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DG Rijkswaterstaat

ADEPTS - User Manual

Version 1.00

May 2000

R3300

WL | delft hydraulics

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A. Hendriks

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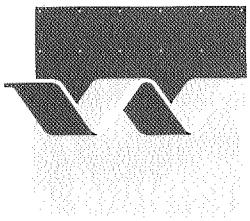

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TITLE:	ADEPTS User Manual / ADEPTS Gebruiksaanwijzing

ABSTRACT:

User Manual for ADEPTS 1.00 (English version and Dutch version)

REMARKS:

These manuals do not conform to the WL "huisstijl" (style). For budgetary reasons they where made from the on-line help using the HelpBreeze™ document wizard, which does not transform easily into the WL style. RIKZ and RIZA approved of this.

REFERENCES:

VER.	ORIGINATOR		DATE	REMARKS	REVIEW		APPROVED BY	
1.00	A. Hendriks		november 18, 1999	see above				
1.00.06	A. Hendriks		may 24, 2000	see above	P. Gijsbers			

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Table of Contents

Introduction

Introduction

ADEPTS, an acronym for "**A** **D**atabase for **E**nvironmental **P**roperties of **T**oxic **S**ubstances", is an application and database for access to information about Physico-Chemical and Ecotoxicologic parameters for various substances in a number of compartments or environmental systems. The physico-chemical parameters stored in ADEPTS are especially relevant for aquatic fate modelling, including sorption, volatilisation, degradation and bioaccumulation. The philosophy behind the database is that a value for a given environmental parameter has no meaning by itself, unless the conditions under which the parameter is measured are carefully characterised. Therefore, every parameter value is accompanied by a number of 'environmental fields'(e.g. pH, temperature, salinity and redox conditions) in order to show it's applicability. While retrieving data from the database, constraints can be specified for these fields. How to specify these constraints is explained in the topic "*Limit the amount of data displayed (see page 19)*". Moreover, the origin of the data is indicated, so that the user can decide whether or not to use review data or QSAR data in addition to real field data. Another unique feature of the database is the quality judgement of the data, which is expressed as a partial score for analytical, methodological and statistical aspects or a score index.

ADEPTS is an integration of the existing applications AQUAPOL and AQUATOX and was developed by BKH Consulting Engineers and WL | Delft Hydraulics for the Dutch *Rijkswaterstaat* (RIZA and RIKZ).

Many of the data in the database have a reliability score. Data from AQUAPOL has separate partial scores for analytical, methodical, statistical and completeness-aspects, assigned by a strict protocol, the data from AQUATOX has been assigned a score-index on the scale from 1 to 4, with the following meaning:

1	excellent
2	reliable
3	unreliable
4	not evaluated

For all enquiries about the protocols you may contact A. de Vries, RIKZ.

Selections and profiles

A Selection is a complete description for a (partial) display of information from the database. It contains information about which substances, parameters and environmental systems to display, as well as information about each column, such as constraints, the width of the column, etc. In this helpfile, each time the word selection is used to describe this complete description, it will be spelled with a capital letter S. A

selection in another sense, like a simple selection from a list, will be written with a small letter s.

An important distinction exists between *Selections* and *Profiles*. A Profile is a Selection that cannot be displayed because one or more items that are necessary to display a Selection are missing. An example is a Selection without any substances: as all information in the database pertains to experiments or norms **for a substance**, nothing can be displayed without specifying a substance. The incomplete Selection can however contain valuable information about which experiments you want to display, which columns you want to display, etc. Profiles (incomplete Selections) can be saved, so all the information can be stored for later use. It is also possible to store a complete Selection as a profile. In that case one of the three main ingredients of a Selection (substances, parameters and environmental systems) will be left out of the file. Which one is determined by the menu *Options/Preferences/Undetermined in profile* in the *Main window (see page 30)*.

The substances shown in the *Main window (see page 30)* are **not** influenced by the constraints as set in the *Constraints window (see page 26)*. E.g. if the Selection or Profile has a constraint on the Molecular Weight of "< 100.0" the substancelist in the Main window and Substances window will still show substances with a weight >= 100.0 g/mol.

Installation

To install ADEPTS you need:

- The CD-ROM with the installation program,
- A Personal Computer with Windows™ 95 B, Windows 98 or Windows NT4 with (at least) Service Pack 3,
- A CD-ROM player,
- At least 20 MegaBytes free on a local harddisk or networkdrive.

A Pentium processor of 300 MHz or better is recommended, as is a screenresolution of at least 1024 * 768 pixels.

Installation of ADEPTS proceeds as follows:

- Close all other applications.
- Put the installation CD in the CD-ROM player (in this example we assume F: is the CD drive)
- Start the program SetupA.exe in the main folder of the CD-ROM (double-click on this file in the Windows Explorer **or** select *Run* from the *start menu* and type "F:\SetupA.exe" after *Open* and push on the OK button.)
- Follow the directions on screen. It is possible you receive some warnings about other versions of the *DelftLng* libraries. If these warnings say it is not save to continue, abort the installation and contact WL | Delft Hydraulics.

After the installation there is a group *ADEPTS* in the *Programs* menu of the *start menu*, which contains shortcuts to the executable and the helpfiles in Dutch and English. You can start the program by selecting the executable in this group. The installation also sets associations for Selection files (`*.dsl`) and Profile files (`*.dpr`), so the program can also be started by *double-clicking* on a Selection file (`*.dsl`) or Profile file (`*.dpr`) in the Windows Explorer.

How to ...

Select substances

Select substances

Several ways exist to decide which substances are included in a Selection. Which way is the most effective, depends on the information you have about the substances you want to include in (or exclude from) your Selection. All these selections are made by pressing the "Substances" button in the *Main window (see page 30)*.

If you know the name you can try to select the substance(s) *directly from the lists (see page 11)* or, if you can not find the name in the list, you can try selection *by synonym (see page 14)*. Selection *by name (see page 12)* is slower, but finds primary names and synonyms at the same time.

