calculation with the dispersion class statistics `anonym.aks` for a wind-induced emission by a stable which is modelled in form of a volume source.

h30a95h1

Simple demonstration of a calculation with complex terrain (idealized hill with a Gaussian shape).

h30a95h0

Like example h30a95h1, but for flat terrain.

h50a95c

Like example h50a95, but with complex terrain (realistic terrain profile).

h50a95n

Like example h50a95, but with automatic generation of nested grids (flat terrain).

h50a95cn

Like example h50a95c, but with automatic generation of nested grids (complex terrain).

house-01

Flow around an u-shaped building with the application of an externally generated wind field library. The calculation period is one single day.

tower-nn

Discharge of SO₂ by a cooling tower. Plume rise is calculated according to guideline VDI 3784 Part 2. In this simple example the influence of the cooling tower as a building is not accounted for in the dispersion calculation (see Section 3.9). The examples refer to the one of guideline VDI 3784 Part 2.

h50a95-sci

Like example h50a95, but the results are written out in scientific notation (option SCINOTAT).

body\h25a95

Calculation with AKTerm `anno95.akterm` for a stack of 25 m height on top of a building complex.

body\h50a95cb

Like example h50a95c, but with a tower-like building close to the stack.

body\raster

Calculation with AKTerm anno95.akterm for a stack of 15 m height on top of a building complex which is specified in a raster file.

odor\h10aksn

Calculation with the dispersion class statistics anonym.aks for a volume source near ground that emits an unrated odorant; nested grids; receptor points.

odor\h50a95

Like example h50a95, but with the emission of an unrated odorant.

odor\h20rated

Example for a calculation with rated odorant classes. Each of two sources emits a rated odorant class (odor_100 and odor_050), the calculation is carried out with the dispersion class statistics anonym.aks.

dust

Test calculations for settling dust, see Annex E.

spread

Test calculations for artificial immission structures, see Annex F.

prfmod

Test calculations for the modified boundary layer model model, see Annex H.

A Verification tests

Guideline VDI 3945 Part 3 (Lagrangian particle model) states in Annex D a series of verification tests. They must be used to check the correct functionality of a program implementation of the model that is described by the guideline. The tests cover special situations for which the correct solutions are known and against which the simulation results can be checked.

Usually it would not be possible to run these tests with *AUSTAL2000* as it is designed to meet the requirements of the *TA Luft*. Therefore some program extensions have been implemented that allow to rerun the verification tests. These extensions are addressed by the input parameter *os*.

Note: These extensions have been exclusively designed and checked for the verification tests and may not be used for dispersion calculations according to TA Luft.

All extensions require the key *NOSTANDARD* as part of the option string (parameter *os*). A corresponding warning message is written to the log file if this key is used.

The key *PERIODIC* enforces periodic boundary conditions. This implies that particles which leave the calculation grid in *x*- or *y*-direction enter into it again on the opposite side. In the *z*-direction at the top of the calculation grid particles are reflected (like at the ground). Thus, no particle can leave the calculation grid.

The key *LIB2* enforces in case of buildings the creation of only two (instead of 36) base fields per stability class for the wind field library. This is useful if only a single meteorological situation is considered.

The key *NOSHEAR* suppresses wind shear with height.

The following parameters can be set in the option string *os* in the form "*Name=Value*;" (case sensitive, no blanks allowed):³⁴

Blm : Version of the boundary layer model (see below).

Groups : Number of particle groups used to estimate the statistical uncertainty.

Kmax : The concentration distribution for all daily means are written out for all layers $1 \leq k \leq Kmax$. The file name has the form *Substance-nnp.dmma*, where *nnn* is a running index and *p* the type of value (a for the concentration, s for the statistical uncertainty).

Kref : Like *Kmax* but only the layer $k = Kref$ is written out.

Rate : Emission rate of simulation particles per second (replaces the setting by *qs*).

³⁴ Additional parameters which may influence the calculation results and are solely designed for test purposes are: *Interval*, *Average*, *MntMax*, *DMKp*, *CHECKVDISP*, *Svf*, *Ftv*, *Tau*, *TRACE*, *TAS*.

Su, Sv, Sw : Direct specification of the wind velocity fluctuations $\sigma_{u,v,w}$.

Tau : Maximum time step for the movement of particles. In the context here it is used to select a value smaller than the one that would be chosen by the program such that a spatially homogeneous time step is applied.

Us : Direct specification of the friction velocity u_* .

Vd : Direct specification of the deposition velocity (replaces the default value of all considered substances).

Vs : Direct specification of the settling velocity (replaces the default value of all considered substances).

The following boundary layer profiles can be selected by the version number **Blm**, they all differ from the default ones described in guideline VDI 3783 Part 8:

Blm=0.1: A homogeneous turbulence field and a homogeneous wind field of strength u_a is created. The velocity fluctuations σ_u , σ_v , and σ_w are defined explicitly by parameters **Su**, **Sv**, and **Sw**, likewise the friction velocity (**Us**). The Lagrange correlation times are calculated as follows:

$$\begin{aligned} T_{u,v} &= 100 \\ T_w &= 10z_0/u_* \end{aligned}$$

Blm=0.5: The following inhomogeneous profiles are used:

$$\begin{aligned} u(z) &= u_a \left(\frac{z}{h_a} \right)^{0.3} \\ \sigma_{u,v} &= 10^{-6} \text{ m/s} \\ \sigma_w(z) &= Sw \sqrt{z/h_a} \\ T_{u,v,w} &= z_0/u_* \end{aligned}$$

Blm=0.7: An inhomogeneous turbulence field is used:

$$\begin{aligned} \sigma_{u,v} &= Su, Sv \\ \sigma_w(z) &= Sw \left[1 - \frac{z_0}{h_a} \sin \left(\frac{z\pi}{2\hat{z}} \right) \right] \\ T_{u,v} &= 20z_0/u_* \\ T_w &= \frac{z_0}{u_*} \left[1 + 20 \sin \left(\frac{z\pi}{2\hat{z}} \right) \right] \end{aligned}$$

$\hat{z}$ is the upper edge of the calculation grid.

Further specifications are described in the sections of the individual verification tests.

A verification test has a 2-digit identification *nn* that refers to the according section in guideline VDI 3945 Part 3. A test is located in the directory `verif\nn`. An individual evaluation program with name `verifnn` exists for each test. The executable programs are located in directory `verif`, the source code (file `verifnn.c`) in directory `source`.

The test calculations are carried out with the command `austal2000 verif/nn`. The results are evaluated with the command `verif\verifnn`. To process all verification tests including evaluation, the commands

```
verif\verify
verif\evaluate
```

can be used. The evaluation results are appended to file `verif\result.txt`. The results shown in the following apply to program version 2.6.11-WG-0.

00 Estimation of the sampling error

A calculated concentration value is subject to a statistical uncertainty that leads to a deviation from the expectation value. Whether a deviation is significant or not can be judged by the sampling error that is automatically estimated by the program. Therefore, at first it has to be checked whether the program correctly estimates the sampling error.

A calculation area of $1000 \times 1000 \text{ m}^2$ with 50×50 horizontal cells is applied. Only a single cell of extension 200 m is defined in the vertical. The calculation runs over a time series of 10 days, particles are emitted in the last hour of the first day across the whole calculation grid. Periodic boundary conditions are applied so that no particle can leave the calculation grid. Turbulence is constant in time and space. The concentration should be the same in all grid cells and deviations purely random.

Calculation grid: $1000 \times 1000 \times 200 \text{ m}^3$, divided into $50 \times 50 \times 1$ cells; periodic boundary conditions.

Meteorology: Homogeneous turbulence with $ua=0.2$, $ra=270$, $z0=0.5$, and
`"Blm=0.1; Su=1.2; Sv=1.0; Sw=0.65; Tau=10; Us=0.2;"`; time series over 10 days.

Source: Volume source extended over the whole calculation grid; emission only in the last hour of the first day; `"Groups=36; Rate=0.01;"` implying that each group only contains a single particle; the total emission is 360 kg, the theoretical mean concentration $1800 \mu\text{g}/\text{m}^3$.

N	Mean	Observed	Estimated
1	37.6	96.6	74.1
2	1800.0	13.8	14.0
3	1800.0	14.5	14.0
4	1800.0	14.9	14.1
5	1800.0	14.3	14.0
6	1800.0	13.8	14.1
7	1800.0	14.1	14.0
8	1800.0	13.6	14.0
9	1800.0	13.5	14.0
10	1800.0	14.7	14.1

The evaluation shown in the table to the left lists for each day N the modelled Mean, the observed sampling error derived from the variation of concentrations in the 50×50 grid cells (column Observed, in percent), and the sampling error estimated by the program for each grid cell (column Estimated, quadratic mean over all cells, in percent). The median of the observed sampling error over all applicable 9 days is 14.1 %, the average of the estimated sampling error is 14.0 %.

01 Calculation of odor hour frequencies

It is checked if the presence of an odor hour is properly identified and if the estimate of the sampling error of the odor hour frequency is correct.

Similar to verification 00, a calculation area of $200 \times 200 \text{ m}^2$ is applied with one vertical cell of size 200m. The calculation covers 10 days with an emission only in the last hour of the first day. Periodic boundary conditions are applied so that no particle can leave the calculation grid. Turbulence is constant in time and space. The concentration should be the same in all grid cells and deviations purely random.

The emission is set such that the average concentration should be 0.25 OU/m^3 , implying that there is a 50% probability for an odor hour. To track beside the odor hour frequency also the mean concentration, the substance xx with the same emission is defined together with substance odor. In addition to the 10 daily means, the time series of concentration and odor hour frequency is reported for 10 receptor points. Here, the frequency (existence of an odor hour) is based on a plain yes/no decision.

Calculation grid: $200 \times 200 \times 200 \text{ m}^3$, divided into $10 \times 10 \times 1$ cells; periodic boundary conditions.

Meteorology: Homogeneous turbulence with $ua=0.2$, $ra=270$, $z0=0.5$, and
 "Blm=0.1; Su=1.2; Sv=1.0; Sw=0.65; Tau=10; Us=0.2;"; time series over 10 days.

Source: Volume source extended over the whole calculation grid; emission only in the last hour of the first day; "Groups=36; Rate=0.1;" implying that each group contains 10 particles; the total emission is 2000 kOU (respectively 2000 kg), and the mean concentration 0.25 OU/m^3 .

Mean daily concentration value:

N	Mean	Observed	Estimated
1	0.005220	5.50	5.96
2	0.250027	0.82	0.83
3	0.250021	0.96	0.82
4	0.250015	0.94	0.84
5	0.250017	0.90	0.83
6	0.250021	0.73	0.82
7	0.250021	0.69	0.83
8	0.250021	0.81	0.83
9	0.250019	0.78	0.82
10	0.250019	0.95	0.82

0.25 OU/m³. The median of the real sampling error over all applicable 9 days is 0.82 %, the average of the estimated sampling error is 0.83 %.

The evaluation shown in the table to the left lists for each day N the modelled mean concentration Mean, the real sampling error derived from the variation of concentrations in the 50 × 50 grid cells (column Observed, in percent), and the sampling error estimated by the program for each grid cell (column Estimated, quadratic mean over all cells, in percent). Given the accuracy of 4 significant places for the numbers in the result files, the calculated mean is just the expected value of

Time series of concentration values:

P	Mean	Observed
1:	0.25079	4.323
2:	0.25050	4.028
3:	0.25030	3.925
4:	0.25106	4.083
5:	0.25024	4.055
6:	0.24866	4.122
7:	0.25141	4.244
8:	0.25069	4.153
9:	0.25002	4.285
10:	0.25002	3.858

The table to the left lists the evaluation of concentration time series at the 10 receptor points (column P) with respect to days 2 to 10. Column Mean contains the concentration average over the 9 days, column Observed the observed sampling error of the hourly mean. The latter should be a factor of $\sqrt{24}=4.9$ larger than the sampling error of the daily mean, i.e. about 4.26 %. The observed value is 4.1 % (median).

Mean daily value of odor hour frequency:

N	Mean	Observed	Estimated
1	0.00	0.00	0.00
2	49.62	10.62	8.26
3	49.29	10.31	8.32
4	48.59	10.16	8.29
5	49.17	11.23	8.32
6	49.21	8.63	8.32
7	50.08	8.92	8.23
8	50.55	9.07	8.21
9	48.66	10.36	8.24
10	48.71	11.15	8.30

percent of the hours of the day). The mean is slightly below the theoretical value of 50%. The median of the real sampling error over the 9 applicable days is 10.31, the average of the estimated error is 8.29.

The evaluation shown in the table to the left lists for each day N the observed mean Mean of the odor hour frequency (percent of the hours of the day). The real sampling error is calculated from the variation of frequencies across the 10 × 10 grid cells (column Observed, percent of the hours of the day). This is compared to the sampling error as estimated by the program for each cell (column Estimated, quadratic mean over all cells, in

The observed sampling error agrees with the expectation: To exactly half of the hourly means an odor hour should be assigned. The mean is therefore 0.5, likewise the average standard deviation. The standard deviation of the daily mean should therefore amount to $0.5/\sqrt{24} = 10.2\%$.

The theoretical value of the sampling error as estimated by the program can be deduced from the following consideration: The parameters of this calculation are chosen such that the expectation value $\bar{c}$ of the single hourly means c is equal to the assessment threshold

$c_{BS} = 0.25 \text{ OU/m}^3$. The single values scatter around this mean with a standard deviation σ which amounts to about 4% of the mean, as shown before. Thus approximately a Gaussian distribution can be assumed,

$$g(c) = \frac{1}{\sqrt{2\pi}\sigma} \exp\left[-\frac{(c - c_{BS})^2}{2\sigma^2}\right] \quad (9)$$

$$G(c) = \int_{-\infty}^c g(c') dc' \quad (10)$$

The following odor hour frequency α with variance v is assigned to a given value c :

$$\alpha(c) = G(c) \quad (11)$$

$$v(c) = \alpha(c)[1 - \alpha(c)] \quad (12)$$

The mean of the variance is

$$\bar{v} = \int_{-\infty}^{+\infty} v(c)g(c) dc \quad (13)$$

$$= \int_{-\infty}^{+\infty} G(c)[1 - G(c)]g(c) dc \quad (14)$$

$$= \frac{1}{6} \quad (15)$$

The integral can be exactly solved by partial integration. The standard deviation of the daily mean (average over 24 single values) is therefore $1/\sqrt{6 \times 24} = 0.083333$, i.e. 8.33% of the hours of the day, in very good agreement with the value estimated by the program.

The observed standard deviation is slightly higher. However, it is not worth the effort to apply here statistically more elaborate methods as the effects discussed in Annex G dominate in practice (calculations based on a AKTerm or AKS). As a consequence, the statistical uncertainty reported by the program for the odor hour frequency is not suitable for an estimate of the accuracy of the result.

Time series of odor hour frequency:

P	Mean	Observed	Counted
1:	52.31	49.95	52.31
2:	51.39	49.98	51.39
3:	50.00	50.00	50.00
4:	49.07	49.99	49.07
5:	50.00	50.00	50.00
6:	46.30	49.86	46.30
7:	59.72	49.05	59.72
8:	50.46	50.00	50.46
9:	49.07	49.99	49.07
10:	50.00	50.00	50.00

The table to the left depicts the evaluation of the time series of odor hour frequencies at the 10 receptor points (column P) for days 2 to 10. Column Mean lists the frequency averaged over the 9 days (median is 50.00% of the total hours), column Observed lists the observed sampling error of the frequency values. For comparison, column Counted lists the frequency of odor hours that results from simply counting the concentration values $c \geq c_{BS}$ in the time series for substance

xx. It is identical to column Mean as the odor hour is determined by a yes/no decision.

02 Rated odor hour frequencies

The correct calculation of the rated odor hour frequency is checked for the case that several odorant classes with different rating factors are applied.

Similar to verification 01, a calculation area of $200 \times 200 \text{ m}^2$ and one vertical cell of size 200 m is applied. However, the horizontal cell size is 200 m so that the grid consists of a single, large cell in order to suppress concentration fluctuations and to provide a very accurate prediction for the occurrence of an odor hour. A time series over 5 days is applied, odorants are emitted only during the 12th hour of each day. Periodic boundary conditions are used so that the particles cannot leave the grid cell. The turbulence is constant in time and space.

The odorant classes odor_100 and odor_050 are emitted. The emission is set such that the mean concentration of each odorant class increases by 0.13 OU/m^3 with each new release. Hence an odorant must be emitted twice for its own contribution to give rise to an odor hour.

Calculation grid: $200 \times 200 \times 200 \text{ m}^3$, consisting of a single cell with periodic boundary conditions.

Meteorology: Homogeneous turbulence with $ua=0.2$, $ra=270$, $z0=0.5$, and
 "Blm=0.1; Su=1.2; Sv=1.0; Sw=0.65; Tau=10; Us=0.2;"; time series over 5 days.

Source: Volume source over the entire calculation grid; emission during the 12th hour of each day; "Groups=36; Rate=0.01;" implying that each group contains one particle; the total emission within one hour is 1040 kOU, the according increase of the mean concentration is 0.13 OU/m^3 .

Time	odor_100	odor_050
0.12	288.9	0.0
1.12	0.0	288.9
2.12	0.0	288.9
3.12	288.9	0.0
4.12	0.0	0.0

The table to the left shows the time of release (format *day.hour*) and the emission strength of the two odorant classes in OU/s.

This yields the following hourly mean concentrations (OU/m^3) over the simulation period of 5 days:

Time interval	odor_100	odor_050	odor
0.01 – 0.11	0.000	0.000	0.000
0.12	0.065	0.000	0.065
0.13 – 1.11	0.130	0.000	0.130
1.12	0.130	0.065	0.195
1.13 – 2.11	0.130	0.130	0.260
2.12	0.130	0.195	0.325
2.13 – 3.11	0.130	0.260	0.390
3.12	0.195	0.260	0.455
3.13 – 4.24	0.260	0.260	0.520

The resulting odor hour frequencies for each of the 5 days are (%):

Day	odor_100	odor_050	odor
0	0	0	0
1	0	0	50
2	0	50	100
3	50	100	100
4	100	100	100
Mean	30	50	70

This gives the following rated odor hour frequency r_b (IG_b in %):

$$r_b = 0.70 \frac{1.0 \times 30 + 0.5 \times (70 - 30)}{30 + (70 - 30)} = 0.5 \quad (16)$$

$$IG_b = 50.0 \quad (17)$$

In agreement with these theoretical considerations the dispersion calculation yields:

Component :	ODOR_100	ODOR_050	ODOR	ODOR_MOD
Expected :	30.0 %	50.0 %	70.0 %	50.0 %
Observed :	30.0 %	50.0 %	70.0 %	50.0 %

11 Homogeneity test: homogeneous turbulence, constant time step

In the absence of external forces, a spatially homogeneous concentration distribution should develop after a certain amount of substance has been released into a closed calculation grid.

