ANNEX 1

User Guide

GWstat

quo data GmbH
Gesellschaft für
Qualitätsmanagement und Statistik

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Disclaimer

Examples and results presented in this report were elaborated on the basis of test data sets provided by project partners to develop proposals for algorithms on the basis of real data.

They serve for demonstration purposes only and do not anticipate assessments by the Member States

Material in this report reflects the discussion and conclusions of the working group and does not necessarily reflect the position of the EU and its Member States.

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1. BACKGROUND

The main goal of the project WFD-GW was to establish methods for the calculation of representative mean concentrations, for data aggregation and trend (reversal) assessment at the groundwater body level respectively for groups of groundwater bodies. The methods had to be suitable for Europe-wide application and implementation based on the provisions of the Water Framework Directive.

The following main aspects were considered (among other points):

- Development of an appropriate data aggregation method for the assessment of groundwater quality at the groundwater body level respectively for groups of groundwater bodies including the determination of minimum requirements for calculation.
- Development of an appropriate statistical method for trend assessment and trend reversal including the determination of the minimum requirements for calculation.
- Concentrations below the detection limit and groundwater pollution that is unevenly distributed within the groundwater body.
- Influences originating from diffuse and/or point sources.

In the discussion it was highlighted that a pragmatic way which can be implemented in different administration systems and applied for different hydrogeological conditions should be preferred as otherwise the proposed procedure could be of minor acceptance in the Member States. To allow for comparable assessment results throughout Europe it was agreed that one assessment method should be developed and proposed for each issue (data aggregation, trend and trend reversal assessment).

The methods and procedures proposed by this Working Group are related to several provisions which are subject of investigation in other EC Working Groups dealing with particular topics of WFD implementation. For example the delimitation of GW-bodies or groups of groundwater bodies and the selection of monitoring stations based on the provisions of the WFD were not subject of investigation in this study, however they will be of vital importance for groundwater quality monitoring and data assessment.

The outcome of the project WFD-GW comprises the algorithm and a software tool for both the proposed procedure for data aggregation and trend/reversal assessment according to the criteria of the WFD.

The software tool *GWstat* developed by the subcontractor *quo data* allows for data aggregation and trend/reversal assessment and includes also the calculation of the network criterion "Representativity Index".

In line with the contract this software tool is available free of charge. This version of the tool does not comprise a database, for analysis data have to be provided in different files.

For the project the comprehensive statistics package *WaterStat* was applied. This package was adapted to the needs of the project and has been in use for the calculation of test data sets. A further adaptation of the *WaterStat* software package with regard to database, data management, reports and report formats and utilities for the network design etc. is possible. This would allow for a harmonised procedure within the EU with regard to the assessment of the chemical status and the trend analyses. The adaptations of the software could be performed by *quo data* and provided at self costs if there is an expressed interest by institutions of the Member States.

1.1 FEATURES

GWstat includes four separate modes for calculation:

- **Representativity index**
  examine the network criterion,
- **Status assessment**
  aggregate the groundwater body mean value from station mean values: calculate the arithmetic mean (AM), the weighted arithmetic mean (wAM), the Kriging mean (KM) and the respective confidence limits CL_{AM}, CL_{wAM} and CL_{KM}.
- **Trend assessment / Monotonic Trend**
  perform trend assessment by the LOESS smoother and perform trend tests based on the LOESS smoother, and
- **Trend assessment / Reversal Trend**
  perform trend reversal assessment.

1.2 HARD- & SOFTWARE REQUIREMENTS

The minimal hardware requirements are:

Intel or AMD CPU ; frequency > 500 MHz

RAM > 64 Mbyte

Free hard disk space: minimal 10 Mbyte

The program works under

WinNT and Win 2000 or higher.

It is not recommended to use Win 98 or Win Me.

1.3 INSTALLATION

Double click on GWstat-Setup.exe to start the installation. Follow the installation instructions on the screen (insert name, destination folder etc.).

The setup-files will be unzipped in a temporary directory, which has to be specified. After unzipping, the setup-routine starts automatically. If the installation is completed, the temporary directory with the setup-files can be deleted manually.

2. PREPARATION OF IMPORT FILES

GWstat includes four separate modes for calculation:

The data structure of the import files is different for the different calculation modes. After selecting a calculation mode, data have to be imported.