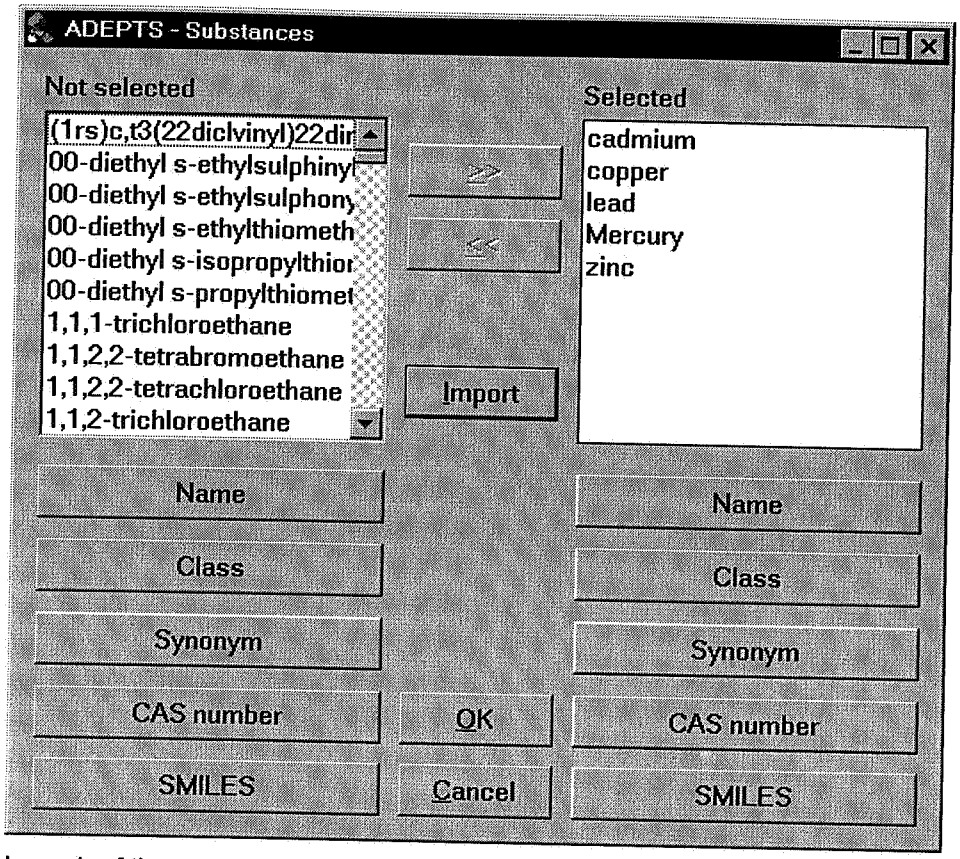
If you want to make a selection based on the (chemical) class substances belong to, you can try selection *by class (see page 13)*.

If you know the CAS number, you can select *by CAS number (see page 15)* or *Import from an ASCII file (see page 17)* with CAS numbers.

The last way to select substances, is by looking for a functional chemical group in the linear notation (SMILES notation) via selection *by SMILES notation (see page 16)*.

Select substances from list

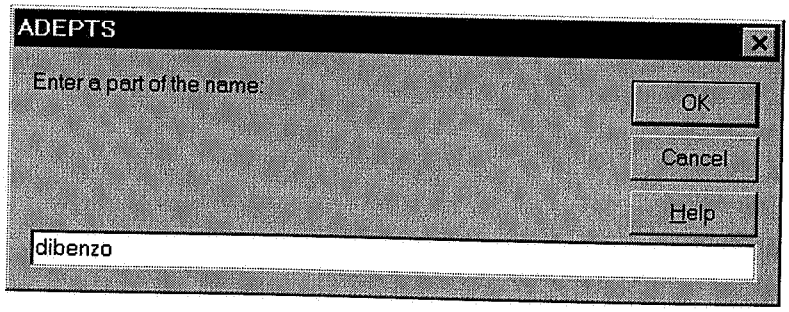
The selection of substances directly from the list, is the fastest way to select and deselect substances if you know the primary name in the database. In the Substances window two lists are displayed: the list on the left side of the window contains the primary names of all substances that are **not** part of the Selection (or Profile), the list on the right contains the primary names of all substances that **are** part of the Selection.



In each of these two lists you can select one or more names. To select one name just click on the name by pointing to it with the mousepointer and click with the left mousebutton. To select a consecutive range of names, click on the first name in the range with the left mousebutton and then click on the last name of the range while pressing the shift key. To select a number of non-consecutive names, click on each one with the left mousebutton, while pressing the ctrl key. After you have selected one or more names, they will appear with a different colour. These 'highlighted' names can then be moved from the left list to the right list (if you selected names to be added to the selection) or from the right list to the left list (if you selected names to be removed from the selection) by pressing the appropriate button between the lists at the top of the window. The changes you make become effective as soon as you press the "OK" button. This button also closes the window.

Select substances by name

The selection of substances by name is slower then selection *directly from the list (see page 11)*, but can be effective if you are not sure whether the name you are looking for is a primary name or a synonym or if you want to search for a partial name. If you want to select substances for inclusion in the Selection, press the button "Name" under the left list, if you want to remove substances from the Selection, press the button "Name" under the right list. The next window will appear:

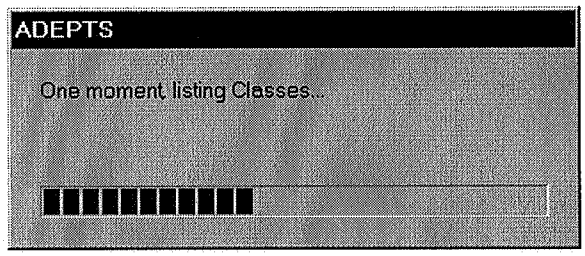


Type the name, or part of the name, in the textbox, and press the "OK" button. A progressbar will appear:

After a few moments the progressbar will disappear and the application will have selected (highlighted) all substances in the appropriate list that contain the string (in this example "dibenzo") in either the primary name or one of the synonyms. The comparison is not case-sensitive and any previously selected substances will still be selected. The 'highlighted' names can then be moved from the left list to the right list (if you selected names to be added to the Selection) or from the right list to the left list (if you selected names to be removed from the Selection) by pressing the appropriate button between the lists at the top of the window. The changes you make become effective as soon as you press the "OK" button. This button also closes the window.