K	Cmin	C	Cmax
1	469.4	489.0	508.6
2	469.4	486.9	504.4
3	474.1	489.8	505.5
4	483.4	498.4	513.4
5	487.6	501.6	515.6
6	486.6	500.6	514.6
7	485.1	498.1	511.1
8	485.0	496.9	508.8
9	490.7	503.8	516.9
10	492.1	505.2	518.3
11	488.7	501.7	514.7
12	492.9	506.1	519.3
13	486.3	499.3	512.3
14	483.7	496.6	509.5
15	478.6	492.4	506.2
16	478.1	491.9	505.7
17	492.2	506.4	520.6
18	491.9	507.1	522.3
19	499.3	516.9	534.5
20	491.8	512.3	532.8

Calculation grid: $1000 \times 1000 \times 200 \text{ m}^3$, divided into $1 \times 1 \times 20$ cells (constant spacing in the vertical); periodic boundary conditions.

Meteorology: Homogeneous turbulence with $ua=0.2$, $z0=0.08$, and
 "Blm=0.1; Su=0.5; Sv=0.5; Sw=0.5; Tau=2; Us=0.2;";
 time series over 10 days.

Source: Volume source extending over the whole calculation grid; emission only during the first hour of the first day;
 "Groups=36; Rate=0.1;" implying 10 particles per group;
 the total emission is 100 kg and the mean concentration therefore $500 \mu\text{g}/\text{m}^3$.

The table to the left shows the vertical profile (index K) of concentration (column C) for the 10th day. At hand of the sampling error as estimated by the program, which ranges between 1% and 2%, the lower bound (column Cmin) and upper bound (column Cmax) of the 95-percent confidence interval are formed. On statistical average it is expected that the correct concentration value $\bar{c} = 500 \mu\text{g}/\text{m}^3$ is only in 1 out of 20 cases outside the given confidence interval.³⁵ In this calculation no value is outside.

12 Homogeneity test: homogeneous turbulence, variable time step

This test cannot be performed with AUSTAL2000 because the time step cannot be explicitly set. The program applies in the case of homogeneous turbulence always a constant time step.

13 Homogeneity test: inhomogeneous turbulence, constant time step

Like test 11, but with inhomogeneous turbulence.

³⁵ This expectation is not entirely correct: the 20 concentration values origin from the same particles and are therefore statistically not independent; this fact becomes particularly evident in the homogeneity test 14.

K	Cmin	C	Cmax
1	473.8	496.6	519.4
2	464.6	483.0	501.4
3	477.9	494.7	511.5
4	483.6	498.6	513.6
5	484.8	498.8	512.8
6	480.7	494.5	508.3
7	479.8	492.6	505.4
8	485.5	499.5	513.5
9	497.5	510.8	524.1
10	492.1	506.3	520.5
11	495.4	510.7	526.0
12	484.4	500.4	516.4
13	474.3	491.0	507.7
14	470.7	487.3	503.9
15	474.3	492.0	509.7
16	473.3	492.0	510.7
17	474.5	494.3	514.1
18	482.4	503.5	524.6
19	499.9	524.0	548.1
20	500.5	530.2	559.9

Calculation grid: $1000 \times 1000 \times 200 \text{ m}^3$, divided into $1 \times 1 \times 20$ cells (constant vertical spacing); periodic boundary conditions.

Meteorology: Inhomogeneous turbulence with $ua=0.2$, $z0=0.8$, $ha=1$, and " $B1m=0.7$; $Su=0.5$; $Sv=0.5$; $Sw=0.5$; $Tau=2$; $Us=0.8$;" time series over 10 days.

Source: Volume source extending over the whole calculation grid; emission during the first hour of the first day; " $Groups=36$; $Rate=0.1$;" implying 10 particles per group; the total emission is 100 kg and the mean concentration therefore $500 \mu\text{g}/\text{m}^3$.

The table to the left shows the vertical profile (index K) of concentration (column C) for the 10th day. At hand of the sampling error as estimated by the program, which ranges between 1% and 3%, the lower bound (column Cmin) and upper bound (column Cmax) of the 95-percent confidence interval are formed. On statistical average it is expected that the correct concentration value $\bar{c} = 500 \mu\text{g}/\text{m}^3$ is only in 1 out of 20 cases outside the given confidence interval. In this calculation one value is outside.

14 Homogeneity test: inhomogeneous turbulence, variable time step

Like test 11, but with inhomogeneous turbulence and variable time step.

K	Cmin	C	Cmax
1	494.9	505.0	515.1
2	497.6	505.7	513.8
3	501.8	508.9	516.0
4	502.9	509.0	515.1
5	494.8	500.8	506.8
6	488.7	494.6	500.5
7	484.7	490.6	496.5
8	486.3	492.2	498.1
9	489.0	495.9	502.8
10	492.0	499.0	506.0
11	487.8	494.7	501.6
12	490.7	497.7	504.7
13	496.6	503.7	510.8
14	490.6	498.6	506.6
15	488.3	496.2	504.1
16	491.0	500.0	509.0
17	492.3	501.3	510.3
18	491.4	500.4	509.4
19	491.0	500.0	509.0
20	494.2	506.4	518.6

Calculation grid: $1000 \times 1000 \times 200 \text{ m}^3$, divided into $1 \times 1 \times 20$ cells (constant spacing in the vertical); periodic boundary conditions.

Meteorology: Inhomogeneous turbulence with $ua=0.2$, $z0=0.8$, $ha=1$, and " $B1m=0.7$; $Su=0.5$; $Sv=0.5$; $Sw=0.25$; $Us=0.8$;" time series over 10 days.

Source: Volume source extending over the whole calculation grid; emission only during the first hour of the first day; " $Groups=36$; $Rate=0.1$;" implying 10 particles per group; the total emission is 100 kg and the mean concentration therefore $500 \mu\text{g}/\text{m}^3$.

The time step chosen by the program varies from 3.2 seconds close to the ground up to 20 seconds in the upper part of the calculation grid. The table to the left shows the vertical profile (index K) of concentration (column C) for the 10th

day. At hand of the sampling error as estimated by the program, which is about 1%, the lower bound (column Cmin) and upper bound (column Cmax) of the 95-percent confidence interval are formed. On statistical average it is expected that the correct concentration value $\bar{c} = 500 \mu\text{g}/\text{m}^3$ is only in 1 out of 20 cases outside the given confidence interval. In this calculation 4 values are outside (see footnote on page 63).

21 Deposition test: deposition, no sedimentation

Dry deposition is parameterised by the deposition velocity v_d (proportionality factor between deposition flux and concentration at the ground). This is not the direct parameter for the algorithm which applies a deposition probability p_d . Therefore it needs to be checked if for a given v_d the probability p_d is calculated such that the deposition takes its correct value.

The depletion of concentration close to the ground due to deposition hampers the determination of the exact concentration value at the ground which in turn could effect the comparison. Therefore a stationary process is studied: an elevated source emits continuously and the substance diffuses within a region of homogeneous turbulence towards the ground where it deposits. In the stationary state as much is emitted as deposited and from the resulting concentration profile one can deduce the correct treatment of deposition.

Only vertical diffusion is considered. The concentration distribution $c(z)$ of a substance with settling velocity v_s and deposition velocity v_d obeys in the case of diffusion in a medium at rest with diffusion coefficient K the following differential equation:

$$-v_s \frac{\partial c}{\partial z} = \frac{\partial}{\partial z} \left(K \frac{\partial c}{\partial z} \right). \quad (18)$$

The solution for constant K reads

$$c(z) = c_0 \exp\left(-z \frac{v_s}{K}\right) + \frac{F_c}{v_s} \left[1 - \exp\left(-z \frac{v_s}{K}\right) \right]. \quad (19)$$

Here, c_0 is the concentration at the ground and F_c is the mass flow density enforced by the source; it is equal to the mass flow density of deposition into the ground, $F_c = c_0 v_d$. Without sedimentation the result reads

$$c(z) = F_c \left(\frac{1}{v_d} + \frac{z}{K} \right) \text{ for } v_s \rightarrow 0. \quad (20)$$

K	Cmin	C	Cmax	Cspec
1	14.3	15.3	16.2	15.0
2	24.5	26.1	27.8	25.0
3	34.0	36.2	38.4	35.0
4	43.9	46.5	49.1	45.0
5	53.5	56.5	59.4	55.0
6	63.1	66.3	69.4	65.0
7	74.2	77.7	81.1	75.0
8	84.4	88.3	92.2	85.0
9	93.8	97.7	101.6	95.0
10	103.3	107.4	111.5	105.0
11	113.6	117.6	121.6	115.0
12	124.8	128.9	133.0	125.0
13	134.5	138.7	142.9	135.0
14	143.3	147.7	152.1	145.0
15	152.4	157.1	161.8	155.0
16	158.6	163.2	167.8	165.0
17	167.4	172.2	177.0	175.0
18	177.1	182.6	188.1	185.0
19	186.9	192.7	198.5	195.0
20	196.9	203.8	210.7	205.0

Calculation grid: $1000 \times 1000 \times 200 \text{ m}^3$, divided into $1 \times 1 \times 20$ cells (constant cell size); periodic boundary conditions.

Meteorology: Homogeneous turbulence with $ua=0.2$, $z0=0.08$, and " $B1m=0.1$; $Sw=0.50$; $Tau=2$; $Vd=0.1$; $Us=0.2$;" time series over 10 days.

Source: Area source at height 200 m; continuous emission with 1 g/s and " $Rate=0.01$;" implying 864 emitted particles per day.

The table to the left contains the vertical profile (index K) of concentration (column C) for the 10th day. At hand of the estimated sampling error, which is between 1% and 3%, the lower bound (column Cmin) and upper bound (column Cmax) of the 95-percent confidence interval are formed.

Column Cspec lists the expected value according to Eq. (20) with $F_c = 1 \mu\text{g m}^{-2}\text{s}^{-1}$, $v_d = 0.1 \text{ m s}^{-1}$, $K = 1 \text{ m}^2\text{s}^{-1}$. All values are within the confidence interval.

22a Deposition test: sedimentation, no deposition

For particles subject to gravitational settling but not deposition, an exponential density profile develops (similar to the barometric height formula) as described by Eq. (19) for $F_c = 0$.

K	Cmin	C	Cmax	Cspec
1	1054.8	1083.0	1111.2	1100.6
2	951.0	972.4	993.8	995.8
3	869.1	886.8	904.5	901.1
4	789.7	805.8	821.9	815.3
5	711.8	726.3	740.8	737.7
6	645.6	658.8	672.0	667.5
7	591.1	604.4	617.7	604.0
8	543.3	556.7	570.1	546.5
9	490.2	503.3	516.4	494.5
10	445.9	458.7	471.5	447.5
11	396.1	408.3	420.5	404.9
12	353.8	365.5	377.2	366.3
13	323.9	334.6	345.3	331.5
14	292.4	303.3	314.2	299.9
15	269.3	279.9	290.5	271.4
16	242.2	253.3	264.4	245.6
17	217.9	228.9	239.9	222.2
18	198.3	209.2	220.1	201.1
19	180.7	192.2	203.7	181.9
20	158.1	169.6	181.1	164.6

Calculation grid: $1000 \times 1000 \times 200 \text{ m}^3$, divided into $1 \times 1 \times 20$ cells (constant cell size); periodic boundary conditions.

Meteorology: Homogeneous turbulence with $ua=0.2$, $z0=0.08$, and " $B1m=0.1$; $Sw=0.50$; $Tau=2$; $Vs=0.01$; $Us=0.2$;" time series over 10 days.

Source: Volume source extending over the whole calculation grid; emission only during the first hour of the first day; " $Groups=36$; $Rate=0.1$;" implying 10 particles per group.

The table to the left contains the vertical profile (index K) of concentration (column C) for the 10th day. At hand of the estimated sampling error, which is between 1% and 3%, the lower bound (column Cmin) and upper bound (column Cmax)

of the 95-percent confidence interval are formed. Column Cspec lists the expected value according to Eq. (20) with $F_c = 0 \mu\text{g m}^{-2}\text{s}^{-1}$, $v_s = 0.01 \text{ m s}^{-1}$, $K = 1 \text{ m}^2\text{s}^{-1}$. One value is outside the confidence interval.

22b Deposition test: deposition and sedimentation

Eq. (19) yields for $v_d = v_s$ a constant concentration distribution. For an emission strength of $1 \mu\text{g m}^{-2}\text{s}^{-1}$ and $v_d = 0.05 \text{ m s}^{-1}$ the concentration is $20 \mu\text{g/m}^3$.

K	Cmin	C	Cmax	Cspec
1	19.2	20.1	21.0	20.0
2	19.0	20.1	21.1	20.0
3	19.3	20.5	21.7	20.0
4	19.6	20.8	22.1	20.0
5	19.3	20.5	21.8	20.0
6	18.8	20.0	21.3	20.0
7	18.8	20.0	21.3	20.0
8	18.7	20.0	21.2	20.0
9	18.9	20.3	21.7	20.0
10	19.0	20.3	21.6	20.0
11	19.1	20.4	21.8	20.0
12	19.0	20.3	21.6	20.0
13	18.5	19.7	20.9	20.0
14	18.9	20.1	21.4	20.0
15	18.9	20.1	21.3	20.0
16	19.2	20.4	21.6	20.0
17	19.2	20.4	21.6	20.0
18	19.1	20.3	21.4	20.0
19	19.0	20.2	21.3	20.0
20	18.9	20.1	21.2	20.0

Calculation grid: $1000 \times 1000 \times 200 \text{ m}^3$, divided into $1 \times 1 \times 20$ cells (constant cell size); periodic boundary conditions.

Meteorology: Homogeneous turbulence with $ua=0.2$, $z0=0.08$, and
 "Blm=0.1; Sw=0.50; Tau=2; Vd=0.05; Vs=0.05; Us=0.2;"; time period over 10 days.

Source: Area source at height 200 m; continuous emission with 1 g/s and "Rate=0.01;" implying 864 emitted particles per day.

The table to the left contains the vertical profile (index K) of concentration (column C) for the 10th day. At hand of the estimated sampling error, which is between 2% and 4%, the lower bound (column Cmin) and upper bound (column Cmax) of the 95-percent confidence interval are formed.

Column Cspec lists the expected value $20 \mu\text{g/m}^3$. All values are within the confidence interval.

31 Test of Taylors theorem

Taylors theorem (see e.g. SEINFELD³⁶) yields for homogeneous turbulence with velocity fluctuations $\sigma_{u,v,w}$ and Lagrange correlation times $T_{u,v,w}$ for the three Cartesian directions (x,y,z) the following spread of an initially point-like particle cloud:

$$\sigma_{x,y,z}^2(t) = 2T_{u,v,w}^2 \sigma_{u,v,w}^2 [t/T_{u,v,w} - 1 + \exp(-t/T_{u,v,w})] . \quad (21)$$

To test this relation for typical values of $\sigma_{u,v,w}$ and $T_{u,v,w}$, the concentration distribution must be studied on a time scale of seconds. This is not possible with AUSTAL2000 as it averages

³⁶J.H. SEINFELD, S.N. PANDIS: *Atmospheric Chemistry and Physics*. New York: John Wiley & Sons 1998, Seite 891.

the concentration distribution over a period of at least one day. Hence turbulence values must be chosen that yield a time constant for the spreading of the order of days.

Calculation grid: $1220 \times 1220 \times 410 \text{ m}^3$, divided into $61 \times 61 \times 41$ cells (constant spacing in the vertical).

Meteorology: Homogeneous turbulence with $ua=0$, $z0=2$ and "Blm=0.1;Us=0.0001; Su=0.8e-4; Sv=0.6e-4; Sw=0.4e-4; Tau=1800;"; time series over 10 days.

Source: Point source in the centre of the calculation grid; 3600 particles are emitted during the first hour of the first day ("Rate=1;").

The spread of the particle cloud is deduced from the second moment of the concentration distribution $c(x, y, z)$, for example

$$\sigma_x^2 = \frac{\int (x - \bar{x})^2 c(x, y, z) dx dy dz}{\int c(x, y, z) dx dy dz} . \quad (22)$$

N	Sx	sx	Sy	sy	Sz	sz
1	6.7	3.3	6.0	2.5	3.3	1.6
2	13.0	10.1	10.4	7.6	6.1	4.6
3	19.0	16.8	15.0	12.6	8.4	7.3
4	25.0	23.5	19.6	17.6	10.5	9.6
5	31.4	30.0	24.0	22.5	12.6	11.8
6	37.6	36.4	28.7	27.3	14.3	13.7
7	44.0	42.8	33.4	32.1	15.9	15.4
8	50.2	49.1	38.0	36.8	17.4	17.0
9	56.4	55.2	42.5	41.4	18.9	18.6
10	62.6	61.3	47.0	46.0	20.2	20.0
11	68.7	67.4	51.6	50.5	21.5	21.3
12	74.6	73.3	55.8	55.0	22.6	22.5
13	80.7	79.2	60.2	59.4	23.7	23.7
14	86.4	84.9	64.4	63.7	24.8	24.9
15	92.3	90.6	68.7	68.0	25.9	25.9
16	98.2	96.3	72.8	72.2	27.0	27.0
17	103.8	101.9	76.7	76.4	27.9	28.0
18	109.4	107.3	81.0	80.5	28.8	29.0
19	115.1	112.8	84.9	84.6	29.6	29.9
20	120.6	118.1	88.6	88.6	30.7	30.8
21	126.1	123.4	92.7	92.6	31.5	31.7
22	131.3	128.7	96.7	96.5	32.4	32.6
23	136.7	133.8	100.4	100.4	33.2	33.4
24	141.9	138.9	104.4	104.2	34.0	34.2
25	146.9	144.0	108.1	108.0	34.7	35.0
26	152.2	149.0	112.1	111.7	35.3	35.8
27	157.2	153.9	115.7	115.4	36.0	36.6
28	162.4	158.7	119.2	119.1	36.7	37.3
29	167.4	163.6	123.0	122.7	37.5	38.0
30	172.1	168.3	126.5	126.2	38.1	38.8

The table above contains for each day N the modelled values S_x , S_y , S_z and the theoretical values s_x , s_y , s_z according to Eq. (21). The deviations at the beginning are mainly due to the finite cell size (20 m horizontally and 10 m vertically).

41 Test of Berljands profiles

The diffusion equation

$$\frac{\partial c}{\partial t} + u \frac{\partial c}{\partial x} + v \frac{\partial c}{\partial y} + w \frac{\partial c}{\partial z} = \frac{\partial}{\partial x} \left(K_{xx} \frac{\partial c}{\partial x} \right) + \frac{\partial}{\partial y} \left(K_{yy} \frac{\partial c}{\partial y} \right) + \frac{\partial}{\partial z} \left(K_{zz} \frac{\partial c}{\partial z} \right) \quad (23)$$

is analysed for the following special case:

- The dispersion is stationary.
- Wind is aligned in the positive x -direction.
- The diffusion coefficients are only a function of z .
- Diffusion in x -direction is neglected.
- The equation is integrated over y .