2.1 IMPORT FORMAT - REPRESENTATIVITY INDEX, STATUS ASSESSMENT

The import file format is CSV or EXCEL 5.0/95

2.1.1 Station co-ordinates, Station mean values

Station co-ordinates and the station mean values for data import have to be prepared according to the following structure. Column headers are only included for explanatory purposes. They need not be included in the actual import files.

station ID	***X***	***Y***	***value***	*sub-body index*	*sub-body area*
AT10001	10	5	1.56	1	87
AT10002	3	24	2.88	1	87
AT10003	22	22	0.98	2	54
AT10004	6	15	1.24	1	87
AT10005	12	6	2.6	1	87

Station ID [*essential*]

X and **Y** [*essential*] - indicate the relative position of stations within the groundwater body (details see next chapter 2.1.2). X and Y rows must not be empty.

Value [*essential*] - station mean value for the investigated time resolution (yearly, half-yearly, quarterly) (example see Table 1)

Sub-body index (1….n) and **sub-body area** (in units of km²) [*optional - required for calculation of the wAM*].

Station co-ordinates

The co-ordinates of the monitoring sites indicate the relative position of the cell within the GW-body where the monitoring site is situated in and are given as relative X and Y. The origin is situated in the upper left corner (see Figure 1).

Station mean values

Before aggregating the groundwater body mean value from station mean values with *GWstat* it is necessary to prepare the import file with the calculated station mean values. The calculation of the station mean values is NOT provided by *GWstat*. The calculation has to consider the proposed treatment of values below the limit of quantification (LOQ) of 50 %LOQ and is done as follows (see Table 1).

Table 1: Example calculation of station mean values

date	AT40706012		AT40706022		AT50707012		AT50707022		AT60707032	
	LOQ=0	LOQ=LOQ	LOQ=0	LOQ=LOQ	LOQ=0	LOQ=LOQ	LOQ=0	LOQ=LOQ	LOQ=0	LOQ=LOQ
12.01.99	0.000	0.003								
13.01.99			0.000	0.003						
02.03.99							0.029	0.029		
15.04.99	0.000	0.003	0.000	0.010	0.000	0.003				
15.07.99	0.000	0.003			0.000	0.003				
17.07.99			0.000	0.003					0.000	0.007
03.10.99	0.000	0.003								
15.10.99			0.000	0.003	0.000	0.003			0.012	0.012

	AM0	AM100	AM0	AM100	AM0	AM100	AM0	AM100	AM0	AM100
station mean	0.000	0.003	0.000	0.005	0.000	0.003	0.029	0.029	0.006	0.009
AM50	**0.0015**		**0.0025**		**0.0015**		**0.0290**		**0.0075**	

2.1.2 GW-body GIS-data

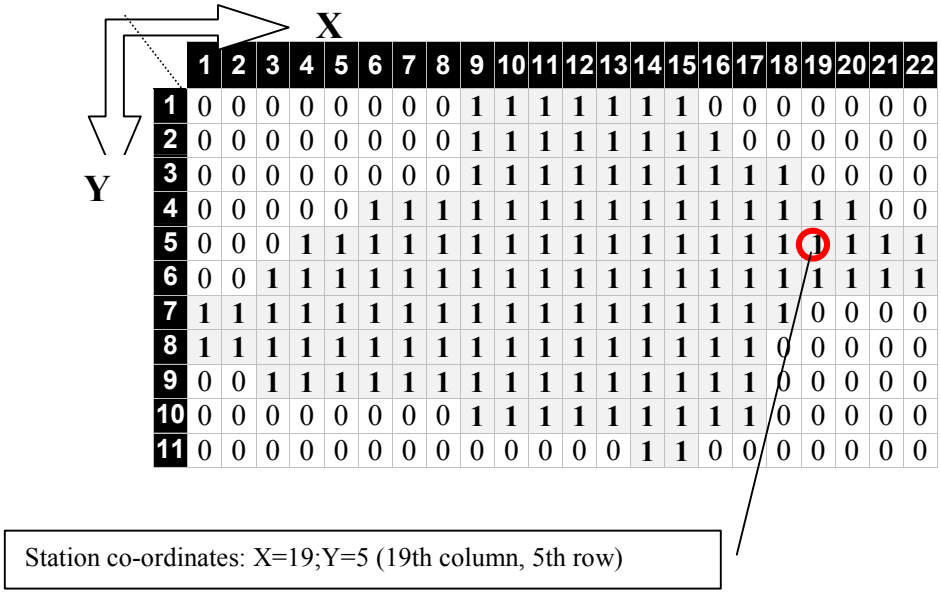
GIS-data of the GW-body as well as the co-ordinates of the monitoring sites are needed for assessing the homogeneity of the network (examine the network criterion Representativity Index R_U) and for the calculation of the Kriging mean (KM).