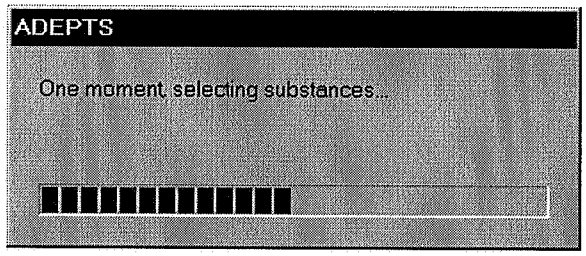
Select substances by class

The selection of substances by class is slower then selection *directly from the list (see page 11)*, but can be effective if you want to include (or exclude) **all** substances in a (chemical) class. If you want to select substances for inclusion in the Selection, press the button "Class" under the left list, if you want to remove substances from the Selection, press the button "Class" under the right list.



The application will show a progress bar while making a list of all classes that have at least one substance in the appropriate list. After this task is completed, the next window will appear:

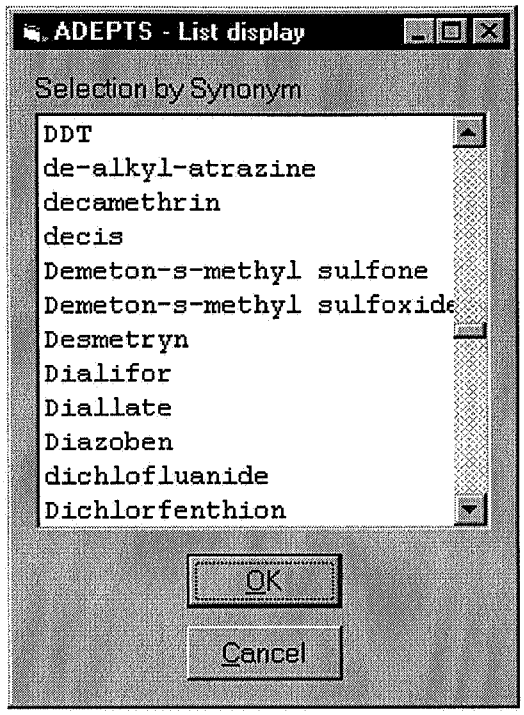
To select one class just click on the name by pointing to it with the mousepointer and click with the left mousebutton. To select a consecutive range of names, click on the first name in the range with the left mousebutton and then click on the last name of the range while pressing the shift key. To select a number of non-consecutive names, click on each one with the left mousebutton, while pressing the ctrl key. After you have selected one or more classes, they will appear with a different colour. To select all substances that belong to one or more of the selected classes, press the "OK" button. A new progressbar will appear:



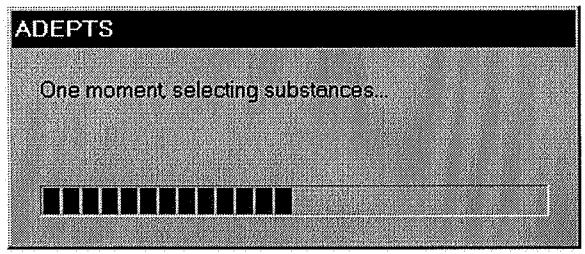
After a few moments the progressbar will disappear and the application will have selected (highlighted) all substances in the appropriate list that belong to the selected class(es). Previously selected substances will still be selected. The 'highlighted' names can then be moved from the left list to the right list (if you selected names to be added to the Selection) or from the right list to the left list (if you selected names to be removed from the Selection) by pressing the appropriate button between the lists at the top of the window. The changes you make become effective as soon as you press the "OK" button. This button also closes the window.

Select substances by synonym

The selection of substances by synonym is slower then selection *directly from the list (see page 11)*, but less sensitive to typing errors than *selection by name (see page 12)*. If you want to select substances for inclusion in the Selection, press the button "Synonym" under the left list, if you want to remove substances from the Selection, press the button "Synonym" under the right list. The application will show a progress bar while making a list of all synonyms for substances in the appropriate list. After this task is completed, the next window will appear:



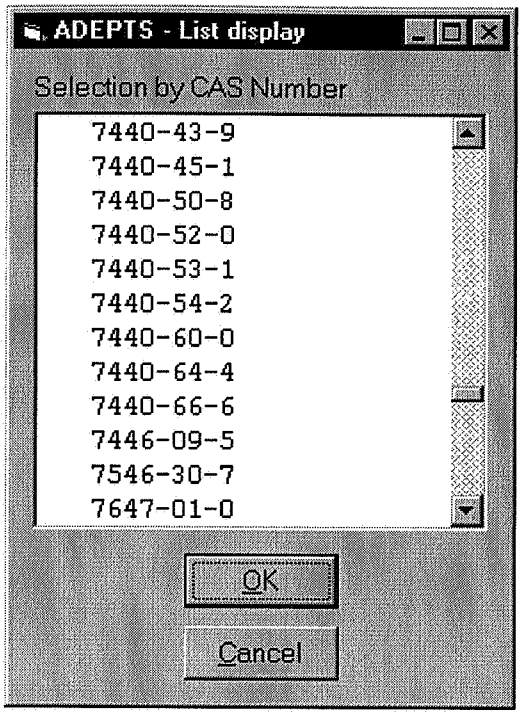
To select one synonym just click on the name by pointing to it with the mousepointer and click with the left mousebutton. To select a consecutive range of names, click on the first name in the range with the left mousebutton and then click on the last name of the range while pressing the shift key. To select a number of non-consecutive names, click on each one with the left mousebutton, while pressing the ctrl key. After you have selected one or more synonyms, they will appear with a different colour. To select all substances that have the selected synonyms, press the "OK" button. A new progressbar will appear:



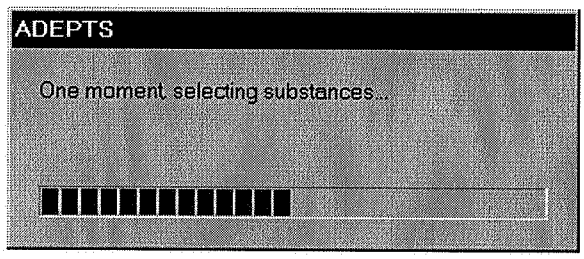
After a few moments the progressbar will disappear and the application will have selected (highlighted) all substances in the appropriate list having the selected synonym(s). Previously selected substances will still be selected. The 'highlighted' names can then be moved from the left list to the right list (if you selected names to be added to the Selection) or from the right list to the left list (if you selected names to be removed from the Selection) by pressing the appropriate button between the lists at the top of the window. The changes you make become effective as soon as you press the "OK" button. This button also closes the window.

Select substances by CAS Number

The selection of substances by CAS number is slower then selection *directly from the list (see page 11)*, but does not depend on language-sensitive names. If you want to select substances for inclusion in the Selection, press the button "CAS number" under the left list, if you want to remove substances from the Selection, press the button "CAS number" under the right list. The application will show a progress bar while making a list of all CAS numbers for substances in the appropriate list. After this task is completed, the next window will appear:



The CAS numbers are listed in ascending order. To select one CAS number just click on the number by pointing to it with the mousepointer and click with the left mousebutton. To select a consecutive range of numbers, click on the first number in the range with the left mousebutton and then click on the last number of the range while pressing the shift key. To select a number of non-consecutive numbers, click on each one with the left mousebutton, while pressing the ctrl key. After you have selected one or more CAS numbers, they will appear with a different colour. To select all substances that have the selected CAS numbers, press the "OK" button. A new progressbar will appear:



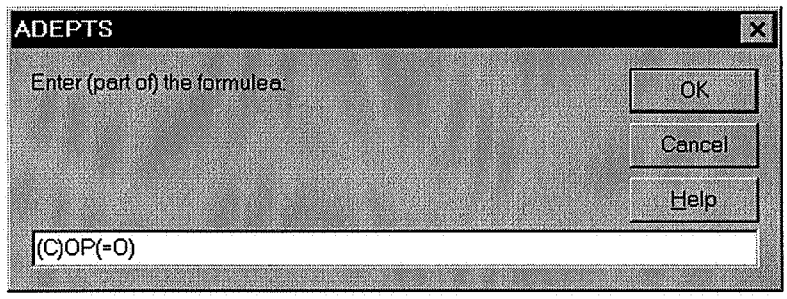
After a few moments the progressbar will disappear and the application will have selected (highlighted) all substances in the appropriate list having the selected CAS number(s). Previously selected substances will still be selected. The 'highlighted' names can then be moved from the left list to the right list (if you selected names to be added to the Selection) or from the right list to the left list (if you selected names to be removed from the Selection) by pressing the appropriate button between the lists at the top of the window. The changes you make become effective as soon as you press the "OK" button. This button also closes the window.

CAS numbers that you want to include in the Selection may also be read from an ASCII file. This is explained in "*Import CAS numbers (see page 17)*".

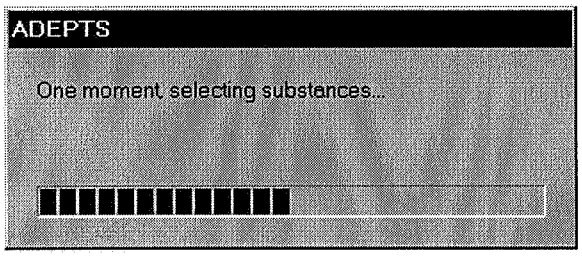
Select substances by SMILES

The selection of substances by functional group in the SMILES notation is slower then selection *directly from the list (see page 11)*, but can be effective if you want to select substances with the same functional group, and this group is written the same way in all notations. If you want to select substances for inclusion in the Selection, press the button

"SMILES" under the left list, if you want to remove substances from the Selection, press the button "SMILES" under the right list. The next window will appear:



Type the group, or part of the group, in the textbox, and press the "OK" button. A progressbar will appear:



After a few moments the progressbar will disappear and the application will have selected (highlighted) all substances in the appropriate list that contain the string (in this example "(C)OP(=O)") as part of the SMILES notation. The comparison is case-sensitive! Any previously selected substances will still be selected. The 'highlighted' names can then be moved from the left list to the right list (if you selected names to be added to the Selection) or from the right list to the left list (if you selected names to be removed from the Selection) by pressing the appropriate button between the lists at the top of the window. The changes you make become effective as soon as you press the "OK" button. This button also closes the window.