The following equation results for $c_y = \int c \, dy$:

$$u \frac{\partial c_y}{\partial x} = \frac{\partial}{\partial z} \left(K_{zz} \frac{\partial c_y}{\partial z} \right) \quad (24)$$

For the case of a point source (emission strength Q) at $x = 0$ and $z = H$, a power law for the wind profile,

$$u(z) = u_H (z/H)^n, \quad (25)$$

linearly increasing K_{zz} ,

$$K_{zz}(z) = K' z, \quad (26)$$

and in the absence of deposition,

$$K_{zz} \frac{\partial c}{\partial z} = 0 \text{ for } z = 0, \quad (27)$$

Eq. (24) can be exactly solved:³⁷

$$\frac{Hu_H}{Q} c_y(x, z) = \frac{1+n}{\xi} \exp\left(-\frac{1+\xi^{1+n}}{\xi}\right) I_0\left(2\frac{\xi^{(1+n)/2}}{\xi}\right) \quad (28)$$

with $\xi = x \frac{(1+n)^2 K'}{Hu_H}$
 $\xi = z/H$

³⁷M.E. Berljand. *Moderne Probleme der atmosphärischen Diffusion und der Verschmutzung der Atmosphäre* (modern problems of atmospheric diffusion and pollution in the atmosphere). Akademie-Verlag, Berlin, 1982.

Here, I_0 is the modified Bessel function.³⁸ Using the parameter settings

$$\begin{aligned} n & 0.3 \\ H & 100 \text{ m} \\ u_H & 6 \text{ m/s} \\ K' & 0.1 \text{ m/s} \end{aligned}$$

a plume is obtained with a near-ground concentration maximum at the distance $x = 2361 \text{ m}$.

If in the Lagrange model the parameters σ_u , σ_v , σ_w and T_u , T_v , T_w are chosen such that the diffusion coefficient described above is reproduced and the travel time of the particles is large with respect to the Lagrange correlation times, the model should exactly reproduce this plume.

Calculation grid: $5000 \times 150 \times 800 \text{ m}^3$, divided into $100 \times 3 \times 80$ cells (constant spacing in the vertical).

Meteorology: Profile with $ua=6$, $z0=2.5$, $ha=100$, and "Blm=0.5;Us=1.0;Su=1.e-6;Sv=1.e-6;Sw=2.0;Tau=2;"; time series over one day.

Source: Point source at (75, 75, 100); 360 000 particles are emitted in the first hour of the day ("Rate=100;") with an emission strength of 24 g/s;³⁹ The average emission strength over the day is therefore 1 g/s.

As the horizontal dispersion perpendicular to the wind direction is suppressed, only layer $50 \leq y \leq 100$ contains non-zero concentration values. The following tables list the vertical concentration profiles up to a height of 400 m for the source distances 500 m, 1000 m, 2000 m, and 4000 m. At hand of the estimated sampling error, which around the concentration maximum is between 0.3% and 0.6%, the lower bound (column Cmin) and upper bound (column Cmax) of the 95-percent confidence interval are formed. Column Cspec lists the theoretical value according to Eq. (28).

Significant deviations only occur close to the ground. This is probably due to the type of wind profile with a strong variation close to the ground that cannot be properly described by linear interpolation.

³⁸W.H. PRESS, B.P. FLANNERY, S.A. TEUKOLSKY, W.T. VETTERLING: *Numerical Recipes in C*. Cambridge University Press 1989.

³⁹In fact an emission strength of 1 200 g/s is used. As this is a factor 50 too high, the concentration listing for the vertical layer $y = 75$ directly yields the value of c_y , which results for this case from a multiplication of c with the cell size of 50 m.

X = 500:

Z	Cmin	C	Cmax	Cspec
5	38.8	43.1	47.4	25.5
15	92.6	97.9	103.2	88.4
25	214.9	221.5	228.1	214.0
35	395.4	402.6	409.8	411.0
45	641.5	650.6	659.7	669.6
55	937.1	948.5	959.9	960.4
65	1208.8	1221.0	1233.2	1241.7
75	1444.4	1456.0	1467.6	1470.8
85	1600.1	1613.0	1625.9	1615.1
95	1644.7	1658.0	1671.3	1659.1
105	1605.1	1618.0	1630.9	1605.4
115	1494.0	1506.0	1518.0	1471.7
125	1297.5	1308.0	1318.5	1284.2
135	1082.1	1093.0	1103.9	1070.7
145	853.4	863.8	874.2	855.8
155	653.5	660.1	666.7	657.6
165	476.8	483.6	490.4	487.0
175	337.9	344.8	351.7	348.4
185	230.2	234.4	238.6	241.1
195	154.4	158.2	162.0	161.8
205	95.4	98.5	101.7	105.4
215	60.2	62.6	64.9	66.8
225	35.4	37.6	39.8	41.1
235	20.9	22.4	23.8	24.7
245	11.7	12.8	13.9	14.5
255	6.2	7.0	7.7	8.3
265	3.2	3.7	4.3	4.6
275	1.7	2.2	2.6	2.5
285	0.7	0.9	1.1	1.4
295	0.5	0.7	0.9	0.7
305	0.2	0.4	0.6	0.4
315	0.0	0.1	0.2	0.2
325	-0.0	0.0	0.1	0.1
335	-0.0	0.0	0.0	0.0
345	-0.0	0.0	0.1	0.0
355	-0.0	0.0	0.1	0.0
365	-0.0	0.0	0.0	0.0
375	0.0	0.0	0.0	0.0
385	0.0	0.0	0.0	0.0
395	0.0	0.0	0.0	0.0

X = 1000:

Z	Cmin	C	Cmax	Cspec
5	298.3	312.0	325.7	261.7
15	404.6	414.5	424.4	391.0
25	536.2	546.0	555.8	546.6
35	692.2	703.5	714.8	709.2
45	838.1	850.0	861.9	863.5
55	976.1	990.0	1003.9	997.0
65	1078.3	1087.0	1095.7	1100.3
75	1148.1	1162.0	1175.9	1167.6
85	1176.1	1188.0	1199.9	1196.9
95	1186.4	1196.0	1205.6	1189.9
105	1154.3	1166.0	1177.7	1150.4
115	1081.1	1092.0	1102.9	1084.3
125	1008.8	1019.0	1029.2	998.5
135	891.2	902.0	912.8	899.8
145	785.7	793.6	801.5	794.7
155	693.4	701.8	710.2	688.8
165	583.2	591.5	599.8	586.5
175	488.6	496.5	504.4	491.1
185	406.6	413.2	419.8	404.8
195	324.7	330.7	336.7	328.6
205	255.2	260.9	266.6	263.0
215	196.7	201.5	206.3	207.6
225	155.7	159.5	163.3	161.8
235	117.6	121.5	125.4	124.5
245	86.7	89.9	93.1	94.6
255	67.6	70.1	72.6	71.1
265	47.6	49.4	51.2	52.8
275	35.4	37.4	39.4	38.8
285	25.3	26.6	27.9	28.2
295	18.1	19.3	20.6	20.3
305	12.4	13.3	14.3	14.5
315	8.9	9.8	10.7	10.2
325	5.3	5.9	6.6	7.2
335	3.7	4.2	4.8	5.0
345	3.0	3.5	3.9	3.4
355	1.7	2.1	2.5	2.3
365	1.1	1.4	1.6	1.6
375	0.6	0.9	1.1	1.1
385	0.4	0.6	0.8	0.7
395	0.2	0.3	0.5	0.5

X = 2000:

Z	Cmin	C	Cmax	Cspec
5	689.1	710.4	731.7	669.6
15	736.9	750.4	763.9	720.9
25	780.7	795.0	809.3	773.9
35	824.7	833.0	841.3	820.9
45	849.0	864.6	880.2	858.1
55	872.4	886.6	900.8	883.5
65	884.5	893.4	902.3	896.5
75	884.6	895.3	906.0	897.0
85	876.1	886.7	897.3	886.0
95	852.1	862.4	872.7	864.4
105	814.8	824.7	834.6	833.8
115	782.1	791.6	801.1	795.8
125	739.7	747.2	754.7	751.8
135	695.8	704.3	712.8	703.6
145	653.9	661.8	669.7	652.7
155	598.0	605.3	612.6	600.3
165	546.3	555.2	564.1	547.7
175	488.3	496.2	504.1	496.0
185	443.2	449.5	455.8	445.8
195	392.3	397.9	403.5	398.0
205	350.7	355.7	360.7	352.9
215	308.4	313.4	318.4	310.9
225	273.0	278.0	283.0	272.3
235	233.7	238.0	242.3	237.0
245	202.0	206.5	211.0	205.1
255	171.8	175.7	179.6	176.6
265	149.0	152.7	156.4	151.2
275	127.9	131.0	134.1	128.8
285	107.0	110.1	113.2	109.1
295	89.5	91.9	94.3	92.0
305	74.0	76.3	78.5	77.3
315	61.5	63.8	66.1	64.6
325	51.9	53.9	56.0	53.7
335	42.4	44.0	45.5	44.5
345	34.4	36.1	37.9	36.7
355	28.2	29.6	30.9	30.1
365	22.4	23.6	24.8	24.6
375	18.5	19.6	20.6	20.1
385	15.1	16.2	17.3	16.3
395	11.7	12.7	13.8	13.2

X = 4000:

Z	Cmin	C	Cmax	Cspec
5	775.1	797.4	819.7	790.0
15	788.2	802.6	817.0	784.1
25	774.4	788.6	802.8	775.6
35	758.3	770.6	782.9	764.6
45	745.1	758.8	772.5	751.0
55	732.9	743.3	753.7	735.0
65	712.7	722.8	732.9	716.8
75	690.8	700.6	710.4	696.4
85	670.5	680.0	689.5	674.1
95	645.3	653.1	660.9	650.3
105	615.3	625.3	635.3	625.1
115	595.7	602.9	610.1	598.8
125	571.1	579.2	587.3	571.6
135	539.1	546.8	554.5	543.9
145	507.7	516.0	524.3	516.0
155	476.9	483.7	490.5	487.9
165	452.4	459.8	467.2	459.9
175	430.8	437.8	444.8	432.3
185	401.3	407.0	412.7	405.2
195	375.9	381.2	386.5	378.7
205	350.4	355.4	360.4	353.0
215	327.0	333.0	339.0	328.2
225	299.2	305.3	311.4	304.3
235	275.0	278.9	282.8	281.5
245	257.4	261.6	265.8	259.7
255	230.2	234.9	239.6	239.1
265	213.2	217.5	221.8	219.6
275	200.0	204.1	208.2	201.2
285	185.5	188.9	192.3	184.0
295	165.6	169.7	173.8	167.8
305	149.3	152.3	155.3	152.8
315	136.6	140.2	143.8	138.8
325	125.1	128.7	132.3	125.9
335	110.2	112.7	115.2	113.9
345	101.0	103.1	105.2	102.9
355	90.2	93.1	96.1	92.7
365	81.5	84.5	87.6	83.4
375	72.2	74.9	77.5	75.0
385	63.7	65.8	67.9	67.2
395	57.2	59.6	62.0	60.1

51a Test of plume rise (VDI 3782 Part 3)

Plume rise is modelled by assigning an additional vertical velocity component U to each particle which then is reduced in each time step τ by the fraction τ/T_U . This yields an exponential decay of U on the time scale T_U . The total vertical displacement Δh of the particle due to the additional velocity component is

$$\Delta h = UT_U \quad (29)$$

Guideline VDI 3782 Part 3 formulates a plume rise proportional to $x^{2/3}$ and states a final rise and a distance $x_{\max}$ at which the final rise is obtained. An exact agreement with this slope cannot be achieved in the simulation. But the parameters U and T_U can be chosen such that the slopes approximately agree.

X	Za	za	Sz	sz
40	68.2	69.8	5.5	3.0
80	80.1	78.5	7.0	5.5
120	90.3	85.8	8.7	7.5
160	99.0	92.4	10.2	9.3
200	106.7	98.4	11.7	10.9
240	113.2	104.0	13.0	12.3
280	118.8	109.3	14.2	13.6
320	123.7	114.3	15.4	14.7
360	128.0	119.2	16.4	15.8
400	131.6	123.8	17.4	16.8
440	134.8	128.4	18.3	17.8
480	137.5	132.7	19.2	18.7
520	139.9	137.0	20.0	19.6
560	142.0	141.2	20.8	20.4
600	143.7	145.2	21.6	21.2
640	145.3	149.2	22.3	22.0
680	146.6	153.1	23.1	22.7
720	147.7	155.0	23.8	23.5
760	148.7	155.0	24.4	24.2
800	149.6	155.0	25.2	24.8
840	150.3	155.0	25.9	25.5
880	151.0	155.0	26.4	26.1
920	151.5	155.0	27.1	26.8
960	152.0	155.0	27.7	27.4
1000	152.4	155.0	28.3	28.0
1040	152.8	155.0	28.8	28.6
1080	153.2	155.0	29.4	29.2
1120	153.5	155.0	29.9	29.7
1160	153.7	155.0	30.5	30.3
1200	154.0	155.0	31.1	30.8
1240	154.1	155.0	31.6	31.4
1280	154.7	155.0	32.2	31.9
1320	155.3	155.0	32.7	32.4
1360	155.3	155.0	33.2	32.9
1400	155.3	155.0	33.7	33.4

Calculation grid: $2000 \times 60 \times 300 \text{ m}^3$, divided into $100 \times 3 \times 30$ cells (constant spacing in the vertical).

Meteorology: Homogeneous turbulence with $ua=6$, $z0=1$, $lm=99999$, and "Blm=0.1;Us=1;Su=1.e-6;Sv=1.e-6;Sw=0.5;Tau=1;"; time series over one day.

Source: Point source at (30, 30, 55); emission occurs only during the first hour of the day; the heat current is $qq=19.17$ (MW) which for neutral stratification yields a plume rise of 100 m according to guideline VDI 3782 Part 3.

The table to the left lists for different source distances X the observed plume height Za , calculated as the centre of mass of the concentration distribution, and the required plume height za according to guideline VDI 3782 Part 3. In addition, the observed plume spread Sz and the theoretical one according to Eq. (21) is listed (sz).

51b Test of plume rise (parameter sq)

To allow a specification of plume rise apart from guideline VDI 3782 Part 3, the parameter sq is provided which defines the characteristic rise time T_U (see verification 51a). Together with parameter vq which defines the initial value of U , the slope of the plume axis $h(z)$ is given as described in verification 51a:

$$h(z) = H_q + UT_U [1 - \exp(-t/T_U)] \quad (30)$$

X	Za	za	Sz	sz
40	70.4	70.4	5.9	3.0
80	83.7	83.3	7.0	5.5
120	94.8	94.3	8.7	7.5
160	104.2	103.7	10.2	9.3
200	112.2	111.5	11.7	10.9
240	118.9	118.2	13.0	12.3
280	124.5	123.9	14.2	13.6
320	129.3	128.6	15.4	14.7
360	133.3	132.7	16.4	15.8
400	136.7	136.1	17.4	16.8
440	139.6	139.0	18.3	17.8
480	142.0	141.5	19.2	18.7
520	144.1	143.5	20.0	19.6
560	145.8	145.3	20.8	20.4
600	147.2	146.8	21.6	21.2
640	148.5	148.1	22.3	22.0
680	149.6	149.1	23.1	22.7
720	150.3	150.0	23.8	23.5
760	151.1	150.8	24.5	24.2
800	151.7	151.4	25.1	24.8
840	152.2	152.0	25.8	25.5
880	152.7	152.4	26.4	26.1
920	153.1	152.8	27.1	26.8
960	153.4	153.2	27.7	27.4
1000	153.7	153.4	28.2	28.0
1040	153.9	153.7	28.8	28.6
1080	154.1	153.9	29.4	29.2
1120	155.2	154.1	29.9	29.7
1160	155.2	154.2	30.5	30.3
1200	155.3	154.3	31.1	30.8
1240	155.3	154.4	31.6	31.4
1280	155.3	154.5	32.2	31.9
1320	155.3	154.6	32.7	32.4
1360	155.3	154.7	33.2	32.9
1400	155.2	154.7	33.7	33.4

Calculation grid: $2000 \times 60 \times 300 \text{ m}^3$, divided into $100 \times 3 \times 30$ cells (constant spacing in the vertical).

Meteorology: Homogeneous turbulence with $ua=6$, $z0=1$, $lm=99999$, and "Blm=0.1;Us=1;Su=1.e-6;Sv=1.e-6;Sw=0.5;Tau=1;"; time series over one day.

Source: Point source at (30, 30, 55); emission occurs only during the first hour of the day; the exit velocity vq is 2.5 m/s, the time scale sq is 40 seconds, yielding a final rise of 100 m.

The table to the left lists for different source distances X the observed plume height Za, calculated as the centre of mass of the concentration distribution, and the required plume height za according to Eq. (30). In addition, the observed plume spread Sz and the theoretical one according to Eq. (21) is listed (sz).

51c Test of plume rise (VDI 3784 Part 2)

For the discharge of exhaust from cooling towers, the calculation of plume rise according to guideline VDI 3784 Part 2 is required. This guideline is applied in practice with the help of the program *VDISP* (provided by the VDI). The result of a calculation with *VDISP* is a text file with the height of the plume axis as a function of source distance. *AUSTAL2000* extracts from the result file the final rise and the distance at which half of the final rise is reached and sets the model parameters *vq* and *sq* accordingly. In this test the modelled plume axis and the one as specified by *VDISP* are compared.

X	Za	za
40	144.4	145.1
80	155.0	154.7
120	165.4	163.9
160	175.2	172.6
200	184.3	180.9
240	192.2	188.8
280	199.1	196.3
320	205.7	203.5
360	211.7	210.3
400	216.9	223.5
440	221.8	229.4
480	226.1	235.1
520	230.0	240.6
560	233.6	245.8
600	236.9	250.6
640	239.8	255.1
680	242.5	259.2
720	244.9	262.7
760	247.0	265.3
800	249.0	266.8
840	250.8	267.4
880	252.4	267.6
920	253.8	267.6
960	255.2	267.6
1000	256.4	267.6
1040	257.4	267.6
1080	258.4	267.6
1120	259.3	267.6
1160	260.1	267.6
1200	260.8	267.6
1240	261.5	267.6
1280	262.1	267.6
1320	262.6	267.6
1360	263.1	267.6
1400	263.6	267.6

The same input data are applied as in the example given in guideline VDI 3784 Part 2, Annex B2.

Calculation grid: $2000 \times 60 \times 300 \text{ m}^3$, divided into $100 \times 3 \times 40$ cells (constant spacing in the vertical).

Meteorology: Homogeneous turbulence with $ua=15.82$ at $ha=130$, $z0=1$, $lm=-200$ (stability class III/2), and
 $”Blm=0.1; Us=1; Su=1.e-6; Sv=1.e-6; Sw=0.5; Tau=1;”$;
time series over one day.

Source: Point source at (30, 30, 130) with a diameter dq of 65 m; emission occurs only during the first hour of the day; exit velocity vq 4.1 m/s, exit temperature tq 36 °C, relative humidity rq 100%, liquid water content lq 0.003 kg/kg.