GIS-data of the GW-body are needed in the form of a **matrix**. Therefore, the GW-body is subdivided into cells. The size of the cells (grid) may depend on the size of the GW-body, on the desired exactness of calculation results and not at least on the power of the computer. For smaller GW-bodies the length of a side of such a cell might be 100 m, for larger GW-bodies the length of a cell might be 250 m.

To form the matrix, all cells within the GW body are assigned by "1" and all cells which are outside the GW-body are assigned by "0".

The co-ordinates of the monitoring sites indicate the relative position of the cell within the GW-body where the monitoring site is situated in and are given as relative X and Y. The origin is situated in the upper left corner.

Figure 1: Example GIS matrix of GW-body and co-ordinates of sampling site



	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	19	20	21	22
1	0	0	0	0	0	0	0	0	1	1	1	1	1	1	1	0	0	0	0	0	0	0
2	0	0	0	0	0	0	0	0	1	1	1	1	1	1	1	1	0	0	0	0	0	0
3	0	0	0	0	0	0	0	0	1	1	1	1	1	1	1	1	1	1	0	0	0	0
4	0	0	0	0	0	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	0	0
5	0	0	0	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1
6	0	0	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1
7	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	0	0	0	0
8	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	0	0	0	0	0
9	0	0	1	1	1	1	1	1	1	1	1	1	1	1	1	1	1	0	0	0	0	0
10	0	0	0	0	0	0	0	0	1	1	1	1	1	1	1	1	1	0	0	0	0	0
11	0	0	0	0	0	0	0	0	0	0	0	0	0	1	1	0	0	0	0	0	0	0

Import file formats for the GIS-data of the GW-body are CSV or EXCEL 5.0/95.

Please note that in EXCEL (5.0/95 format) the number of columns is limited. The GIS-matrix has to be smaller than 256 columns. For larger GIS-matrixes it is necessary to prepare ASCII files (CSV).

Please note: If the GIS-matrix is saved as EXCEL 5.0/95, it has to be in the same EXCEL workbook together with the measured values, as two separate spreadsheets.

2.2 IMPORT FORMAT - TREND ASSESSMENT, TREND REVERSAL ASSESSMENT

The import file format is CSV or EXCEL 5.0/95

The structure of the table for trend assessment is shown in Table 2. Column headers are only included for explanatory purposes. They need not be included in the actual import files.

Table 2: Structure of table for trend assessment and trend reversal assessment

year	*value*	*quarter of a year*
1988	23.5	1
1988	26.8	2
1988	20.7	3
1988	21.8	4
1989	22.5	1

Year [*essential*]

Value [*essential*] - GW-body mean value for the investigated time resolution (yearly, half-yearly, quarterly)

Quarter of a year [*essential*] - index denotes the respective time resolution of the year (1 for yearly; 1, 2 for half yearly; 1, 2, 3, 4 for quarterly)

For aggregating GW-body mean values please refer to chapter 4.

3. REPRESENTATIVITY INDEX

This mode is required to:

- calculate the Representativity Index R_U of the monitoring network.

Station co-ordinates and **GW-body GIS data** are necessary for the calculation of the Representativity Index R_U and have to be prepared according to chapter 2.1. **Station mean values** are not necessary for the calculation of the Representativity Index but the respective column in the data file must not be empty.

3.1 DATA IMPORT

For necessary data format refer to chapter 2.1.

(1) Select *Representativity Index* from the *File* menu. (see Figure 2).

(2) Click on *Import* in the *File* menu or click on the button *Import data* to open the Import Window.