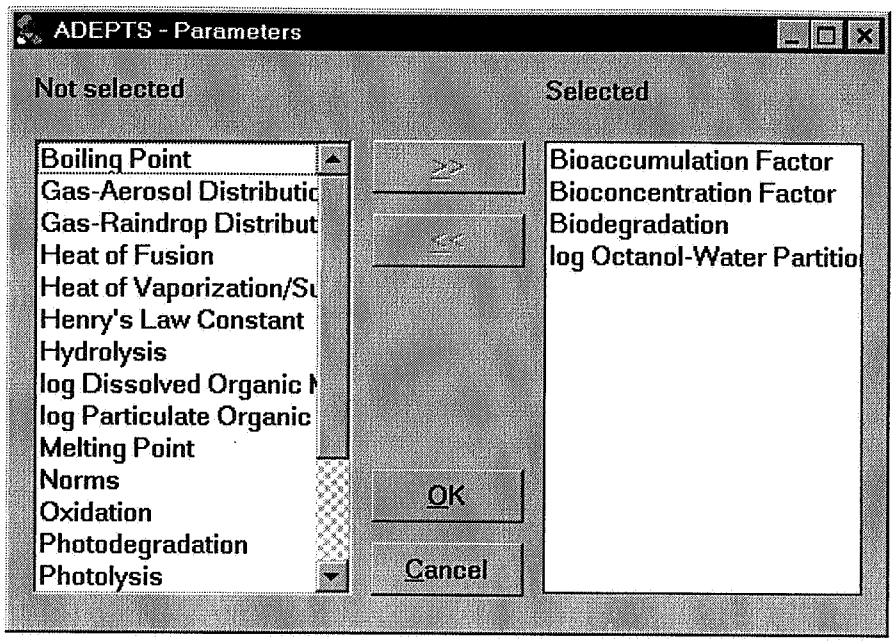
Import CAS numbers

To select substances based on a text-file with CAS numbers, press the "Import" button between the two lists in the *Substances window (see page 40)*. A dialog will ask for the name of the ASCII file (see "*Open ASCII import dialog (see page 32)*"). This file should contain lines with only CAS numbers, one number per line. Lines that cannot be resolved to a valid CAS number will be ignored, for all other lines the application will try if the given CAS number belongs to a substance in the left list, and if so, will select this substance. A log file with the name "Import.log" is generated in the 'user' folder (see "*The ADEPTS ini file (see page 42)*").

Select parameters

Select parameters

The Parameter selection is made by pressing the "Parameters" button in the *Main window (see page 30)*. Pressing it will show the next window:



In the Parameters window two lists are displayed: the list on the left side of the window contains the names of all parameters that are **not** part of the Selection (or Profile), the list on the right contains the names of all parameters that **are** part of the Selection.

In each of these two lists you can select one or more names. To select one name just click on the name by pointing to it with the mousepointer and click with the left mousebutton. To select a consecutive range of names, click on the first name in the range with the left mousebutton and then click on the last name of the range while pressing the shift key. To select a number of non-consecutive names, click on each one with the left mousebutton, while pressing the ctrl key. After you have selected one or more names, they will appear with a different colour. These 'highlighted' names can then be moved from the left list to the right list (if you selected parameters to be added to the selection) or from the right list to the left list (if you selected parameters to be removed from the selection) by pressing the appropriate button between the lists at the top of the window. The changes you make become effective as soon as you press the "OK" button. This button also closes the window.

Select compartments

Select compartments

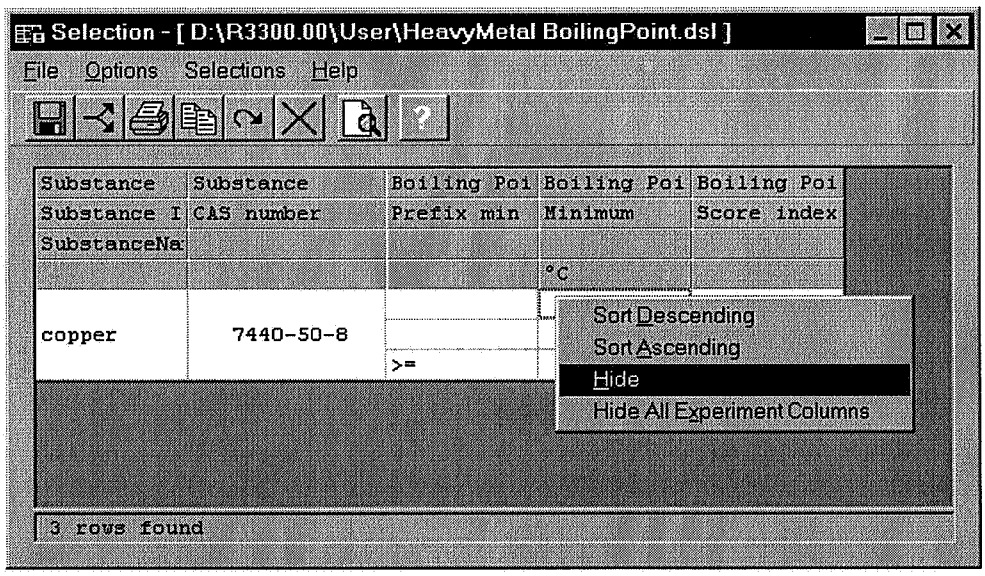
Compartments, also called Environmental systems, are selected and deselected by clicking on the checkboxes in the rightmost frame (System) of the Main window. Changes are effective immediately, unlike the selection of substances and parameters, where you can "Submit" or "Cancel" your changes when leaving the selection window. Be aware of the fact that not all parameters have to be defined for all compartments: in release 1.00 of ADEPTS oxidation is defined only for the three water compartments and air, whereas the boiling point is only defined for the compartment "not applicable".

Display the selection

Limit the amount of data displayed

After selecting substances, parameters and compartments in the *Main Window (see page 30)*, the button "Show" will display all data for the Selection. The data is displayed in a grid (see the example in the paragraph "*Selection window (see page 37)*"), and for a selection with more than one parameter there might easily be 50 or more columns. Not all columns in this window will be of importance for the question at hand, and also not all rows in the display will contain relevant data. For instance, when displaying data for pKa experiments, you might not be interested in the column "pKa/Origin ID/Origins/Description", which describes the origin of the data in a row, because you want to display only those experiments that have "Measured" as their origin. How to hide and show columns is described in the paragraph "*Show or hide columns (see page 19)*", while the paragraph "*Set constraints for a column (see page 21)*" describes how to filter out rows by specifying constraints.

Show of hide columns



Hiding columns

Columns in the Selection window can be hidden in a number of ways.