The table to the left lists for different source distances *X* the observed plume height *Za*, calculated as the centre of mass of the concentration distribution, and the plume height according to *VDISP*, *za*. The final rise as specified by *VDISP* is approached only asymptotically, therefore at larger distances the rise as calculated by *AUSTAL2000* is slightly lower than the one of *VDISP*.

61 Test of the particle trace in a three-dimensional wind field

The trajectory of a particle is analysed as it moves in a wind field that corresponds to a rigid rotation around the z -axis of the coordinate system:

$$V_x = -\omega y \quad (31)$$

$$V_y = \omega x \quad (32)$$

$$V_z = 0 \quad (33)$$

The wind field is defined on the Arakawa-C grid, i.e. V_x is defined on the faces of the grid cells with a normal vector parallel to the x -axis, likewise V_y on faces perpendicular to the y -axis. Within a cell, V_x is linearly interpolated in x -direction and V_y is linearly interpolated in y -direction.

The terrain is flat and there is no turbulence. The setting $\omega = \pi/60 \text{ s}^{-1}$ yields a flow which rotates counter-clockwise with a cycle period of 120 s.

The verification test requires the key TRACE in the option string os. In this case, the coordinates of the particles at each time step are written to the log file. In addition, turbulence is ignored and the time step is not adjusted.

The wind field has been stored in the library `verif\61\lib` as file `w3001a00.dma`. Because the program formally requires at least 2 base fields, it has been copied once more into the library as file `w3002a00.dma`. This provokes a warning message that the base fields are linearly dependent but has no other negative consequences.

Calculation grid: $310 \times 310 \times 10 \text{ m}^3$, divided into $31 \times 31 \times 1$ cells; the terrain is defined as complex, but with constant terrain height $z_g = 0 \text{ m}$.

Meteorology: Turbulence is ignored, "Blm=0.1;Tau=1;"; the wind field is read from the library and scaled according to `ua=7.328 m/s` and `ra=90 deg` (in fact, the wind field already takes these values at the anemometer position); time series over one day.

Source: Point source at (0, 70, 5); emission occurs only during the last hour of the day; "Groups=1;Rate=0.0001;" implying that only a single particle is created.

T	X	x	Y	y
0	0.00	0.00	70.00	70.00
5	-18.32	-18.11	67.91	67.62
10	-35.34	-34.99	60.58	60.63
15	-49.73	-49.49	49.32	49.50
20	-60.73	-60.61	34.93	35.01
25	-67.79	-67.61	17.91	18.13
30	-69.89	-70.00	-0.41	0.02
35	-67.27	-67.62	-18.73	-18.09
40	-59.94	-60.64	-35.49	-34.98
45	-48.69	-49.52	-49.88	-49.48
50	-34.03	-35.03	-60.88	-60.60
55	-17.01	-18.15	-67.42	-67.60
60	1.31	-0.04	-69.51	-70.00
65	19.63	18.07	-66.90	-67.63
70	36.12	34.96	-59.57	-60.65
75	50.52	49.46	-47.79	-49.53
80	61.51	60.59	-32.87	-35.05
85	68.06	67.60	-15.85	-18.17
90	69.63	70.00	2.47	-0.06
95	66.48	67.63	20.79	18.05
100	59.16	60.66	37.28	34.94
105	47.38	49.55	51.15	49.45
110	32.46	35.07	61.62	60.58
115	15.44	18.19	68.17	67.59
120	-2.88	0.08	69.74	70.00

The table to the left lists the coordinates X and Y of the particle for different times T as given in the log file of the calculation. The corresponding coordinates for the trajectory on an ideal circle is given by x and y. The particle is slightly ahead of the ideal trajectory, but after 120 seconds still less than one time step (about 2.4 deg, i.e. 0.7 %). The agreement for the circle radius is even better (deviation 0.4%).

B File formats

B.1 DMNA files

All files that contain an input or an output table are constructed in the same manner. They consist of a data header with information on the structure and the representation of the table, followed by the table part. The table part can be appended directly to the header if the table is written out in formatted form. For unformatted (binary) output, the table part is a separate file that contains the table elements in the way they are internally handled, without separators or control commands. A table element can consist of a single value (data element) or it can represent a set of several values (record).

The data header is a text file with file name extension `".dmna"` and consists of a series of lines, each line defining one parameter. The parameter name is stated at the beginning of the line, followed by one or more values. Valid separators are a blank, tabulator, and semicolon which can be used separately or in combined form. The line can be terminated by a LF or a CR+LF.

Beside the parameters required by the program the header may contain additional parameters. Parameters which are not recognized are ignored. The header ends with a line that has a star (*) as the first character. The following line starts the table part if it is part of the file. The (formatted) table elements are separated by a blank, tabulator, semicolon, CR or LF. The table terminates with a line that consists of three stars.

The following parameters of the data header are recognized and interpreted by the program (lower case letters required, n_v denotes the number of values within a record):

`buff integer(1)`

Internal size in byte of the buffer used to read in data (default: 4000). Increasing the buffer may result e.g. in faster reading of large compressed files.

`cmpr integer(1)`

Compression level of a compressed data part (values 0 to 9, default: 0). A GZIP compressed data part with the file name extension `".dmnt.gz"` (formatted output) respectively `".dmnb.gz"` (binary output) is expected for a value larger 0.

`cset string (1)`

Character set that has been used for the output of strings. Only for information.

`data string(1)`

Name of the file that contains the table part. If `data` is not specified or has the value `"*"` then the table part is in the same file as the header part in case of formatted output; in case of unformatted (binary) output the file name is the one of the header part with the extension `".dmna"` being replaced by `".dmnb"`. If `data` is set and contains a path information, it is interpreted as relative to the directory that contains the header file.

`dims integer(1)`

Number of dimensions of the data part (maximum 5).

fact *float*(1)

Factor by which all data elements of type *float* or *double* are multiplied before written out in formatted form. On reading formatted data the data elements are divided again by **fact**. The factor only acts on those data elements to which no individual factor is assigned in the format string (see **form**).

form *string*(n_v)

Format used for formatted output of data. If the table elements are records, then each element of the record requires a format specification and **form** consists of the series of single formats which are either written in combined form or as separate strings.

Format = *Format*₁ *Format*₂ ...

*Format*_{*i*} = *Name*%(**Factor*)*Length*.*PrecisionSpecifier*

Meaning:

Name Name of the data element (optionally).

Factor Scaling factor (optionally, including the parentheses).

Length Length of the data field.

Precision Number of decimal positions (for floats).

Specifier Type specifier.

The scaling factor acts as parameter **fact**. The length specification *Length* refers to the minimum length of the data field; the length is exceeded if this is required for a correct presentation of the element; in any case elements are separated by at least one separator.

The following type specifiers are available:

<i>Spec.</i>	Type	Length	Meaning
c	<i>character</i>	1	single characters
d	<i>integer</i>	4	integer number
x	<i>integer</i>	4	hexadecimal number
f	<i>float</i>	4	floating point number (without exponent)
e	<i>float</i>	4	floating point number (with exponent)
t	<i>integer</i>	4	time specification (without date)

The specifiers **f** and **e** may be preceded by a **l** (double of length 8 bytes). The specifiers **d** and **x** may be preceded by a **h** (short integer of length 2 bytes).

Time format for binary output: The time specification without date (specifier **t**) is the number of passed seconds. If the specifier **t** is preceded by a **l**, the number (double of length 8 bytes) is interpreted as time specification with date: the value represents the number of days passed since 1899-12-30.00:00:00 plus 10⁶.

Time format for text output: with specifier **t** the time is formatted as **dd.hh:mm:ss** or **hh:mm:ss**, with **lt** date and time are formatted as **yyyy-MM-dd.hh:mm:ss**.

Similar format specifications can be merged:

`vx%5.2fvy%5.2fvz%5.2f` is equivalent to `vx%[3]5.2f`⁴⁰

hghb *integer(dims)*

Higher bound for the different indices.

loc1 *string(1)*

Representation of float numbers: **C** (default) indicates that a point is used as decimal separator, **german** indicates a comma. An input file that uses a comma as decimal separator must have **loc1** set to **german**.

lowb *integer(dims)*

Low bound for the different indices.

mode *string(1)*

Output mode: **binary** (unformatted) or **text** (formatted).

sequ *string(1)*

Index sequence for the data output. Usually, the fastest index is the one at the far-right side (C convention). For a three-dimensional field A_{ijk} , this corresponds to the specification **i+, j+, k+**. FORTRAN saves data according to **k+, j+, i+**. A minus sign instead of a plus sign denotes an index running backwards.

Example: For a formatted two-dimensional data table (e.g. terrain heights) with the values oriented like in a map (north at the top etc.), **sequ** must have the value **j-, i+**.

Subranges can be selected as well:

j=10..1/1, i=5..25/1, k=1. The optional setting **/n** specifies the starting value of the corresponding index. If a subrange is selected with **sequ**, the index boundaries **lowb** and **hghb** still refer to the original index definitions.

size *integer(1)*

Size of the binary data record in bytes. For formatted output the sum of the element sizes resulting from the format specification must be equal to **size**.

vldf *string(1)*

Identifier of the type of data: **volume average (V)**, **point value (P)**, **area average (Arakawa-C grid, X, Y, S)**.

Strings containing blanks must be enclosed in quotation marks, otherwise quotation marks are optional for strings.

Example:

A field with floating point numbers $A_{ijk} = 100i + 10j + k$, $i = 1..3$, $j = 2..4$, $k = 0..1$ is saved in form of horizontal layers:

⁴⁰For merged formats, the specified *Name* applies to the first element only. For the following elements, the last character of *Name* is increased by one alphabetical position.

```

form  "%4.1f"
mode  "text"
sequ  "k+,j-,i+"
fact  1.000e-001
dims  3
size  4
lowb  1 2 0
hghb  3 4 1
*
    14.0  24.0  34.0
    13.0  23.0  33.0
    12.0  22.0  32.0

    14.1  24.1  34.1
    13.1  23.1  33.1
    12.1  22.1  32.1
***

```

B.2 Quantities defined on the Arakawa-C grid

For quantities defined on a Cartesian Arakawa-C grid the following conventions apply:

A point raster (x_i, y_j, z_k) is defined in each of the Cartesian directions x, y, z :

$$\begin{aligned}
 x_i & \text{ for } i = 0..n_x \\
 y_j & \text{ for } j = 0..n_y \\
 z_k & \text{ for } k = 0..n_z
 \end{aligned}$$

The centre points of these intervals have the coordinates

$$\begin{aligned}
 \hat{x}_i &= (x_{i-1} + x_i)/2 \text{ for } i = 1..n_x \\
 \hat{y}_j &= (y_{j-1} + y_j)/2 \text{ for } j = 1..n_y \\
 \hat{z}_k &= (z_{k-1} + z_k)/2 \text{ for } k = 1..n_z
 \end{aligned}$$

The intervals in the directions of the three axes, $D_{x;i}$, $D_{y;j}$, $D_{z;k}$, have the same index as their centre point. For example, $D_{x;i}$ includes all x -values between x_{i-1} and x_i , i.e.

$$D_{x;i} = \{x \mid x_{i-1} \leq x \leq x_i\}$$

The three point raster constitute a three-dimensional grid. The grid cells V_{ijk} of the three-dimensional grid have the same index as their corresponding axis intervals, i.e.

$$\begin{aligned}
 V_{ijk} &= \{(x, y, z) \mid x_{i-1} \leq x \leq x_i, y_{j-1} \leq y \leq y_j, z_{k-1} \leq z \leq z_k\} \\
 &\text{for } i = 1..n_x, j = 1..n_y, k = 1..n_z
 \end{aligned}$$

In an Arakawa-C grid, the velocity components are defined at the grid points for the axis direction that corresponds to the component and at the centre points for the two other directions. For example, v_x is defined on the points $(x_i, \hat{y}_j, \hat{z}_k)$. The values of v_x have the same index as the points on which they are defined, thus

$v_{x;ijk}$ is the value of v_x at $(x_i, \hat{y}_j, \hat{z}_k)$ with $i = 0..n_x$, $j = 1..n_y$, $k = 1..n_z$

$v_{y;ijk}$ is the value of v_y at $(\hat{x}_i, y_j, \hat{z}_k)$ with $i = 1..n_x$, $j = 0..n_y$, $k = 1..n_z$

$v_{z;ijk}$ is the value of v_z at $(\hat{x}_i, \hat{y}_j, z_k)$ with $i = 1..n_x$, $j = 1..n_y$, $k = 0..n_z$

If a data table contains index values for which a data element is not defined, the placeholder 0 is used. For example, the table record W_{ijk} for the wind vector W contains the data elements z_k , $v_{x;ijk}$, $v_{y;ijk}$, $v_{z;ijk}$ and the index values are $i = 0..n_x$, $j = 0..n_y$, $k = 0..n_z$. Therefore at $j = 0$ or $k = 0$ the value 0 is written instead of v_x , likewise for v_y at $i = 0$ or $k = 0$, and for v_z at $i = 0$ or $j = 0$.

For the calculation of the divergence on a grid cell see Annex D.1.1.

B.3 Register of roughness lengths

AUSTAL2000 can determine the roughness length according to *TA Luft* on the basis of the CORINE landuse register. The determined length is the average over a circular area centred around the stack, where the circle radius is 10 times the stack height.

The stack height is taken here as the mean construction height which is defined by the sum of construction height h_q and half the vertical extension c_q . The minimum value is 10 m. For a horizontally extended source, the centre of the source base is taken as source location. If more than one source is defined, separate values of z_0 are calculated for each source and then the average is taken with the square of the stack height as weighting factor. The applied register of roughness lengths and the calculated value for z_0 are written to the log file.

The register of roughness lengths has been set up based on the CORINE Land Cover 2006 (CORINE 2006). It is provided in form of a DMNA file with formatted and compressed data part. The data part reveals a North-oriented table of the roughness class R (values 1..9) for small quadratic areas which in total cover a rectangular area.⁴¹

The values in x -direction are stored in form of a single string (one character for one square) without blanks. The data part is formally two-dimensional: Index i addresses the x -direction and takes only one value (one string per row), index j addresses the y -direction and runs from the bottom to the top. The data header must contain the following parameters:

xmin Absolute x -coordinate of the lower left corner of the lower left square in metres.

ymin Absolute y -coordinate of the lower left corner of the lower left square in metres.

delta Side length of the squares in metres.

⁴¹ A roughness class 0 is replaced by the program by class 3 (roughness length 0.05 m).

ggcs Geographic coordinate system to which the absolute values **xmin** and **ymin** refer. Possible values are GK for Gauß-Krüger coordinates and UTM for UTM coordinates.

form data format in the form *Name%Print.Storage*, where *Name* is an arbitrary identifier (e.g. *Class*), *Print* the length of the data field if formatted output is applied, and *Storage* the required storage capacity for a data element (including the terminating null byte for strings). As the roughness classes are stored as characters in one string without blanks, *Print* is the number of elements (columns of the underlying register table) and *Storage* is *Print*+1.

dims Dimension of the data part, here 2.

lowb Smallest index value, here 0 for *i* (first entry) and 1 for *j* (second entry).

hghb Largest index value, here 0 for *i* (first entry) and the number of data lines for *j* (second entry).

sequ Index sequence, here *j- , i+* as the data refer to a North-oriented table.

Note:

For Gauß-Krüger coordinates, the stripe index must be part of the coordinate specification.

For UTM coordinates in the register, it is optional to include the zone index in the coordinate specification. However, the roughness length register and user coordinate specifications must apply the same convention. For the UTM register provided for Germany, the zone index is not included, see below.

The flexible dimensions open the possibility for modifications of the register or for applying registers for other regions. To identify the register, the check sum (CRC32 code) of the data part (in natural order *i+*, *j+*) of the current register is listed in the log file *austal2000.log* in form of a 8-digit hexadecimal number which uniquely identifies the data part.

The register must be located in the main directory of *AUSTAL2000*. It can be provided for the Gauß-Krüger coordinate system (files *z0-gk.dmna* and *z0-gk.dmnt.gz*) or the UTM coordinate system (files *z0-utm.dmna* and *z0-utm.dmnt.gz*).

The calculation of the average roughness length can lead to different values depending on the coordinate system being used (grid miss match). The differences are usually small but may result in a different class assignment at the border between two roughness length classes of the *TA Luft*.

The register can also be used in uncompressed form (current size about 60 MB). In this case, file *name.dmnt.gz* must be uncompressed, parameter *cmpr* in file *name.dmna* must be set to 0, and parameter *data* must be set to *name.dmnt*.

If *AUSTAL2000* is called in combination with option *-v4*, the log file lists for each source the (possibly transformed) centre coordinates and the part of the register used to determine

the average roughness length (in form of a North-oriented data table). This allows to inspect and check details or later modifications of the register.

The register that is distributed with *AUSTAL2000* version 2.6.11 covers Germany and is based on the landuse register CORINE 2006:

Register in Gauß-Krüger coordinates (3rd stripe)

- The check sum of the data part is **3b0d22a5**.
- The file header contains the following entries:


```
xmin  3278000.0
ymin  5228000.0
delta 100.0
ggcs  "GK"
form  "Classes%6690.6691s"
size  6691
mode  "text"
cmpr  9
buff  1000000
dims  2
sequ  "j-,i+"
lowb  0      1
ghhb  0      8920
```

The data table consists of 8920 lines each with 6690 entries referring to squares of size 100 m. The covered area is defined in the 3rd stripe of the Gauß-Krüger coordinate system and extends in *x*-direction from 3278000 to 3947000 and in *y*-direction from 5228000 to 6120000.

- If source coordinates are specified in one of the meridian stripes 1 to 5, they are internally translated to coordinates of the stripe of the register.
- The reference point *gx* and *gy* must be set in the input file *austal2000.txt* to apply this register.

Register in UTM coordinates (zone 32)

- The check sum of the data part is **7e0adae7**.
- The file header contains the following entries:


```
xmin  278000.0
ymin  5226000.0
delta 100.0
ggcs  "UTM"
form  "Classes%6690.6691s"
size  6691
mode  "text"
cmpr  9
buff  1000000
dims  2
```

```
sequ  "j-,i+"  
lowb  0      1  
hghb  0  8920
```

The data table consists of 8920 lines each with 6690 entries referring to squares of size 100 m. The covered area extends in x -direction (easting) from 278000 to 947000 and in y -direction (northing) from 5226000 to 6118000.

- The source coordinates must refer to the same zone as the register.
- The reference point ux and uy must be set in the input file `austal2000.txt` to apply this register.

A warning message is given by *AUSTAL2000* if a register different of one of these two is used.

B.4 Settings file

The list of substances, their properties and some model parameters are defined in the text file `austal2000.settings` which is read by the program.

The program lists in the log file the check sum (CRC code) of the settings file and checks whether it agrees with the standard settings. If not, a warning is given.

Note: File `austal2000.settings` should not be modified unless you know exactly what you are doing. Changes may result in a loss of compliance with the TA Luft.

The settings file is structured in sections and processed line by line. Three types of text lines are distinguished:

Head line: First character is a squared, opening brace ([).

Data line: First character is a letter.

Comment line: All other lines.