Figure 2: File menu, Representativity index mode chosen

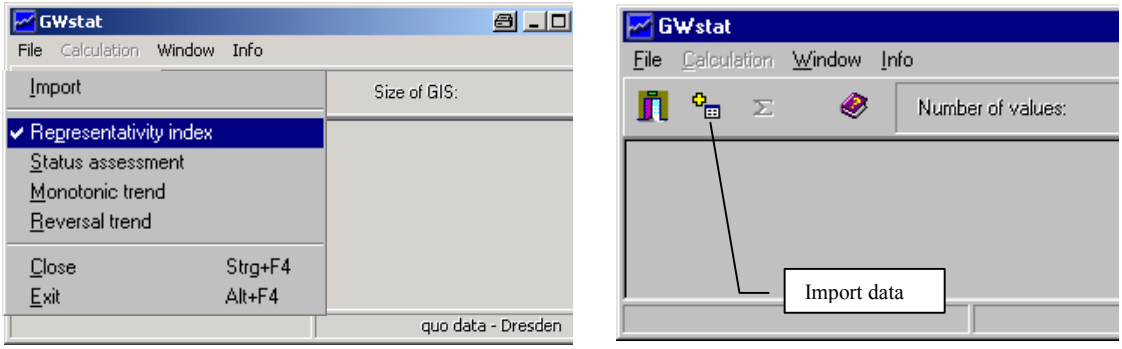
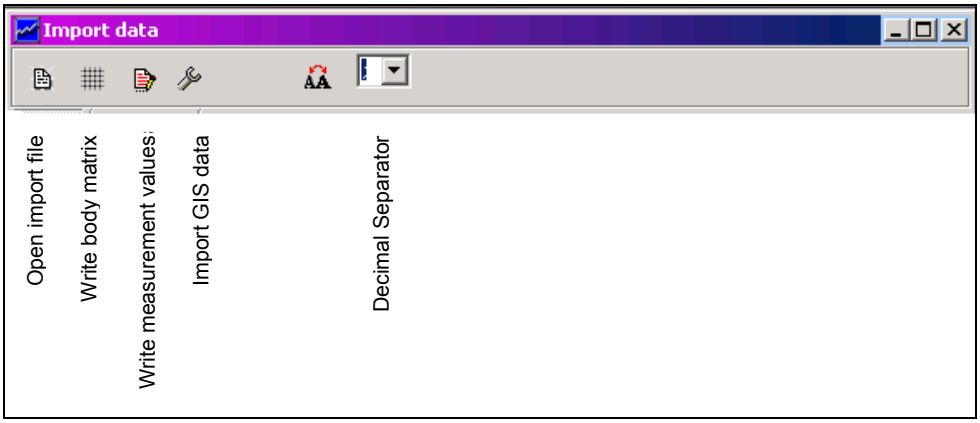


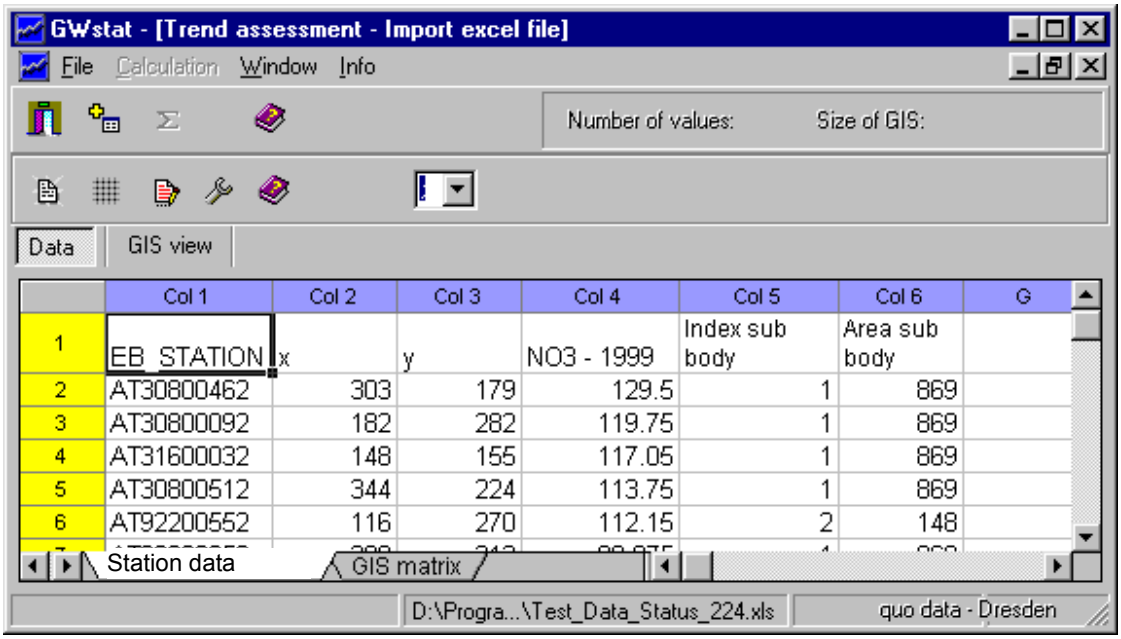
Figure 3: Buttons of the Import Window



If Station data (station co-ordinates and station mean values) and GIS data are stored in the same EXCEL 5.0/95 workbook:

(3) Click on the button *Open import file* and select and open the EXCEL 5.0/95 workbook to be imported.