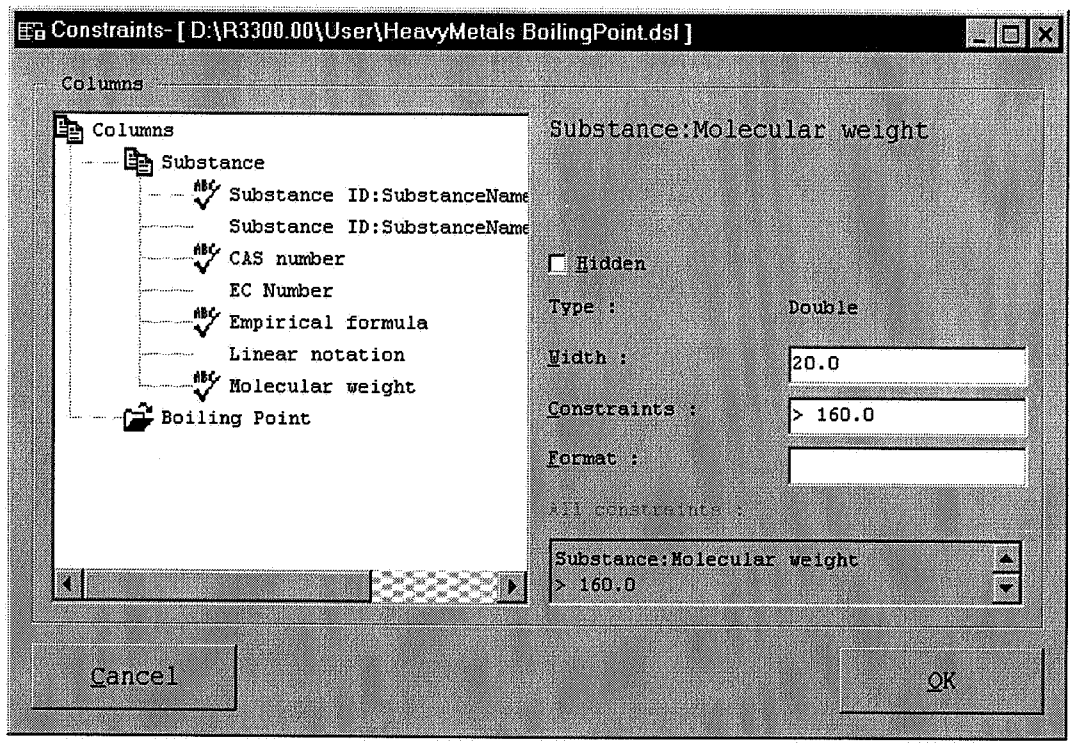
- Perhaps the most intuitive way is by pointing to a column with the mousepointer and clicking the right mousebutton. The menu shown in the above picture will pop-up and by selecting the item "Hide" the column will be hidden.
- The same menu can also be found via the main menu for this window: select *Options/Column options*. In this case the command influences the current column, the column that you last clicked on with the mouse or last accessed via the keyboard. The current column has a 'selection rectangle' around the current cell, but this rectangle might be in a part of the grid that is not visible at that moment.
- The third way of making a column invisible is by reducing the width of the column to 0. When the mousepointer is placed on the top rows **between** two columns it changes to a vertical beam with two arrows pointing to the left and to the right. If you press the left mousebutton you can move the right border of the left row to influence the size of that row. If you move the right border to the same position as the left border the width becomes 0, effectively hiding the column.

- The last way to hide a column is by pressing the button "Set criteria and show/hide" on the toolbar ( ) or selecting menu *Options/Constraints*. This will display the "Constraints window" where you can also hide each column. This is covered in the next section.

Hiding a column does **not** influence the constraints for that columns. See "*Set constraints for a column (see page 21)*" for an explanation about setting constraints.

Showing columns

In the Constraints window all details for each column in the grid are shown and most of these details may be edited. This includes the checkbox "Hide", which can be found in the right pane of this window. Checking it will make the column identified by the highlight in the left pane **and** by the larger caption at the top of the right pane invisible (in our example this is the column "Substance:Molecular weight"), unchecking it will make the column visible (if the width given is larger than 0). The visibility can also be toggled by clicking on the column name in the left pane using the **right** mousebutton. A checkmark before the column name identifies a visible column.



More about this window is explained in the paragraph "*Setting constraints for a column (see page 21)*".

The value for the width is measured in millimetres. The value given will not be exact due to different screen sizes and differences in printers.

Sizing a column may also be done directly in the Selection window, as explained in the section "hiding columns" above.

Set constraints for a column

A constraint for a column is like the WHERE clause in an SQL query: it formulates which records (rows) will be displayed as the result of a database query operation. In the constraint textbox in the right pane of the *Constraints window (see page 26)* you may enter a valid 'sQL WHERE clause'-like string (without fieldnames) as the constraint. What is valid and not is determined by the type of the column (which is displayed two rows above the constraint textbox).

Examples of valid constraints are:

Type of field	Constraint	Comments
single, double	< 160.0	Select all rows where the value for the field is less than 160.0
single, double	> 100.0 AND < 150.0	Select all rows where the value for the field lies between 100 and 150.
Single, double	<= 100.0 OR > 150.0	Select all rows where the value for the field is smaller than or equal to 100 or larger than 150.
Single, double	<> 100.0	Select all rows where the value for the field is not equal to 100.0. Beware that using the comparisons '=' and '<>' with floating point numbers may give unexpected results due to rounding errors.
Single, double	MEAN	Special case, see later in this paragraph.
text	="Janssen"	Select all rows where the value for the field is exactly "Janssen" (not case-sensitive).
text	="Janssen" OR IsNull	Select all rows where the value for the field is exactly "Janssen" (not case-sensitive) or the field is empty.
text	LIKE "Jans*"	Select all rows where the value for the field starts with "Jans" (not case-sensitive).
text	NOT LIKE "Jans*"	Select all rows where the value for the field does not start with "Jans" (not case-sensitive).
text	LIKE "*jans*"	Select all rows where the value for the field contains "jans" anywhere in the field.
text	LIKE "P[A-F]###"	Select all rows where the value for the field begins with the letter P, followed by any letter between A and F and three digits.
text	LIKE " 7*"	Select all rows where the value for the field starts with three spaces and a 7" (e.g. CAS Numbers less than "1000000-00-0" start with spaces)
long	= 8	Select all rows where the value for the field equals 8.
long	IN (8, 9, 12)	Select all rows where the value for the field equals 8 or 9 or 12.