A hash mark (#) in a head or data line starts a comment. It extends to the end of the line and is ignored on reading.

Every section starts with a head line that contains in squared braces the name of a substance. The data lines of the section contain the parameter name and its value (or values), separated by one or more blanks. If the value is a string it must be enclosed in quotation marks. Thus, file `austal2000.settings` has the following structure:

```
# Comment line
# Comment line
#
[Substance]
Parameter Value # Comment
Parameter Value # Comment
#
[Substance]
Parameter "Value" # Comment
Parameter Value-1 Value-2
#
```

The following table lists the parameters that can be defined for a substance:

Name	Type	Meaning
fc	Number	Conversion factor for concentration from natural units (g/m^3 , 1) to the unit specified by uc.
fn	Number	Conversion factor for deposition from natural units ($\text{g/m}^2\text{s}$) to the unit specified by un.
grps	String	Range of aerosol groups in which the substance can appear, in the form " g_1 - g_2 ". Example: "0-0" (gas only) or "1-2" (only size classes 1 and 2).
rn	Number	Reference value for deposition in the unit specified by un (≤ 0 : no evaluation).
ry	Number	Reference for concentration in the unit specified by uc (≤ 0 : no evaluation).
uc	String	Output unit for concentration.
un	String	Output unit for deposition.
unit	String	Unit in which the emission per second is specified.
vd	Number	Deposition velocity of the gaseous component in m/s.
we	Number	Washout exponent κ of the gaseous component.
wf	Number	Washout factor Λ_0 of the gaseous component in 1/s.
dy	Number	Number of decimal positions for the annual mean (< 0 : scientific notation).
nd	Number	Number of exceedances for the daily mean.
rd	Number	Reference value for the daily mean (≤ 0 : no evaluation).
dd	Number	Number of decimal positions for the daily mean (< 0 : scientific notation).
nh	Number	Number of exceedances for the hourly mean.
rh	Number	Reference value for the hourly mean (≤ 0 : no evaluation).
dh	Number	Number of decimal positions for the hourly mean (< 0 : scientific notation).
dn	Number	Number of decimal positions for the deposition (< 0 : scientific notation).

Section names starting with a point indicate a special section:

- [.astl] The section contains default values for all substance parameters. The default value is applied if the parameter is not explicitly set in a substance definition.
- [.system] The section contains relevant parameters for the dispersion model such as the settling velocity for the different diameter size classes.

File `austal2000.settings` must be located in the same directory as program `austal2000`.

The default substances and their properties of Version 2.6.11 are listed in the table on the following page.

The following default settings are applied for the 5 diameter size classes (vd: deposition velocity in m/s; vs: settling velocity in m/s):

	-1	-2	-3	-4	-u
vd	0.001	0.010	0.050	0.200	0.070
vs	0.000	0.000	0.040	0.150	0.060
wf	0.0	0.0	0.0	0.0	0.0
we	0.8	0.8	0.8	0.8	0.8

Note: The check sum (CRC code) of the settings file for program version 2.6.11 is:

fdd2774f

Name	grps	unit	fc	uc	ry	dy	nd	rd	dd	nh	rh	dh	vd	wf	we	fn	un	rn	dn
S02	0-0	g	1.e6	ug/m3	50	1	3	125.0	0	24	350.0	0	0.0	0.0	0.8	86400	g/(m2*d)	0.0	-1
NOX	0-0	g	1.e6	ug/m3	30.0	1	-1	0.0	-1	-1	0.0	-1	0.0	0.0	0.8	86400	g/(m2*d)	0.0	-1
NO2	0-0	g	1.e6	ug/m3	40.0	1	-1	0.0	-1	18	200.0	0	0.0	0.0	0.8	86400	g/(m2*d)	0.0	-1
NO	0-0	g	1.0	g/m3	0	-1	-1	0.0	-1	-1	0.0	-1	0.0	0.0	0.8	86400	g/(m2*d)	0.0	-1
NH3	0-0	g	1.e6	ug/m3	3.0	2	-1	0.0	-1	-1	0.0	-1	0.010	0.0	0.8	3.154e8	kg/(ha*a)	4.0	2
HG0	0-0	g	1.e6	ug/m3	0.0	-1	-1	0.0	-1	-1	0.0	-1	0.0003	0.0	0.8	86.4e9	ug/(m2*d)	1.0	3
BZL	0-0	g	1.e6	ug/m3	5.0	2	-1	0.0	-1	-1	0.0	-1	0.0	0.0	0.8	86400	g/(m2*d)	0.0	-1
F	0-0	g	1.e6	ug/m3	0.4	3	-1	0.0	-1	-1	0.0	-1	0.0	0.0	0.8	86400	g/(m2*d)	0.0	-1
TCE	0-0	g	1.e6	ug/m3	10.0	2	-1	0.0	-1	-1	0.0	-1	0.0	0.0	0.8	86400	g/(m2*d)	0.0	-1
PM	1-5	g	1.e6	ug/m3	40.0	1	35	50.0	1	-1	0.0	-1	0.0	0.0	0.8	86.4e3	g/(m2*d)	0.35	4
PB	1-5	g	1.e6	ug/m3	0.5	3	-1	0.0	-1	-1	0.0	-1	0.0	0.0	0.8	86.4e9	ug/(m2*d)	100.0	1
AS	1-5	g	1.e6	ug/m3	0.0	-1	-1	0.0	-1	-1	0.0	-1	0.0	0.0	0.8	86.4e9	ug/(m2*d)	4.0	2
CD	1-5	g	1.e6	ug/m3	0.02	4	-1	0.0	-1	-1	0.0	-1	0.0	0.0	0.8	86.4e9	ug/(m2*d)	2.0	3
NI	1-5	g	1.e6	ug/m3	0.0	-1	-1	0.0	-1	-1	0.0	-1	0.0	0.0	0.8	86.4e9	ug/(m2*d)	15.0	2
HG	0-5	g	1.e6	ug/m3	0.0	-1	-1	0.0	-1	-1	0.0	-1	0.005	0.0	0.8	86.4e9	ug/(m2*d)	1.0	3
TL	1-5	g	1.e6	ug/m3	0.0	-1	-1	0.0	-1	-1	0.0	-1	0.0	0.0	0.8	86.4e9	ug/(m2*d)	2.0	3
XX	0-5	g	1.0	g/m3	1.0	-1	-1	0.0	-1	-1	0.0	-1	0.0	0.0	0.8	86400	g/(m2*d)	1.0	-1
ODOR	0-0	OU	100.0	%	10.0	1	-1	0.0	-1	-1	0.0	-1	0.0	0.0	0.8	86400	g/(m2*d)	0.0	-1
ODOR_040	0-0	g	1.0	g/m3	1.0	-1	-1	0.0	-1	-1	0.0	-1	0.0	0.0	0.8	86400	g/(m2*d)	0.0	-1
ODOR_050	0-0	g	1.0	g/m3	1.0	-1	-1	0.0	-1	-1	0.0	-1	0.0	0.0	0.8	86400	g/(m2*d)	0.0	-1
ODOR_060	0-0	g	1.0	g/m3	1.0	-1	-1	0.0	-1	-1	0.0	-1	0.0	0.0	0.8	86400	g/(m2*d)	0.0	-1
ODOR_075	0-0	g	1.0	g/m3	1.0	-1	-1	0.0	-1	-1	0.0	-1	0.0	0.0	0.8	86400	g/(m2*d)	0.0	-1
ODOR_100	0-0	g	1.0	g/m3	1.0	-1	-1	0.0	-1	-1	0.0	-1	0.0	0.0	0.8	86400	g/(m2*d)	0.0	-1
ODOR_150	0-0	g	1.0	g/m3	1.0	-1	-1	0.0	-1	-1	0.0	-1	0.0	0.0	0.8	86400	g/(m2*d)	0.0	-1

C Structure of the program system

The program system AUSTAL2000 consists of the programs *AUSTAL2000* and *TALdia*, both located in the main directory *A2K*. The according file names on a Windows system are *austal2000.exe* and *taldia.exe* and on a Linux system *austal2000* and *taldia*. In addition, the programs *verifx* for the evaluation of the verification tests are required, where *x* denotes the test ID. They are located in subdirectory *A2K\verif*.

All programs are written in the programming language C; extensions to the ANSI-C standard are applied only in module *TalUtl.c*. The source code is identical for Windows and Linux, differences only occur in the according make files. They all apply file *rules.make* in the source directory. The file describes the interdependencies of the different program modules and the rules required for their compilation. Details regarding the language packages are described in Annex C.2.

The directory tree of the program files has the following structure:

```
A2K/  
A2K/source/  
A2K/source/austal2000.c  
A2K/source/austal2000.h  
A2K/source/rules.make  
...  
A2K/source/nls/  
A2K/source/nls/austal2000.text  
...  
A2K/source/nls/en/  
A2K/source/nls/en/austal2000_en.text  
...  
A2K/wg-0/  
A2K/wg-0/austal2000.exe  
A2K/wg-0/Makefile  
...  
A2K/wg-0/nls/  
A2K/wg-0/nls/en/  
A2K/wg-0/nls/en/A2K_en.nls  
...  
A2K/wg-0/nls/en@latin1/  
A2K/wg-0/nls/en@latin1/A2K_en@latin1.nls  
...
```

C.1 Compiler

The source codes are written such that they can be translated without modification by all supported compilers. For Windows, the GNU-C compiler is available free of charge at the web site www.mingw.org, for Linux it is usually part of the system distribution. The Intel compiler is a commercial product by Intel.

Care must be taken that the structures are packed during compilation without gaps (which implies the compiler option `-fpack-struct`) and that the data type `char` is defined as `unsigned`.

The required submodules and their interdependencies are specified in the file `rules.make`. For each supported compiler a `Makefile` and a library for handling compressed data is provided in a separate directory.

All executables are created by calling `make` (of the GNU distribution) in the subdirectory of the desired compiler:

```
make          creates all executables
make clean    deletes all executables
```

Afterwards the executables must be copied into the corresponding directory, i.e. *AUSTAL2000* and *TALdia* to *A2K* and the evaluation programs for the verification tests to *A2K\verif*.

The following calculation time for verification test 11 have been observed with the different compilers (GNU-C without and Intel-C 13.0 with optimization):

System	Compiler	Zeit
Windows 7 (64 bit)	WG-0	150 s
Xeon W3530/2.8 GHz	WI-x	40 s

C.2 Native Language Support

All language-specific text used in *AUSTAL2000*, *TALdia*, and the verification routines is stored in separate text files which are located in subdirectory `source\nls`. The file name is the one of the corresponding program module and the extension is `.text`. The text files contain by default the English text versions without special characters.⁴² They are compiled into the programs but may be replaced by external text packages for other languages at execution time.

For a language other than English, the language file of module *Subprogram* (for example *TalUt1*) is placed in a subdirectory *Language* (short description by 2 characters, for example

⁴²I.e. 'u' instead of 'μ', '2' instead of '²', '3' instead of '³'.

de for German), the file name is *Subprogram_Language.text*. All text files are coded in UTF8. The make file for creating the programs can also be used to combine the language files into language packages for the different programs. These packages can then be read in and applied by *AUSTAL2000*, *TALdia*, and the verification routines. The command for the creation of a package is

```
make NLS LAN=Language VRS=Version
```

Language is the desired language and *Version* denotes the version of *AUSTAL2000* (for example 2.6.9). The created language packages are stored to subdirectory *nls\Language* in the directory of the executable programs,⁴³ the package names are *A2K_Language.nls* for *AUSTAL2000*, *DIA_Language.nls* for *TALdia*, and *VRF_Language.nls* for the verification routines. The language files created during compilation can be deleted by the command `make clean_nls`.

As the language packages are plain text files, their encoding can be modified with a suitable text editor. In this case, the applied encoding should be marked in the file name by appending *@Encoding*, for example *A2K_de@latin1.nls* for ISO-8859-1. This change must be made also in the first comment line of the language package file, because the programs take the encoding information from this line and not from the file name (e.g. "nls/de/A2K_de", i.e. default encoding/UTF8, replaced by "nls/de/A2K_de@latin1").

Note: The programs check the first two comment lines of a language package file. The first line must contain the correct encoding information and the second line the correct version number.

A program uses the language package that is located in the program directory. Therefore the user must copy the desired language package from subdirectory *nls\Language* to the program directory. If no package is found, the program applies the builtin English text versions.⁴⁴

The German distribution of *AUSTAL2000* is delivered for Windows systems (DOS shell) with package *A2K_de@latin1* (encoding ISO-8859-1) and for Linux systems with package *A2K_de* (encoding UTF8). The same applies to *TALdia*.

It is also possible to specify a language package on the command line using the option `--language=Language`. In this case the programs (*AUSTAL2000*, *TALdia*, verification routines) search for the specified package in the current directory. If not found, subdirectory *nls\Language* is scanned. Option `--language=-` suppresses the use of any language package, i.e. the builtin English text is applied.

For Windows systems and language selection *de@latin1*, the output to the DOS shell is automatically converted to **cp850** as this is the default encoding for German DOS systems.

⁴³The subdirectory must be created by hand prior to the package call.

⁴⁴The built-in text contains no special characters. For better readability also an English language package is provided that resorts to special characters and thus depends on the applied encoding.

The conversion can be suppressed with the option `-X0`.⁴⁵

Note: If a program starts in English instead of the desired language, the language package is either missing or located in the wrong subdirectory.

The following table lists the language-specific file identifiers for the German and the English language system:

Description	German	English
Time series file	<code>zeitreihe.dmna</code>	<code>series.dmna</code>
Result type <i>year</i>	<code>j</code>	<code>y</code>
Result type <i>day</i>	<code>t</code>	<code>d</code>
Result type <i>hour</i>	<code>s</code>	<code>h</code>
Type <i>additional load</i>	<code>z</code>	<code>a</code>
Type <i>statistical uncertainty</i>	<code>s</code>	<code>s</code>
Time series type <i>background</i>	<code>zbpv</code>	<code>tmpp</code>
Time series type <i>additional load</i>	<code>zbpz</code>	<code>tmpa</code>
Time series type <i>statistical uncertainty</i>	<code>zbps</code>	<code>tmps</code>

Note: It is recommended to apply for languages other than German always the English file identifiers.

⁴⁵In this case a correct output requires codepage 1250 and a font type suited for this encoding (for example *Lucida Console*).

Example:

The following steps implement Romanian language support:

1. Create the subdirectory `ro` in directory `source\nls`.
2. Copy the language files `Subprogram_en.text` from directory `source\nls\en` to this directory and replace in the file names the language identifier `en` by `ro`.
3. Translate the English text in the language files to Romanian:
 - The files contain in each line an assignment of the form *Key=Text*; only *Text* is translated.
 - Assignments (lines) may be deleted, in which case the built-in English text will be used.
 - Care has to be taken that the percent signs which act as place holders (for example `%d` in `'and %d more cases'`) are preserved in the translated text.
 - The text should be read, modified, and stored in encoding UTF8 (for example using the free text editor JEdit).

4. Create the new language packages with the program `make` of the GNU distribution:

```
make NLS LAN=ro VRS=2.6.9
```

The command must be executed in a directory which is at the same level as the source directory `source`, for example `wg-0`.

The language packages `A2K_ro.nls`, `DIA_ro.nls`, `VRF_ro.nls` are written to subdirectory `nls\ro` which must have been created before the command call.

5. The encoding can be changed if required, for example from UTF8 to ISO-8859-2:

Change the encoding with a suitable text editor, change the encoding information in the first comment line of the language package file (e.g. `"nls/ro/A2K_ro"` replaced by `"nls/ro/A2K_ro@latin2"`), then copy the packages to the main directory of AUSTAL2000, for example as files `A2K_ro@latin2.nls` and `DIA_ro@latin2.nls`. File `VRF_ro.nls` must be copied to the verification directory `verif` which contains the verification routines.

Select in the DOS shell codepage 28592 (command `chcp 28592`) and select a font for the shell that is suitable for all characters of this encoding (for example *Lucida Console*).

Alternatively, the language package `A2K_en.nls` could be translated. However, then the source code may not be modified because the text output or its order might change. It is therefore recommended to apply the translation on the level of the individual language files as outlined above.

D Wind field model *TALdia*

The diagnostic wind field model *TALdia* creates a library of divergence-free wind fields based on a given initial wind profile and a given terrain profile and/or set of building shapes.

TALdia has its origin in the diagnostic mesoscale wind field model *TALdiames* of the distribution AUSTAL2000 version 2.1, which has been extended to account for building effects by means of the microscale model DMK.⁴⁶

TALdia requires the settings file `austal2000.settings`. The program is started either directly with the command

```
taldia ProjectDirectory
```

or via

```
austal2000 ProjectDirectory -l
```

The three-dimensional wind and turbulence fields produced by *TALdia* are written to DMNA files with binary data part. The option `-t` enforces formatted text output. With option `-oGRIDONLY`, only the files with the tuned calculation grids are written to the library. For both options, *TALdia* must be started directly and not via `austal2000`.

The log file `taldia.log` lists for each grid and each created wind field the maximum residual divergence in scaled form. If the calculation grids are not explicitly specified, it also contains the grid parameters and vertical intervals that have been automatically created.⁴⁷

In this context, the following checks are performed in order to prevent the usage of unrealistic wind fields: The program aborts if

- the wind speed at the anemometer position is smaller than 0.5 m/s,
- a vertical component has an absolute value larger than 50 m/s,⁴⁸
- The sum of squares of the superposition factors for two base fields is larger than 100 or smaller than 1/400.

A wind field is calculated in the following sequence:

- An almost homogeneous, incoming flow field is generated. If a terrain profile is applied, a terrain-adjusted coordinate system is set up.
- If a terrain profile is applied, the flow is adjusted to the profile, taking into account the atmospheric stability, and a divergence-free wind field is created (here, the average terrain height is taken as characteristic height).

⁴⁶See final report (English) `taldmk.pdf` on web site `www.austal2000.de`.

⁴⁷The amount of control information that is written to the log file can be increased with option `-vLevel`.

⁴⁸The vertical component is the component V_s of the terrain-adjusted coordinate system; it is also influenced by the terrain steepness and the horizontal wind component.

- The logarithmic profile of the Prandtl layer is impressed on the wind profile.
- A diagnostic wind field is generated by removing (for the second time) the divergence. the wind field calculation terminates with this step in the absence of buildings.
- This step and the following one apply if buildings are defined: If a terrain profile is used, the wind field of the preceding step is transformed to a plain coordinate system, otherwise the field of step 1 is used; the buildings, rastered on the calculation grid, are inserted (removal of building cells from the flow volume, adjustment of boundary conditions, insertion of the recirculation zones).
- A diagnostic wind field is created by removing the divergence (for the third time), which, if necessary, is transformed again to the terrain-adjusted coordinate system.