(4) Select the spreadsheet with the Station data first and click on the button *Write measurement values*.



	Col 1	Col 2	Col 3	Col 4	Col 5	Col 6	G
1	EB_STATION	x	y	NO3 - 1999	Index sub body	Area sub body	
2	AT30800462	303	179	129.5	1	869	
3	AT30800092	182	282	119.75	1	869	
4	AT31600032	148	155	117.05	1	869	
5	AT30800512	344	224	113.75	1	869	
6	AT92200552	116	270	112.15	2	148	

(5) Select the spreadsheet with the GIS matrix and click on the button *Write body matrix*. (Import might take some time depending on the size and the format of the file)

If Measurement data are stored in EXCEL 5.0/95 and GIS data are stored as ASCII file:

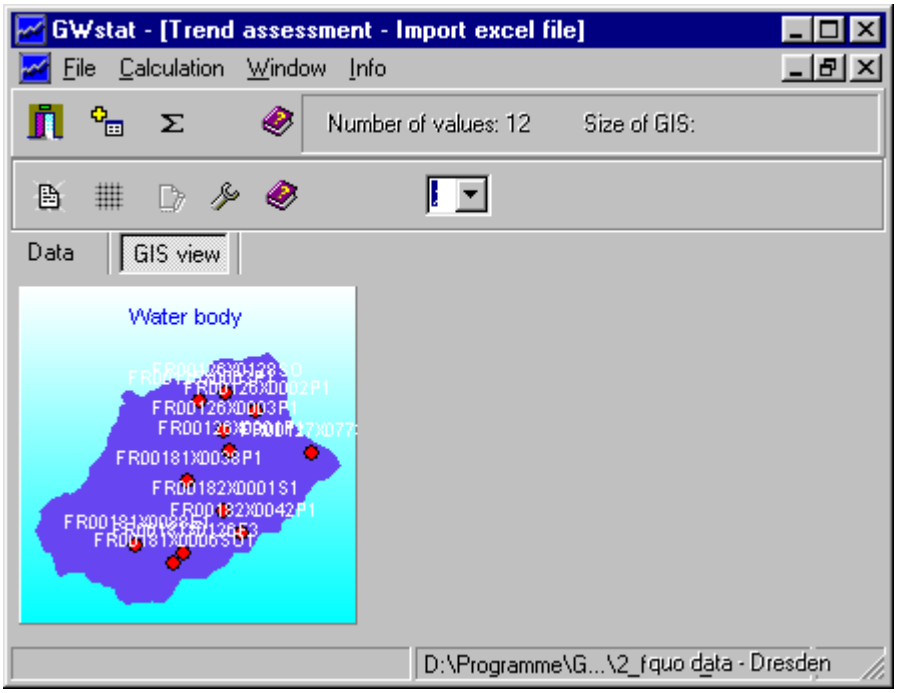
(6) Click on the button *Open import file* and select and open the EXCEL 5.0/95 with the Station data to be imported.

(7) Select the spreadsheet with the Station data and click on the button *Write measurement values*.

(8) To import the GIS ASCII file click on the button *Import GIS data* and select and open the respective ASCII-file with the GIS matrix. (Import might take some time depending on the size and the format of the file)

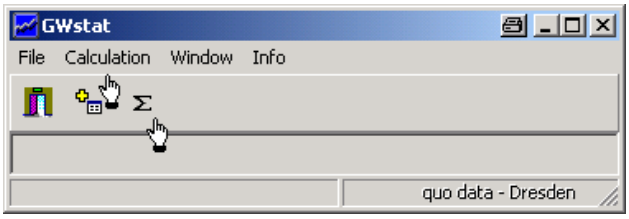
Successful data import of both Station data and GIS data can be checked on the *GIS view* page in the Import Window. The area of the GW-body is highlighted blue and the monitoring sites are indicated as red dots (see Figure 4).

Figure 4: GIS View. Checking successful data import. GW-body (blue area) and sampling sites (red dots)

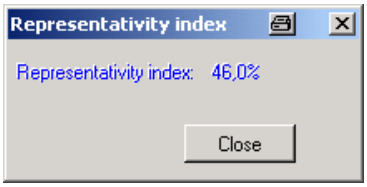


3.2 CALCULATE REPRESENTATIVITY INDEX

(9) For calculation of the Representativity Index click on the *Calculation* menu or click on the button [Σ] .



The result will be displayed in a window with the calculated Representativity Index.