The keywords that may be used are AND, IN, ISNULL, LIKE, NOT and OR. Keywords are not case-sensitive. The ISNULL keyword is only practical alone or in combination

with OR. E.g. a phrase like "LIKE 'P*' AND ISNULL" will never return records, because there never will be records where a field is empty and at the same time contains a string starting with a 'P'.

The comparison operators that may be used are =, <, <=, <>, > and >=.

Parenthesis may be used to group statements.

Three special constraints are valid for numeric fields: the words **MIN**, **MEAN** and **MAX**, spelled with capital letters and **alone** as constraint for a field have special meaning: the rows resulting from all other constraints will be reduced to one row. In the case of the keyword MIN by displaying the row with the lowest value for that column, in case of the keyword MAX by displaying only the row with the highest value for that column and in the case of the keyword MEAN by taking the mean of al rows for that column.

By pressing the F2 key a list with all possible values for a field will pop-up. By selecting one or more of these values a constraint will be generated by the application. Not very useful if many values are possible, but nice if the number of possible values is lower than ca. 10.

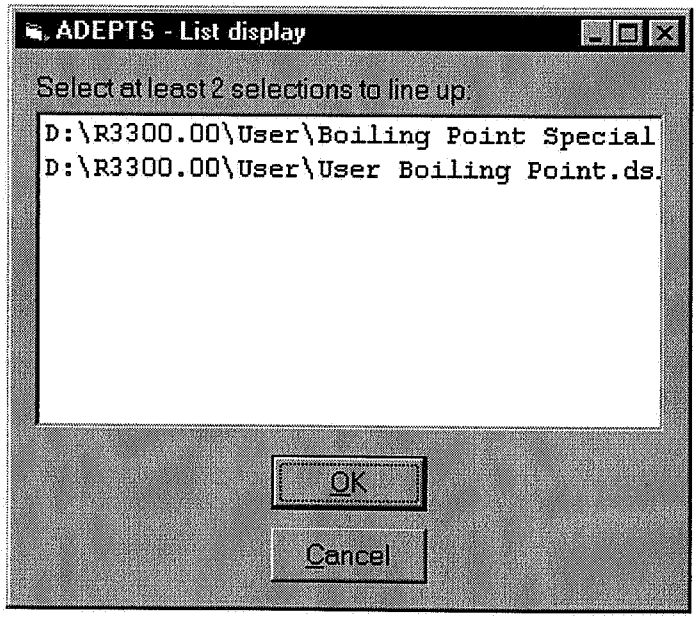
By pressing the F4 key, the application will check the constraint, and if any doubtful parts are detected, these will be 'highlighted'.

When constraints on more than one column are defined, they are combined using 'AND'.

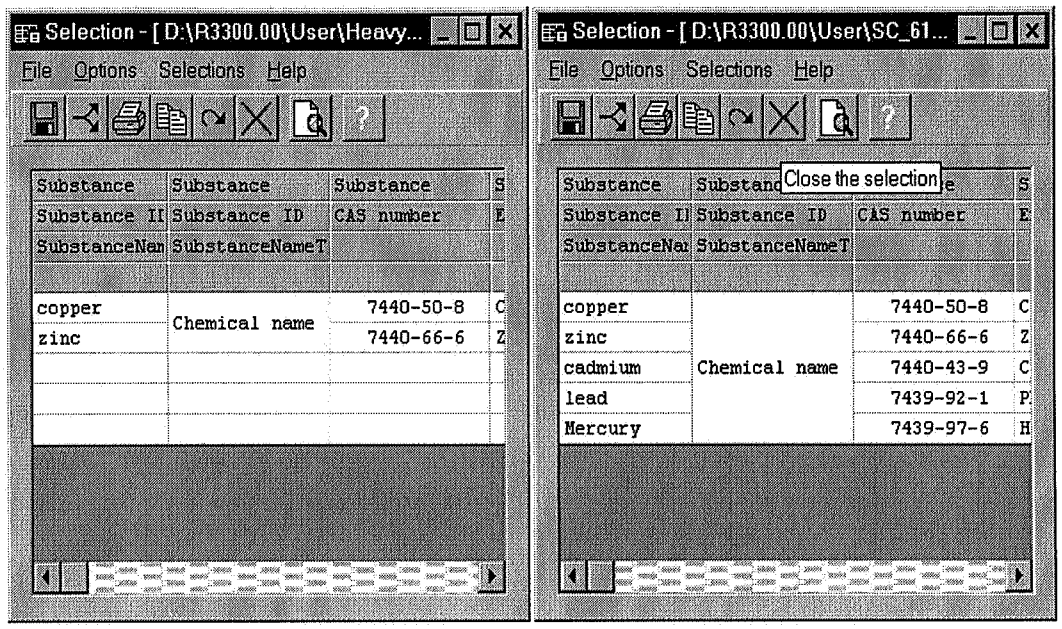
The total length of a constraint may not exceed 1000 characters.

Line up Selections

When two or more Selections are visible on the screen, it is possible to display rows with equal data on the same position in all *Selection windows (see page 37)*. This is done by selecting the menu *Selections / Line up* in one of the Selection windows. A list with all the Selections on screen will appear:



Select two or more of these Selections by clicking on them with the mouse while keeping the Ctrl key down and press the Close button. After positioning the windows with the tile or cascade option, the screen will show something like the following example:



For each row that is present in the right Selection, but not in the left Selection, an empty row is displayed in the left Selection. Also, if the left collection would have had rows that are not present in the right Selection, empty rows would have been added to the right Selection. In this way all the Selections will display the same records on the same rows. Differences between the Selections are thus easy to spot. Sorting any of the Selections on a column will not remove the empty rows, but rows will not be in the same position in all Selections any longer!