D.1 Mathematical calculation of the diagnostic wind field

D.1.1 Terrain-adjusted coordinates

With the terrain heights defined in Cartesian coordinates,

$$z = b(x, y) , \quad (34)$$

and an upper limit of the calculation area given by $z = \hat{z}$, the vertical coordinate z is substituted by a coordinate s that is proportional to the distance from the ground $h = z - b$,

$$s = \hat{s} \frac{z - b(x, y)}{\hat{z} - b(x, y)} , \quad (35)$$

$$z = b(x, y) + \frac{s}{\hat{s}} [\hat{z} - b(x, y)] . \quad (36)$$

TALdia only applies the special case $\hat{z} \rightarrow \infty$, $\hat{s} \rightarrow \infty$, $\hat{z}/\hat{s} \rightarrow 1$, i.e. $s \equiv h$.

The vertical component of the wind vector v_z is substituted by

$$v_s = \frac{ds}{dt} \quad (37)$$

and thus

$$v_z = \phi v_x + \chi v_y + \psi v_s \quad (38)$$

$$\text{with } \phi = (1 - \rho) \frac{\partial b}{\partial x}, \quad (39)$$

$$\chi = (1 - \rho) \frac{\partial b}{\partial y}, \quad (40)$$

$$\psi = \frac{\hat{z} - b(x, y)}{\hat{s}}, \quad (41)$$

$$\rho = s / \hat{s}. \quad (42)$$

Note: The coordinates x , y , and s are independent, but they do not form a Cartesian system. A displacement in x - or y -direction does not change the coordinate s , thus the displacement is parallel to the ground. Likewise, a displacement in s -direction does not change the coordinates x and y .

By defining $v_s = 0$ for $s = 0$ it is guaranteed that the flow is exactly parallel to the terrain surface.

The divergence of a wind field with respect to a grid cell is calculated by means of the Arakawa-C components of the field, v_x , v_y , and $\tilde{v}_s = \psi v_s$: According to Gauss' integral theorem, the divergence is equivalent to the net flux through the grid cell divided by the cell volume. The flow through a vertical face of a cell is given by the product of the face area and the according Arakawa-C component; the flow through the top or bottom face (in general a curved surface) is given by the product of the horizontal projection of the face (here the square of the cell size) and the according Arakawa-C component $\tilde{v}_s$.

In discrete coordinates, the divergence D_{ijk} for each grid cell V_{ijk} ($i = 1..n_x$, $j = 1..n_y$, $k = 1..n_z$) is calculated as follows:

$$D_{ijk} = \frac{1}{V_{ijk}} \left[F_{x;i,j,k} v_{x;i,j,k} - F_{x;i-1,j,k} v_{x;i-1,j,k} + F_{y;i,j,k} v_{y;i,j,k} - F_{y;i,j-1,k} v_{y;i,j-1,k} + \Delta^2 \tilde{v}_{s;i,j,k} - \Delta^2 \tilde{v}_{s;i,j,k-1} \right]. \quad (43)$$

The vertical faces of a grid cell, $F_{x;i,j,k}$ perpendicular to the x -axis and $F_{y;i,j,k}$ perpendicular to the y -axis, and the cell volume, V_{ijk} , can be determined from the height values $Z_{i,j,k}$ of the grid intersections (corner points of the grid cells):

$$F_{x;i,j,k} = \frac{\Delta}{2} (Z_{i,j-1,k} + Z_{i,j,k} - Z_{i,j-1,k-1} + Z_{i,j,k-1}) \quad (44)$$

$$F_{y;i,j,k} = \frac{\Delta}{2} (Z_{i-1,j,k} + Z_{i,j,k} - Z_{i-1,j,k-1} + Z_{i,j,k-1}) \quad (45)$$

$$V_{i,j,k} = \frac{\Delta^2}{4} (Z_{i-1,j-1,k} + Z_{i-1,j,k} + Z_{i,j-1,k} + Z_{i,j,k} - Z_{i-1,j-1,k-1} - Z_{i-1,j,k-1} - Z_{i,j-1,k-1} - Z_{i,j,k-1}) \quad (46)$$

D.1.2 Diagnostic procedure

Given a terrain profile $b(x, y)$ and an initial flow field $\mathbf{u}(\mathbf{r})$, the diagnostic procedure determines a field $\mathbf{v}(\mathbf{r})$ that satisfies the conditions

$$\nabla \cdot \mathbf{v} = 0, \quad (47)$$

$$\int \frac{1}{2} \{a_h(v_x - u_x)^2 + a_h(v_y - u_y)^2 + a_v(v_z - u_z)^2\} d^3\mathbf{r} = \min! \quad (48)$$

The factors a_v and $a_h = 1/a_v$ control whether more weight is given to the vertical or horizontal velocity component on minimizing. If $\mathbf{u}$ is a horizontal, homogeneous field, $a_v = 1$ yields a potential flow. With $a_v \gg 1$, a field is created with an enhanced sideways flow around obstacles as it is the case for stable stratification.

With the Lagrange parameter $\lambda(\mathbf{r})$, Equations (47) and (48) yield a variational problem of the form

$$\delta \left\{ \int \frac{1}{2} [a_h(v_x - u_x)^2 + a_h(v_y - u_y)^2 + a_v(v_z - u_z)^2] d^3\mathbf{r} + \int \lambda(\mathbf{r}) \nabla \cdot \mathbf{v} d^3\mathbf{r} \right\} = 0 \quad (49)$$

For the unknown $\mathbf{v}(\mathbf{r})$ it follows that

$$\begin{aligned} v_x &= u_x + \frac{1}{a_h} \frac{\partial \lambda}{\partial x} \\ v_y &= u_y + \frac{1}{a_h} \frac{\partial \lambda}{\partial y} \\ v_z &= u_z + \frac{1}{a_v} \frac{\partial \lambda}{\partial z} \end{aligned} \quad (50)$$

provided that

$$\oint \lambda \delta \mathbf{v} \cdot d\mathbf{f} = 0. \quad (51)$$

The last condition implies that everywhere at a border surface, where the normal component of $\mathbf{v}$ is not explicitly defined, λ must be 0.

For a numerical computation, $\lambda(\mathbf{r})$ is discretized on the centre points of the cells of the calculation grid. The condition of vanishing divergence for $\mathbf{v}(\mathbf{r})$ is transformed into the condition of vanishing flow through the total surface of a grid cell. This yields the same number of equations as variables λ_{ijk} and the resulting equation system can be iteratively solved.

D.1.3 Terrain profile

The divergence needs to be removed which is created by the implementation of the boundary conditions for the terrain profile and by the introduction of the Prandtl layer. Here, the ADI method (alternate directions implicit) is used instead of the common SOR method (successive overrelaxation); although not as effective in some situations, it shows better convergence properties for steep terrain and strongly varying cell sizes in the vertical.

Parameter a_v is a function of the Strouhal number S_r and – like in other diagnostic models – it is parameterised in the form

$$a_v = \sqrt{\frac{a_v}{a_h}} = \frac{1}{2} S_r^2 + \sqrt{1 + \frac{1}{4} S_r^4}. \quad (52)$$

The Strouhal number is the product of the Brunt-Väisälä frequency N_{BV} ,

$$N_{BV} = \sqrt{\frac{g\vartheta'}{\vartheta}} \quad (53)$$

(potential temperature ϑ , vertical gradient ϑ' , gravitational acceleration $g = 9.81 \text{ m/s}^2$), and a characteristic time t_c ,

$$S_r = N_{BV} t_c. \quad (54)$$

In the context of the present model only neutral and stable atmospheric stratification is considered, thus $\vartheta' \geq 0$.

The characteristic time t_c can be defined as the quotient of a characteristic length L_c and a characteristic velocity v_c ,

$$t_c = \frac{L_c}{v_c}. \quad (55)$$

Here, the length L_c is set to the geometrical average of the characteristic height of the terrain, h_c , and its characteristic horizontal extent l_c ,

$$L_c = \sqrt{l_c h_c}. \quad (56)$$

For $v_c(z)$, the velocities of the undisturbed, 1-dimensional wind profile without logarithmic part is used. Height h_c is calculated from the average variance of the terrain height $b(x, y)$, length l_c from the average square of the terrain slope, $\gamma(x, y)$.⁴⁹

$$h_c = 4 \sqrt{\int [b(x, y) - \bar{b}]^2 dx dy / F} \quad (57)$$

$$\text{with } F = \int dx dy = (x_{\max} - x_{\min})(y_{\max} - y_{\min}) \quad (58)$$

$$\bar{b} = \int b(x, y) dx dy / F \quad (59)$$

$$l_c = \frac{h_c}{2\gamma} \quad (60)$$

$$\gamma^2 = \int \left[\left(\frac{\partial b}{\partial x} \right)^2 + \left(\frac{\partial b}{\partial y} \right)^2 \right] dx dy / F \quad (61)$$

With the substitutions $a_v v_z \rightarrow v_z$, $a_v z \rightarrow z$ and for $u_z \equiv 0$ one obtains again Equations (47) and (48) for the case $a_h = a_v = 1$. This implies that – assuming $\mathbf{u}$ is constant – the introduction of parameter a_v causes a scaling of the terrain profile, then a potential flow is calculated for this profile, and finally the terrain profile is scaled back again. This also shows the limits of the model: Even a high value of a_v does not prevent the overflow over a hill, it only reduces it. This is different for a real flow at stable stratification.

D.1.4 Prandtl layer

The Prandtl layer is included after the terrain profile has been considered. This seems to be more accurate than providing the incoming flow with a complete wind profile from the beginning:

The divergence is effectively removed by adding a suitable gradient field $\nabla \lambda$ (for neutral stratification with $a_h = a_v = 1$). This leaves the rotation of the original field unchanged. A substantial part of the rotation is caused by the wind shear in the Prandtl layer, especially its logarithmic part (increasing wind velocity with increasing distance from the ground). Conservation of rotation implies that the velocity difference between the lower and the upper bound of the Prandtl layer is preserved.

⁴⁹For nested grids these values are determined from the coarsest grid and then used for all grids.

For a flow across a ridge, an increased wind speed over top of the ridge develops. Because the rotation is conserved, an increase must occur as well close to the ground on top of the ridge, leaving an unrealistically high wind velocity at the ground if the initial wind field already includes the Prandtl layer.

Conversely, for the flow over a building, reduced wind velocities occur behind the close wake of the building. If in this region the wind velocity down to the ground is decreased due to the Prandtl layer by the same amount as in the undisturbed case, the wind velocity becomes negative, resulting in a reversed flow direction at the ground. This is not realistic and can – for sources at ground level – lead to completely wrong conclusions with respect to the dispersion.

Application of the Prandtl layer after the diagnostic procedure by means of a height-dependent factor is likewise not satisfactory from a theoretical point of view, but at least it seems to avoid some of the presented systematic errors. In practice, the profile of the incoming flow is determined from the boundary layer model, but its logarithmic part in the lower 200 metres is eliminated by division with $\ln(z/z_0)/l_{200}$, where $l_{200} = \ln(200/z_0)$. In the penultimate step of the wind field calculation for structured terrain, the values of the lowest 200 metres are multiplied again by this factor.

D.2 Building effects

Building effects are included as follows:

1. Take the wind field that describes the flow without the buildings (zero field $\mathbf{u}_0$).
For flat terrain, this field is just a horizontally homogeneous field describing the incoming flow; for structured terrain it is the diagnostic wind field calculated as discussed before, but projected on a plain coordinate system; in both cases the zero field does include the Prandtl layer.
2. Introduce the boundary conditions (vanishing normal component at the building faces) and add a recirculation field $\mathbf{R}$ that represents in a simplified manner the recirculation zones in the lee of the buildings as observed in the wind tunnel (empirical wind field $\mathbf{u} = \mathbf{u}_0 + \mathbf{R}$).
3. Find the divergence-free wind field that comprises the boundary conditions and constraints while deviating as little as possible from the empirical wind field $\mathbf{u}$ (diagnostic wind field $\mathbf{v}$).

This step corresponds to the solution of the set of equations for the Lagrange parameters λ_{ijk} described in Section D.1.2. In contrast to the treatment of terrain profiles, not an ADI method (alternate directions implicit) but the simpler SOR method (successive over relaxation) is applied. In the proximity of buildings their influence on the flow field dominates effects of stratification, therefore neutral stratification ($a_h = a_v = 1$) is assumed.

4. Determine the auxiliary fields that allow to take into account in a dispersion calculation the additional turbulence induced by the buildings.

D.2.1 Lee recirculation

The recirculation field is created with the help of a field that corresponds to the electrical field of a homogeneous surface charge attached to the lee face of a building. The use of an electrical field has the advantage that a series of desired properties (see below) are automatically fulfilled.

Only faces are taken into account that are located on the lee side of a building, i.e. those for which $\mathbf{n}_i \cdot \mathbf{u}_0 > 0$, where $\mathbf{u}_0$ is the zero field and $\mathbf{n}_i$ is the normal vector of the partial face with index i (directed outwards of the building). Attached to the partial face is a homogeneous charge density $\rho_i = 2(\mathbf{n}_i \cdot \mathbf{u}_0)/|\mathbf{u}_0|$. The field created by this surface charge is denoted by $\mathbf{g}_i$. The overall field $\mathbf{E}$ results from the superposition of all partial fields $\mathbf{g}_i$,

$$\mathbf{E}(\mathbf{r}) = \sum_i \mathbf{g}_i(\mathbf{r}) \quad \text{with} \quad \mathbf{g}_i(\mathbf{r}) = \frac{\rho_i}{4\pi} \int_{\mathcal{A}_i} \frac{\mathbf{r} - \mathbf{a}}{|\mathbf{r} - \mathbf{a}|^3} d^2a . \quad (62)$$

The integral runs over all points $\mathbf{a}$ of the partial face $\mathcal{A}_i$. To ensure that the normal component of $\mathbf{E}$ vanishes at the ground level, the sum includes also the fields of the partial faces that are the mirror images of the original faces with respect to the ground plane.

The field $\mathbf{E}$ has the following desirable properties:

- It is rotation-free.
- In the centre in front of an (isolated) face it is orthogonal to the face and its absolute value approaches unity at the face.
- Its extent scales with the size of the face.
- It is independent of whether and how a face is divided into smaller partial faces (superposition principle).
- At some distance from the face its form does not depend on whether the base of the face is defined in its exact or in rastered form.

The recirculation field $\mathbf{R}$ is obtained by trimming $\mathbf{E}$:

Step 1: Reduction of the z -component,⁵⁰

$$\mathbf{E}_1 = (\mathbf{I} - a_5 \mathbf{z}\mathbf{z}) \cdot \mathbf{E} . \quad (63)$$

⁵⁰Vectors written side by side without operator symbol form a tensor. The components of $\mathbf{ab}$ are $[\mathbf{ab}]_{ij} = a_i b_j$, the scalar product is $[\mathbf{ab} \cdot \mathbf{cd}]_{ij} = \sum_k a_i b_k c_k d_j$, and the twofold scalar product is $\mathbf{ab} \cdot \cdot \mathbf{cd} = \sum_{i,j} a_i b_j c_j d_i$. The unity tensor is denoted by $\mathbf{I}$, i.e. $I_{ij} = \delta_{ij}$.

Step 2: Enhancement of the component parallel to the undisturbed flow direction,

$$\mathbf{E}_2 = \left(\frac{\mathbf{E}_1 \cdot \mathbf{u}_0}{|\mathbf{E}_1| |\mathbf{u}_0|} \right)^{\frac{a_2}{|\mathbf{E}_1|}} \mathbf{E}_1 . \quad (64)$$

Step 3: Limitation of the range of absolute values,

$$\mathbf{E}_3 = \min(a_3, |\mathbf{E}_2|) \frac{\mathbf{E}_2}{|\mathbf{E}_2|} \text{ and } \mathbf{E}_3 = 0 \text{ for } |\mathbf{E}_2| < a_4 . \quad (65)$$

Step 4: Scaling with the mean speed of the incoming flow,

$$\mathbf{R} = -a_1 \bar{u}_0 \mathbf{E}_3 . \quad (66)$$

The mean speed of the incoming flow $\bar{u}_0$ in the last step results from the local zero field averaged vertically over $|\mathbf{E}_3|$.

The first two steps introduce a rotation into the field so that in the diagnostic field a vortex can develop at the lee side. The enhancement in step 2 stretches the field along the undisturbed flow direction. Here, reduction of the z -component in step 1 prevents the field from being reduced too strongly near the top of the building. The factors a_1 and a_3 in the last two steps determine size and magnitude of the recirculation.⁵¹ The factors (mainly the product $a_1 a_3$, a_2 , and a_5) were fixed by comparisons with experimental data sets.

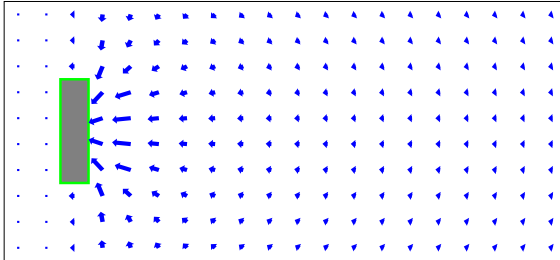
The following safety precautions were introduced to improve robustness of the model in practice and to avoid artifacts for complex built-up structures:

1. The buildings are represented internally only in rastered form on the calculation grid in order to correct in a reliable way imprecise building specifications like overlaps or small gaps. Hence, the partial faces $\mathcal{A}_i$ always have the orientation and extent of the cell faces of the grid. This procedure is justified by the fact that exact and rastered building shapes yield almost the same wind fields as demonstrated in some verification tests.
2. In order to account for shadowing effects of other buildings, the field produced by face $\mathcal{A}_i$ only acts on grid cells that are visible by that face.⁵²
3. The total field $\mathbf{R}$ is restricted to the overall geometrical lee produced by the zero field.

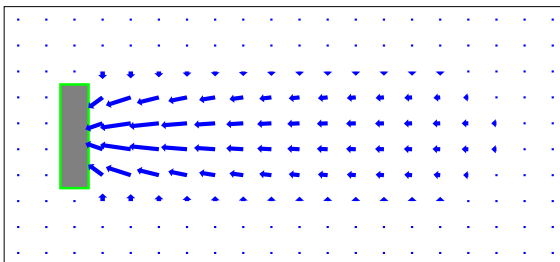
⁵¹The cut-off parameter a_4 has only little influence on the result provided that it is small enough.

⁵²For every grid cell it is checked whether the connection line between its centre point and the centre point of the area cuts a grid cell that is part of a building, the latter point being shifted by half a cell size in flow direction.

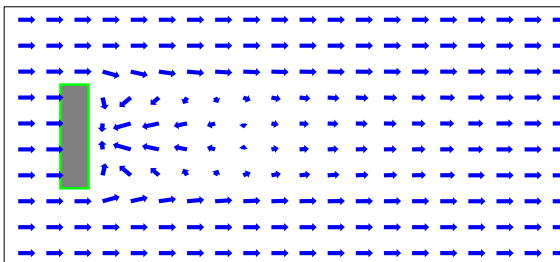
The steps that yield the diagnostic wind field $\mathbf{v}$ are depicted schematically in the following figures.