4. STATUS ASSESSMENT

This mode is required in order to:

- assess the chemical status of the ground water body (CL_{AM}, CL_{wAM} or CL_{KM}) or
- calculate the annual or quarterly mean values for the GW-body (AM, wAM or KM) that are required for the trend (-reversal) assessment.

Station co-ordinates, Station mean values and **GW-body GIS data** are necessary for status assessment and have to be prepared according to chapter 2.1.

GIS data are required for the calculation of the Representativity Index R_U and for the calculation of the Kriging mean (KM). For the calculation of the arithmetic mean (AM) or the weighted arithmetic mean (wAM) the import of GIS data is not essential.

4.1 DATA IMPORT

For necessary data format refer to chapter 2.1.

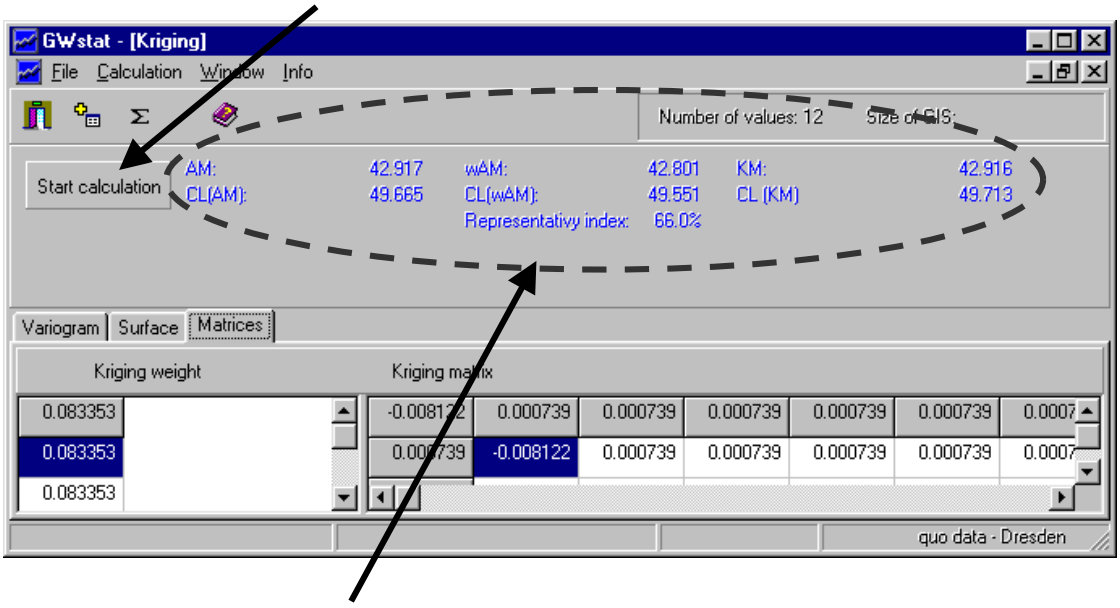
(1) Select *Status assessment* from the *File* menu (see Figure 2).

(2) Follow steps (2) to (8) of chapter 3.1

4.2 CALCULATE STATUS ASSESSMENT

(3) For Status assessment click on the *Calculation* menu or click on the button [Σ] *Status assessment*

(4) Start calculation by clicking on the button *Start calculation*



Calculation results are displayed in blue (AM, CL_{AM}, wAM, CL_{wAM}, KM, CL_{KM}. Furthermore, the Kriging matrix, the Kriging surface as well as the Kriging Variogramm are displayed in the respective window below.

5. TREND ASSESSMENT / MONOTONIC TREND

This mode is required in order to:

- perform trend assessment by the LOESS smoother and perform trend tests based on the LOESS smoother

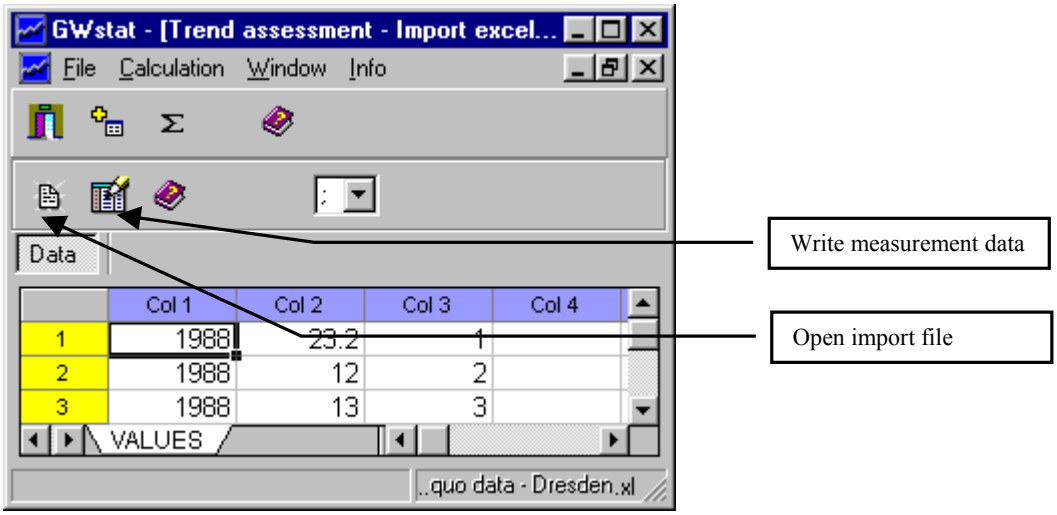
5.1 DATA IMPORT

For necessary data format refer to chapter 2.2.

(1) Select *Monotonic trend* from the *File* menu. (see Figure 2).

(2) Click on *Open import file* and select and open respective file to be imported.

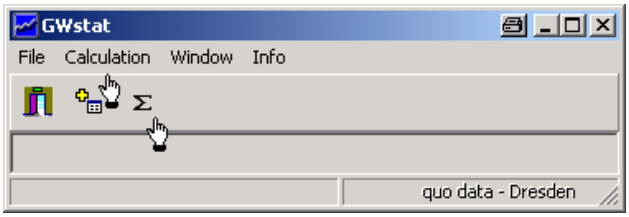
(3) Select the spreadsheet with the GW-body mean values and click on the button *Write measurement values*.



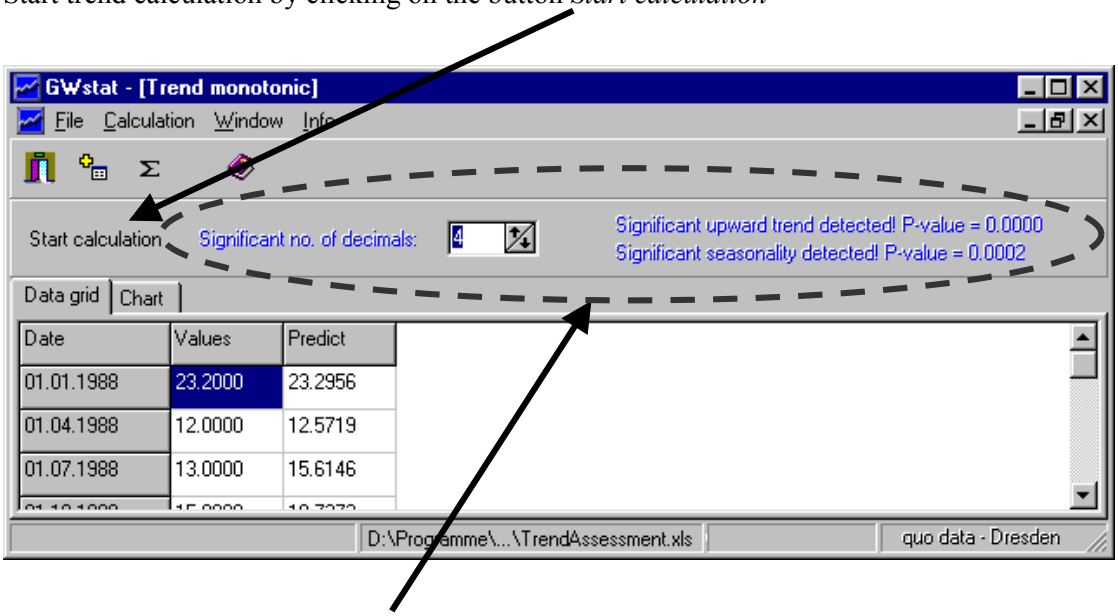
5.2 CALCULATE TREND ASSESSMENT

After data import, which might take some time, depending on the size and format of the file, calculation can be started.