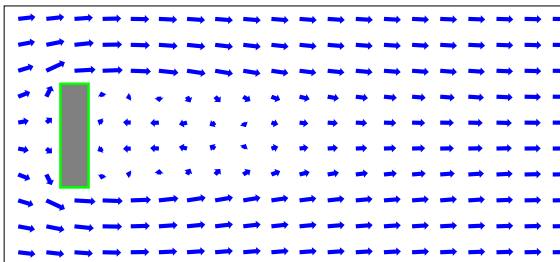
1. Determine the auxiliary field $\mathbf{E}$.



2. Define the recirculation field $\mathbf{R}$.



3. Add it to the zero field $\mathbf{u}_0$.



4. Calculate the diagnostic wind field $\mathbf{v}$.

D.2.2 Prandtl layer and frontal vortex

The zero field usually contains a Prandtl layer. If such a flow approaches an obstacle, a frontal vortex develops. Origin of the vortex is the pressure gradient that is produced by the vertically inhomogeneous incoming flow. In contrast, a vertically homogeneous incoming flow does not produce a frontal vortex.⁵³ In the vicinity of the obstacle, the vortex extends

⁵³See Hosker, R.P., *Flow and diffusion near obstacles*, in: Atmospheric Science and Power Production, SOE/TIC-27601, ISBN 0-87079-126-5, 1984.

from the ground to about 50% to 60% of the obstacle height, further in front of the obstacle its vertical extent depends on the vertical profile of the incoming flow. The horizontal extent of the frontal vortex is determined by the obstacle height and its extension perpendicular to the flow direction.

A vertically inhomogeneous zero field contains a rotation which is conserved in the calculation of the diagnostic wind field. In the near wake, this initial rotation must be compensated for in order to avoid the appearance of an artificial flow in direction of the incoming one. In contrast, in front of the obstacle the initial rotation produces – very much like in nature – a frontal vortex in the diagnostic wind field with dimension and magnitude similar to the observed one.

Therefore, when adding the recirculation field, the zero field is replaced at all locations with non-vanishing recirculation field (i.e. primarily in the wake of the obstacle) by a vertically constant field $\bar{u}_0$ (the zero field vertically averaged over the recirculation field) .

D.2.3 Enhanced turbulence due to the building

The flow around a building causes an enhanced turbulence and diffusion in the wake zone which can be accounted for in an dispersion calculation by means of additional fields for the velocity fluctuations and diffusion coefficients. Similar to the procedure in LASAT, these additional fields are set up on the basis of the recirculation field. The standard deviations of the additional velocity fluctuations are defined as

$$\hat{\sigma}_{u,v,w}(\mathbf{r}) = \sqrt{|E_2(\mathbf{r})|} f_s \bar{u}_0(\mathbf{r}) , \quad (67)$$

and the addition diffusion coefficients in the form

$$\hat{K}_{h,v}(\mathbf{r}) = f_k \bar{h} \hat{\sigma}_u(\mathbf{r}) . \quad (68)$$

Here, $\bar{u}_0$ is again the vertically averaged zero field, f_s and f_k are coefficients of order unity and $\bar{h}$ denotes the average height of the buildings.

In analogy to the setup of the recirculation field, the square root of $|E_2|$ is restricted to values smaller a_3 and set to zero for values smaller a_4 . Hence, the maximum value of $\hat{\sigma}_{u,v,w}$ is $a_3 f_s \bar{u}_0$ and the one of $\hat{K}_{h,v}$ accordingly $a_3 f_s f_k \bar{h} \bar{u}_0$.

Like the recirculation field, the additional fields are confined to the geometrical wake produced by the zero field. However, for a better agreement with experimental observations, they are extended above the top of the building with a linearly decreasing magnitude down to zero at h_s times the building height, and horizontally the geometrical wake is enlarged to an opening angle of a_s degree.

D.2.4 Model parameters

The default values for the model parameters are the ones described in the final report of the DMK model:

Parameter	Value
a_1	6.0
a_2	1.0
a_3	0.3
a_4	0.05
a_5	0.7
a_s	15
f_k	0.3
f_s	0.5
h_s	1.2

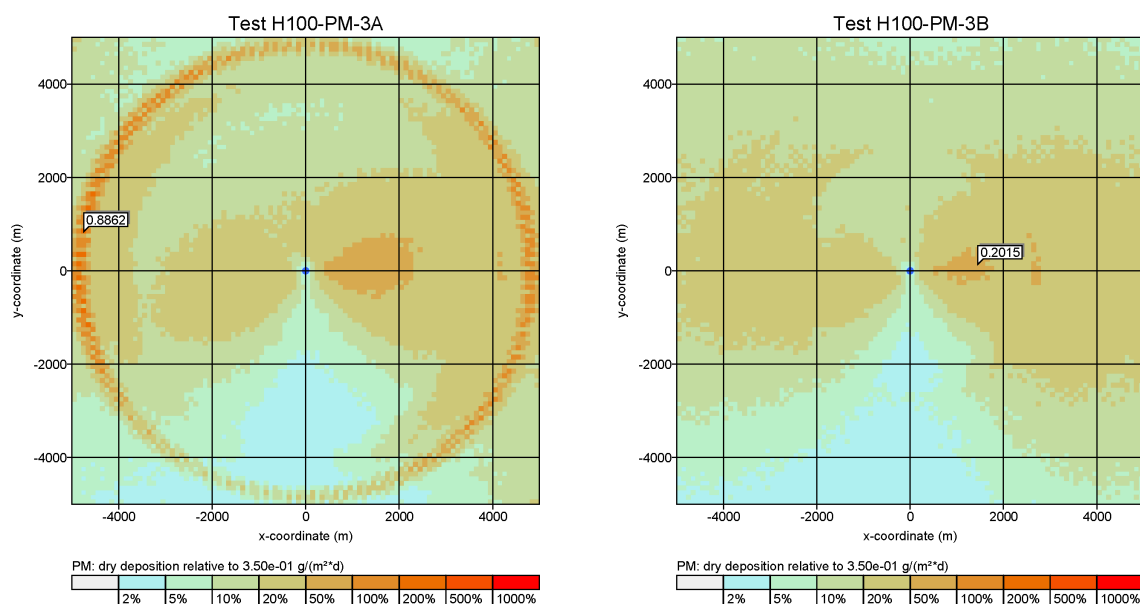
E Artificial ring structures in the deposition distribution of sedimenting dust

The *TA Luft* specifies only a single settling velocity for each of the diameter classes of sedimenting dust (classes 3, 4, and u). This implies that for a given wind speed the trajectories of all particles of a class have the same vertical mean slope. This may result in a ring-like structure of the spatial deposition distribution. The conditions for its appearance are:

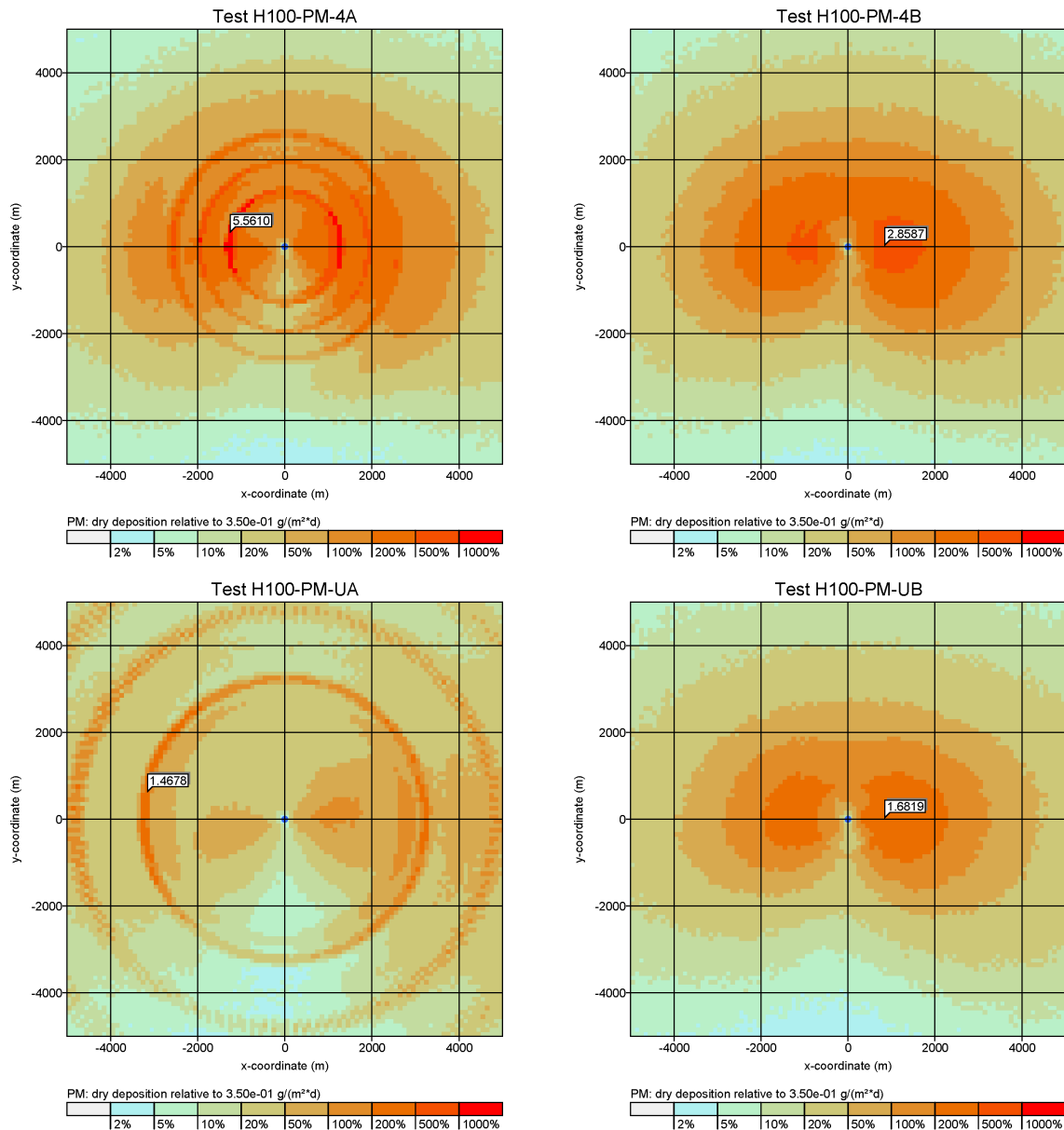
- Dispersion calculation based on a AKS,
- frequent situations of stable stratification at low wind speeds,
- large source heights without plume rise,
- small surface roughness,
- small contribution of PM-10 to total PM.

In all other cases, the ring structures are either not visible, or not of importance for the assessment, or outside the calculation area of interest.

The following figures depict the annual mean of deposition for the three test runs⁵⁴ H100-PM-3A, H100-PM-4A, and H100-PM-UA; three diameter classes are emitted by a source at height 100 m without plume rise, $z_0 = 0.1$ m; the calculation utilizes a AKS for a location in South Germany. In addition to the ring structure, a star structure is visible, e.g. in H100-PM-3A; it is caused by plumes at stable stratification with a width smaller than 2 degree, so that the footsteps of these plumes become visible when applying a wind rose of this resolution.



⁵⁴The runs are located in directory test\dust.



In such cases, the simplification of using only a single settling velocity for each class is not appropriate and a better way of modelling is to apply a continuous diameter spectrum in each class; in practice, for classes 4 and u (unknown) an upper bound of the aerodynamic diameter of $100\mu\text{m}$ is applied. The settling velocity v_s is then calculated for each particle separately according to its diameter; the calculation method is specified in guideline VDI 3782 Part 1. The deposition velocity v_d is set 0.01 m/s higher than v_s .

This modelling procedure is activated by the NOSTANDARD option SPECTRUM. The test runs H100-PM-3B, H100-PM-4B, and H100-PM-UB show that both the ring and the star structure disappear.

F Artificial star structures in the concentration distribution

The meteorological boundary layer profiles according to guideline VDI 3783 Part 8 lead to extremely narrow concentration plumes for emissions at larger altitudes in combination with a stable stratification. The plumes can be so narrow that a star-like structure appears in the concentration distribution for a calculation based on an AKS. This structure reflects the applied 2-degree-sectors and may considerably hamper an assessment of the concentration. This effect can particularly occur for calculations with an AKS and sedimenting dust emitted at larger heights.

The NOSTANDARD option SPREAD has been introduced to suppress the appearance of such artificial structures when using the boundary layer model according to guideline VDI 3783 Part 8; it modifies the lower bound of the horizontal velocity fluctuations σ_v and of the horizontal diffusion coefficient K_v based on the following aspects:

The concentration plume should reveal a certain minimum spread. Close to the source this implies a minimum value for σ_v which is determined by the wind speed u :

$$\sigma_{v,\min} = f_{v,\min} u$$

This spread should hold up to a source distance of at least $x = F_{x,\min} z$. The transport time up to this distance, x/u , is then the minimum Lagrange correlation time,

$$T_{v,\min} = F_{x,\min} \frac{z}{u} .$$

This yields a lower bound for the horizontal diffusion coefficient $K_v = T_v \sigma_v^2$,

$$K_{v,\min} = F_{x,\min} f_{v,\min}^2 z u .$$

This lower bound is not violated if the Lagrange correlation time resulting from the boundary layer profile is set to at least

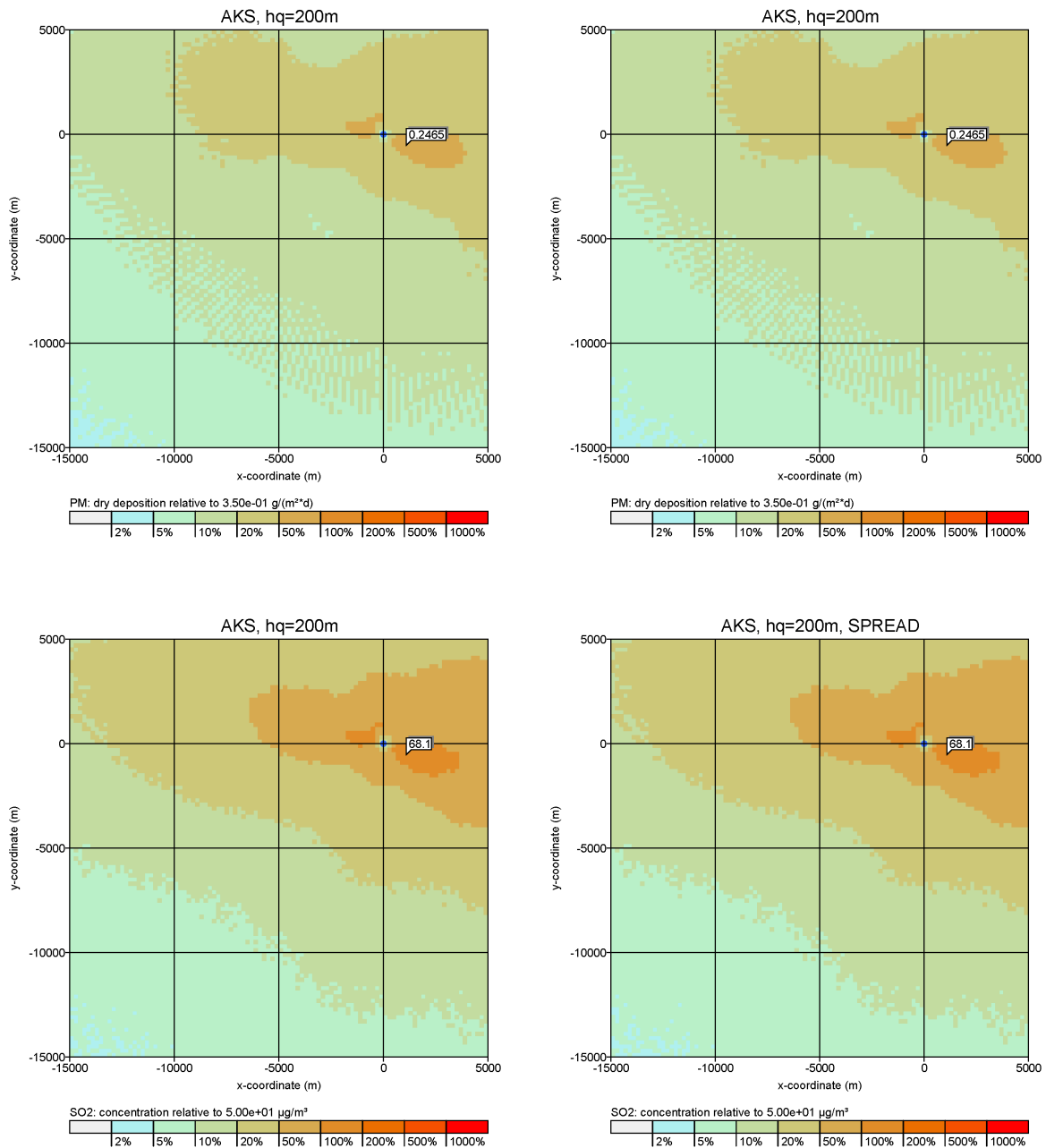
$$T_{v,\min} = \frac{F_{x,\min} f_{v,\min}^2 u z}{\sigma_v^2} ,$$

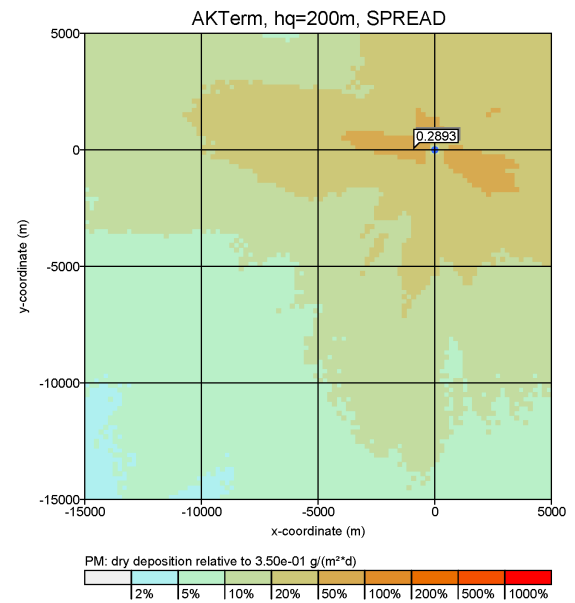
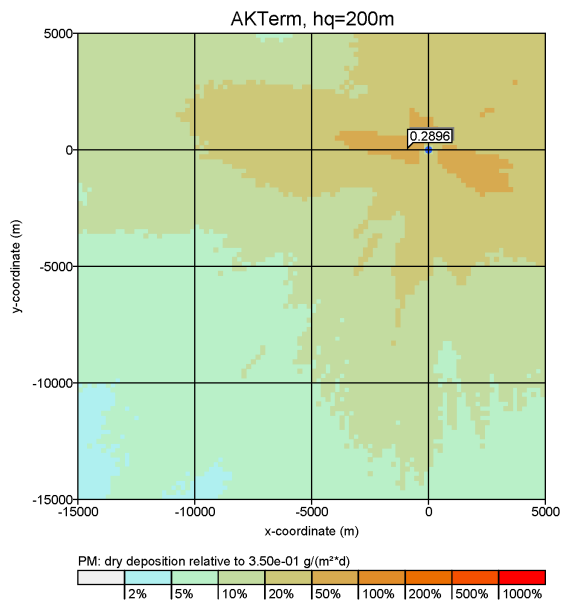
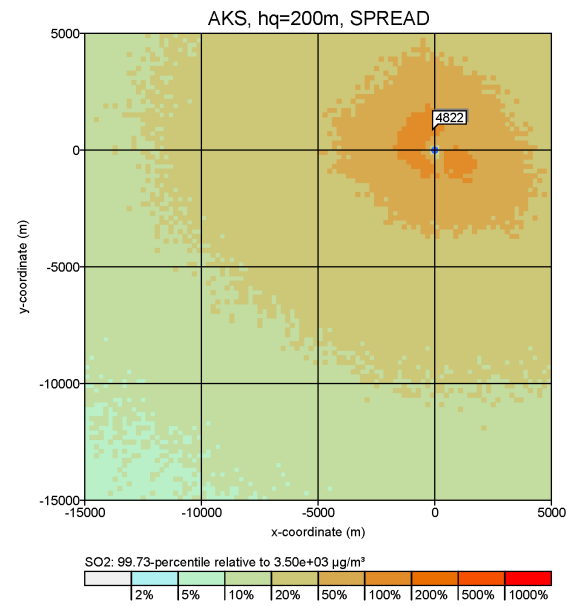
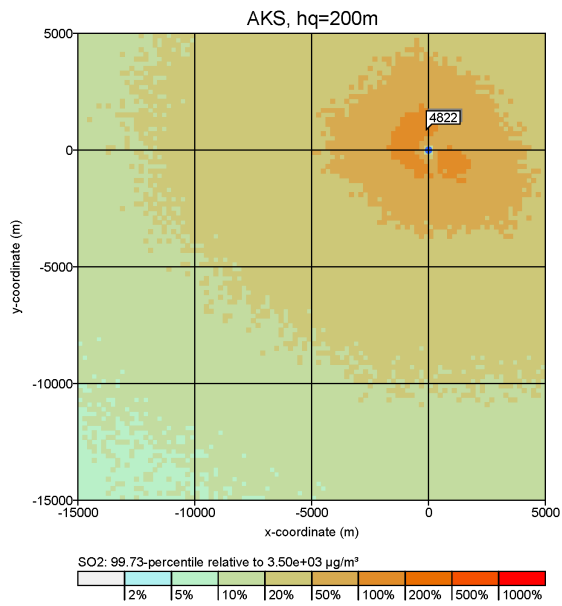
where σ_v ($\geq \sigma_{v,\min}$) denotes the actual velocity fluctuations. This approach avoids modifications close to the ground and acts mainly at larger heights.

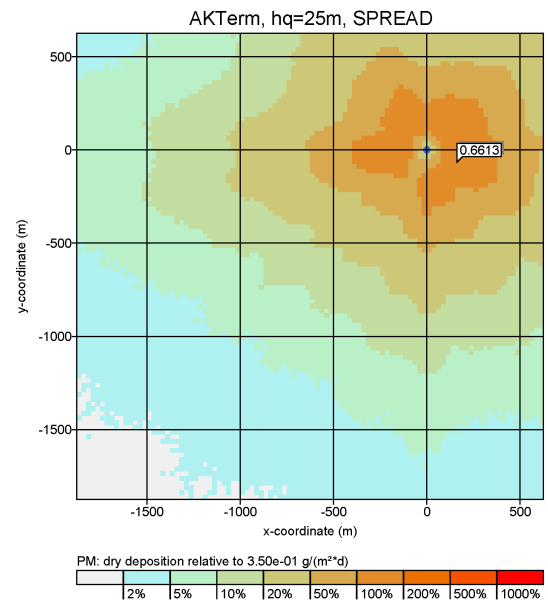
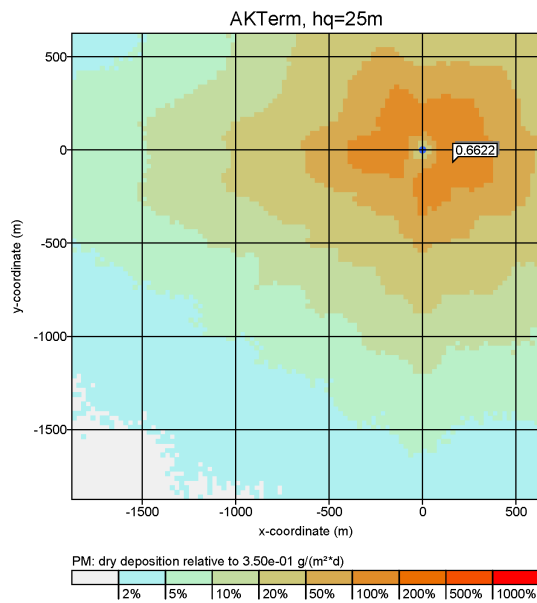
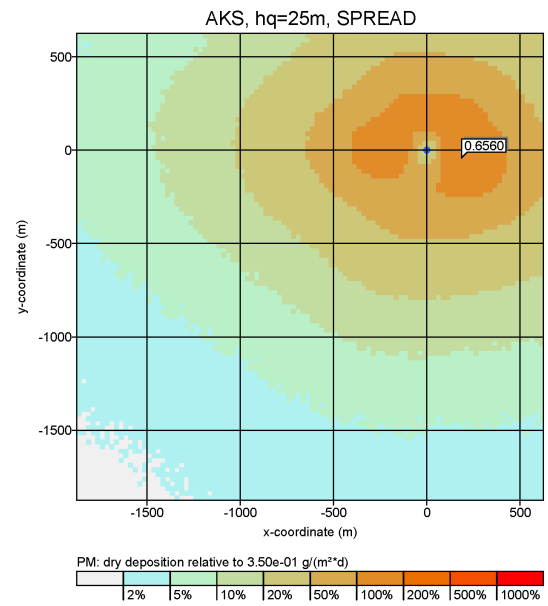
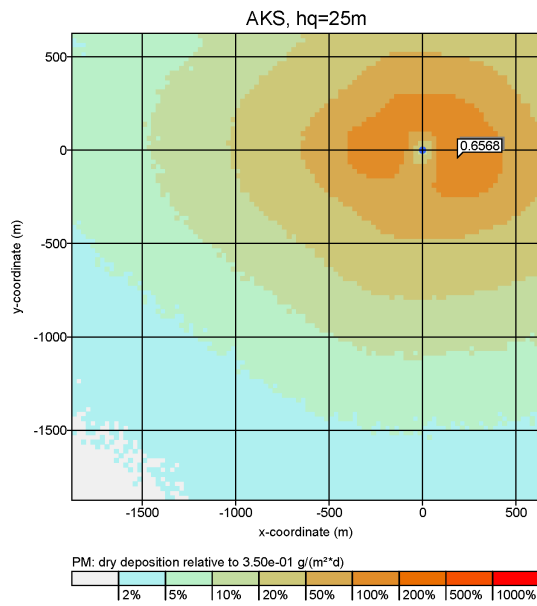
The plume spread (half the width) should be at least 2 degrees to avoid the star structure in a calculation based on an AKS. This implies $f_{v,\min} = 0.035$. Test calculations have shown that for $F_{x,\min}$ a value of 10 is sufficient.

The following graphs show some results of test calculations with AUSTAL2000 for a passive gas (so₂), sedimenting dust (pm-3), a passive source at height 25 m (emission strength 27.8 g/s), at height 200 m (emission strength 2777.8 g/s), a calculation using an AKS

(anonym.aks), and a calculation using an AKTerm (anno95.akterm), each with and without the NOSTANDARD option SPREAD. The results show that the chosen procedure eliminates the star structures where required without modifying the near-ground concentration and deposition at other places.







G Accuracy of the calculation of odor hours

If a dispersion calculation for determining the frequency of odor hours is carried out with too small a number of particles, a systematic error is introduced: The resulting odor hour frequency is too low and the deviation with respect to the real value is significantly larger than the designated statistical uncertainty.

This effect can be demonstrated using a simple example of a point-like, elevated source with the settings

```
az ".../anno95.akterm"
z0    0.2
hq    15
vq    10
dq    1
odor 28000
```

The program AUSTAL2000 (Version 2.1) defines the following simulation grid:

```
dd    16
x0    -1008
nx    126
y0    -1008
ny    126
nz    19
```

When varying the quality level qs between -4 and +2 (particle rates between 0.125 and 8 per second), the following values are obtained for the maximum odor hour frequency $h_{OH,max}$, its absolute standard deviation $s_{OH,max}$, and the corresponding values at point P = (-500 m, 500 m) (grid cell $i=32$, $j=95$):

	Version 2.1				Version 2.2			
Level	Maximum value		Point P		Maximum value		Point P	
qs	$h_{OH,max}$	$s_{OH,max}$	$h_{OH,P}$	$s_{OH,P}$	$h_{OH,max}$	$s_{OH,max}$	$h_{OH,P}$	$s_{OH,P}$
-4	7.1	0.13	1.3	0.059	8.2	0.13	1.6	0.059
-2	9.8	0.13	2.1	0.069	10.7	0.13	2.4	0.069
0	11.0	0.11	2.6	0.067	11.0	0.11	2.6	0.067
+1	11.3	0.09	2.6	0.063	11.4	0.09	2.7	0.063
+2	11.3	0.08	2.6	0.053	11.3	0.08	2.7	0.053

Whereas in version 2.1 the occurrence of an odor hour is calculated as a probability (see project report), in version 2.2 a simple yes/no decision is applied that only indicates whether the hourly average of the odorant concentration exceeds the assessment threshold c_{AT} (0.25 OU/m³) or not. The more primitive approach shows in practice a lower underestimation and has therefore been adopted as the standard approach in version 2.2.

To understand the effect of systematical underestimation one must reconsider the approach taken by *AUSTAL2000* for the calculation of the hourly average concentration and thus the probability for the occurrence of an odor hour.

The simulation grid consists of cells that are used as counting volumes. Every time the trajectory of a particle, which represents the quantity m of a substance, intersects a cell (width b , depth d), the particle contributes to the concentration. These contributions are added in form of the dose D . The contribution of the i -th particle to the dose is the quantity m_i multiplied with the time t_i that the particles remains within the cell,

$$D_i = m_i t_i . \quad (69)$$

If the (horizontal) wind speed is u , $t_i \approx b/u$. The substance quantity m_i , that is transported by a particle, is the total emission q divided by the emission rate r , thus

$$D_i = \frac{qb}{ru} . \quad (70)$$

To obtain the average concentration C for this cell from the total dose D , D must be divided by the cell volume $V = b^2 d$ and the averaging time t_H (3600 s). The contribution of the i -th particle to the concentration is therefore

$$C_i = \frac{q}{rubdt_H} . \quad (71)$$

To reach a concentration that is equal to the assessment threshold c_{AT} of an odor hour, $n = c_{AT}/C_i$ trajectories must intersect the cell,

$$n = \frac{c_{AT} rubdt_H}{q} . \quad (72)$$

Into this estimate the numbers of the considered example are now inserted:

c_{AT}	0.25	OU/m ³
r	0.125	s ⁻¹
u	0.2	m/s
b	16	m
d	3	m
t_H	3 600	s
q	28 000	OU/s

For u an approximate value at ground level is applied under the assumption that a weak wind is blowing with 0.7 m/s at a height of 10 m above ground. The emission rate corresponds to

the quality level -4 (particle rate 0.125 per second). This yields

$$n \approx 0.04, \quad (73)$$

implying that a cell, for which a concentration equal to the assessment threshold is expected, is intersected with a probability of only 4% and then by just one trajectory, whereas it actually should be 50%.

However, if a cell is intersected by a trajectory, the particle contributes to the concentration value by an amount that is 25 times the assessment threshold. Nevertheless, the program in version 2.1 does not treat this event as a full odor hour, because it recognizes this value originating from only a single event and therefore assigns it an uncertainty of 100%. Accordingly the probability for the occurrence of an odor hour is set to less than 1. This effect does not take place with a simple yes/no decision, thus the results in version 2.2 tend to a less pronounced underestimations.

For the cases in which the cell is not intersected by any trajectory (in this example 24 out of 25 cases) both versions register the concentration value 0. The program is certain that no odor hour is present and does not have any reason to doubt it. Therefore the zero values, that actually may be just accidental ones, are treated as being highly accurate and yield in total an estimate of the statistical uncertainty that is too low.

For a calculation with a complete AKTerm this result is not as dramatic, as most situations are characterized by a significantly higher wind speed. Equation (72) further shows that a larger cell size b and a higher emission rate r mitigate this problem. Hence one should use nested grids, a cell size as large as possible (but still suited to the problem), and a high quality level. Special care needs to be taken for situations with several sources as the particles are distributed over these corresponding to the emission rates.

A rule of thumb is that the value of n , calculated according to Equation (72), should not be less than 1. Therefore in this example the emission rate should be increased by a factor 25, i.e. the quality level set to +1 (emission of 4 particles per second). This coincides with the empirical results of the AKTerm calculation described at the beginning of this section.

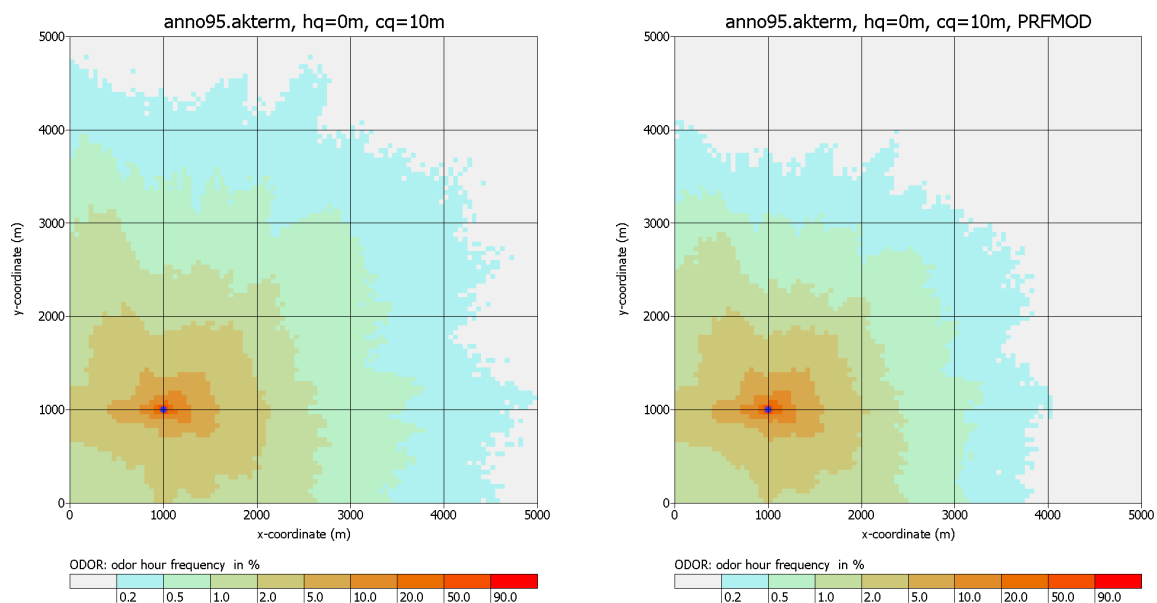
The ultimate test is to repeat the dispersion calculation with a quality factor increased by 1 and to check whether the predicted frequencies of odor hours change significantly. If not, the chosen quality level is sufficient.

H Modified boundary layer model (option PRFMOD)

Experiences with the boundary layer model of guideline VDI 3783 Part 8, which is implemented in *AUSTAL2000*, have shown that it yields for certain situations plumes that are too narrow (see also Annex F). In particular when determining odor hour frequencies at larger source distances this may result in a systematic overestimation.

The main reason for the narrow plumes is the postulated decrease of the velocity fluctuations with height which is too strong. A more detailed discussion can be found in *Reports on Environmental Physics* No 7 (2011).⁵⁵ The modifications of the boundary layer profiles as discussed in the annex of the report⁵⁶ is activated with the NOSTANDARD option PRFMOD (since version 2.5.0).

The following pictures depict as an example the odor hour frequency for a near-ground source (vertical extent 0 m to 10 m above ground, emission rate 10000 OU/s) and the AK-Term anno95.akterm. Left: default boundary layer model. Right: modified boundary layer model.



⁵⁵JANICKE, U., JANICKE, L.: *Some aspects of the definition of meteorological boundary layer profiles and comparisons with measurements* (German), Reports on Environmental Physics, No 7, ISSN 1439-8222, Edt. Janicke Consulting, Überlingen (February 2011), see web site www.janicke.de.

⁵⁶Reduced decrease of the exponential decay $\exp(-z/h_m)$ (height above ground z , mixing layer height h_m) to $\exp(-0.3z/h_m)$ and increase of the factor f_v for the horizontal velocity fluctuations σ_v from 1.8 to 2.0.

I Changes in preceding versions

I.1 Update information for version 2.5.0

Major changes to the last distribution 2.4.7:

- Updated roughness length register (based on CORINE 2006), see Section B.3.
- Compilation with the current compiler Intel-C 12.0.
- Warning message if a roughness length register different from the standard register is applied.
- Files in temporary subdirectory `work` in DMNA format with concentration values instead of the deprecated ARR format with dose values.
- NOSTANDARD option PRFMOD (modified boundary layer model according to *Reports on Environmental Physics* No 7, 2011), see Annex H.
- Additional example `h50a95gap` (time series with measurement gaps).
- Header entries of output DMNA files corrected and adjusted.
- Upper bound of the statistical uncertainty listed in log file `austal2000.log` for the maximum odor hour frequency corrected.
- Problem 2011-07-29 solved (grid localization of monitor points in nested grids improved).
- Problem 2011-04-13 solved (now project title up to 255 characters).
- Problem 2009-04-17 solved (corrected unit for the deviation in monitor time series).

I.2 Update information for version 2.4.7

Changes with respect to the last distribution 2.4.4:

- Problem 2008-11-28 solved (no time-dependent definition of parameter `lq`).
- Problem 2008-12-04 solved (wrong statistical uncertainty of odor hour frequencies at monitor points in case of an AKS).
- Problem 2008-12-18 solved (abort of TALdia with English text output in case of an AKS).

- When using UTM coordinates: Assuming stripe 32 in case the stripe information is not part of the coordinate specification.
 - Harmonized additional information that is written to the header of DMNA files:
 - Parameter names T1, T2, XMIN, YMIN, DELTA, ZSCL, SSCL, SK now in small caps.
 - Instead of PGM now `prgm` for the program core ID.
 - Instead of `ident` now `idnt` for the project ID.
 - Instead of `gakrx` and `gakry` now consistently `refx` and `refy` for the reference point.
 - Time interval (one hour, 1:00:00) now consistently as parameter `dt`.
 - Reference date as parameter `rdat`.
 - Geographical coordinate system as parameter `ggcs`.
 - Array type Z (parameter `artp`) for time series.
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