(4) For Trend assessment click on the *Calculation* menu or click on the button [Σ] *Trend assessment*

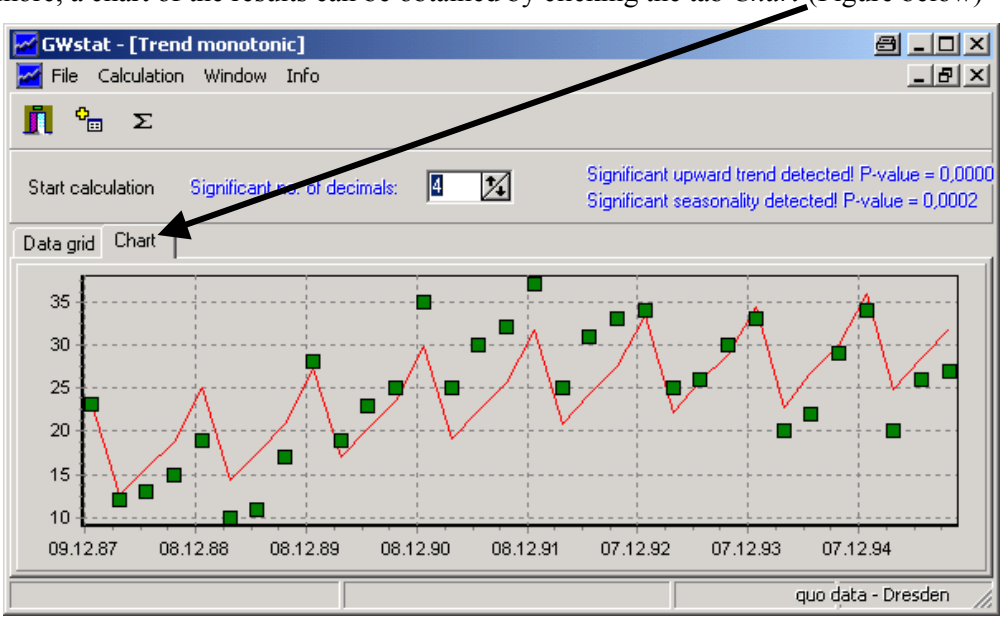


(5) Start trend calculation by clicking on the button *Start calculation*



Calculation results are displayed in blue (Detection of a trend and significance of detection of trend and seasonality).

Furthermore, a chart of the results can be obtained by clicking the tab *Chart* (Figure below)



6. TREND ASSESSMENT / REVERSAL TREND

This mode is required in order to perform trend reversal assessment.

6.1 DATA IMPORT

For necessary data format refer to chapter 2.2.

The analysis of a trend reversal is very similar to the assessment of a monotonic trend.

(1) Select *Reversal trend* in the *File* menu (see Figure 2).

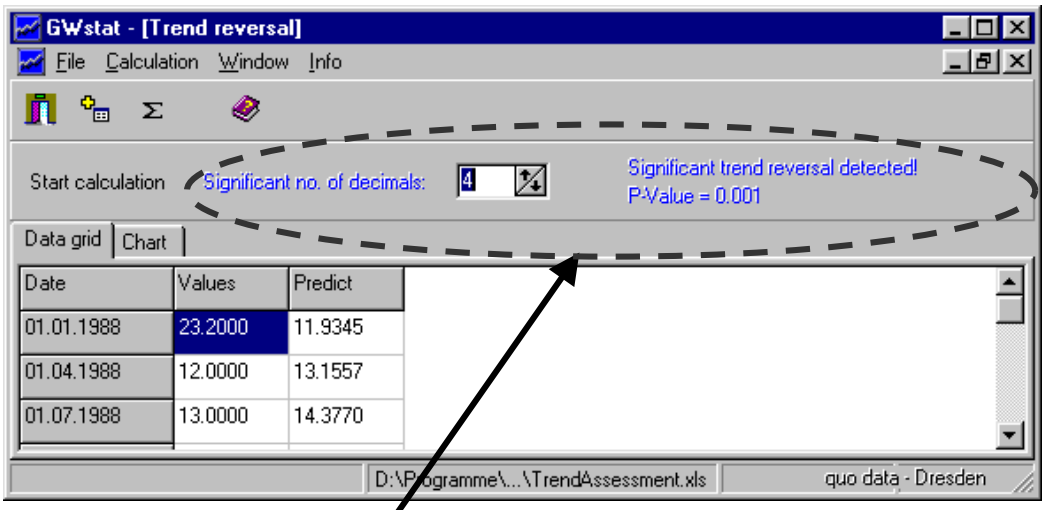
(2) Follow steps (2) and (3) of chapter 5.1

6.2 CALCULATE TREND REVERSAL ASSESSMENT

(3) For Trend reversal assessment click on the *Calculation* menu or click on the button Σ *Trend assessment*

(4) Start trend calculation by clicking on the button *Start calculation*

Results are presented as follows:



Calculation results are displayed in blue (Detection of a trend reversal and significance)

Furthermore, a chart of the results can be obtained by clicking the tab *Chart* (Figure below)