Print or export the data

Print the data

Printing of the data is possible from the *Selection window (see page 37)*. To print the Selection either

- press the button "Print" on the toolbar ( )
- select the menu *File/Print* , or
- press Ctrl-P

The *Print Preview window (see page 35)* will appear. Here you can click on the button "Print" to print the Selection on the current printer or use the button "Setup" to show the *Page Setup window (see page 34)* where you can change the page set-up and the printer.

Export the data

Export of the data to a CSV file, which can be read by Microsoft Excel® and other spreadsheet programs, is possible from the *Selection window (see page 37)*. To export the Selection either

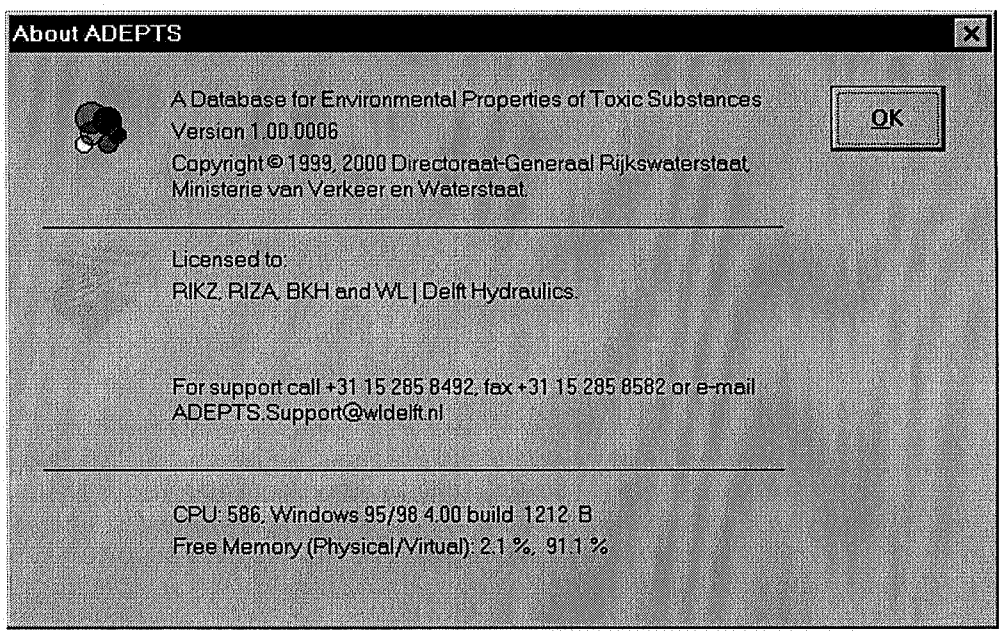
- press the button "Export" on the toolbar ( ) or

- select the menu *File/Export...*

The *Export dialog (see page 27)* will appear. Here you can enter the name of the file you want to export the Selection to.

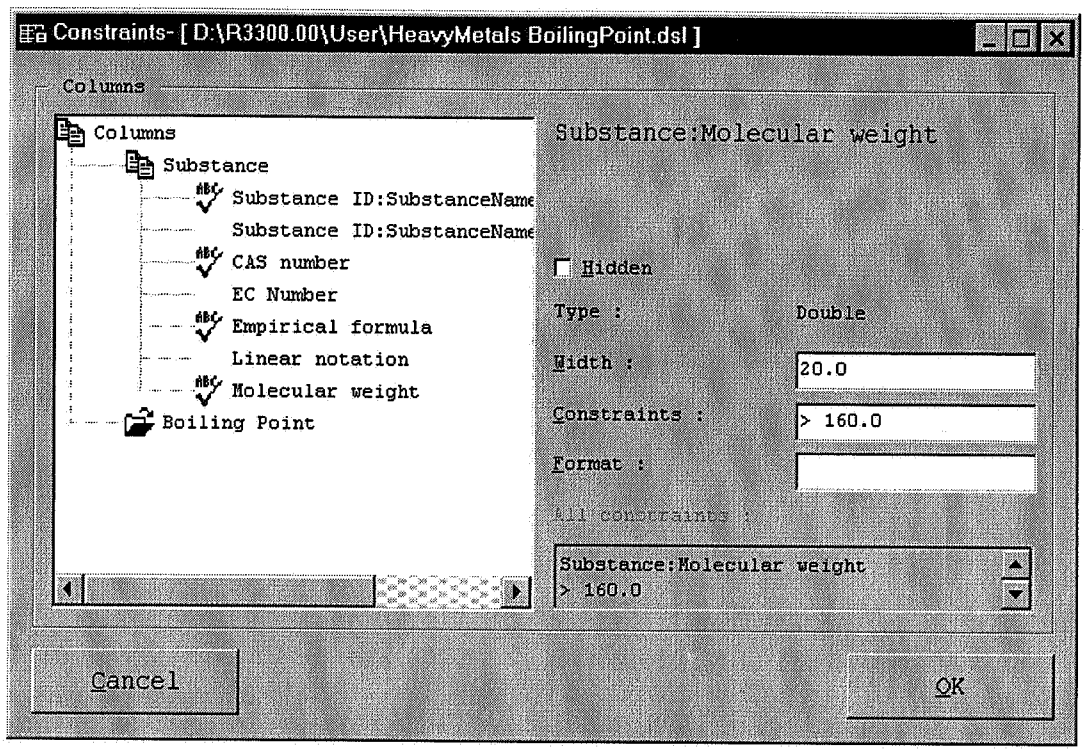
The windows in detail

About dialog



This dialog is shown when initialising the program, or in response to selecting *About ADEPTS...* on the *Help* menu in the Main window or Selection Window. It not only shows the exact version of the application, which is important when reporting problems, but also the version and build of the Windows™ operating system.

Constraints window



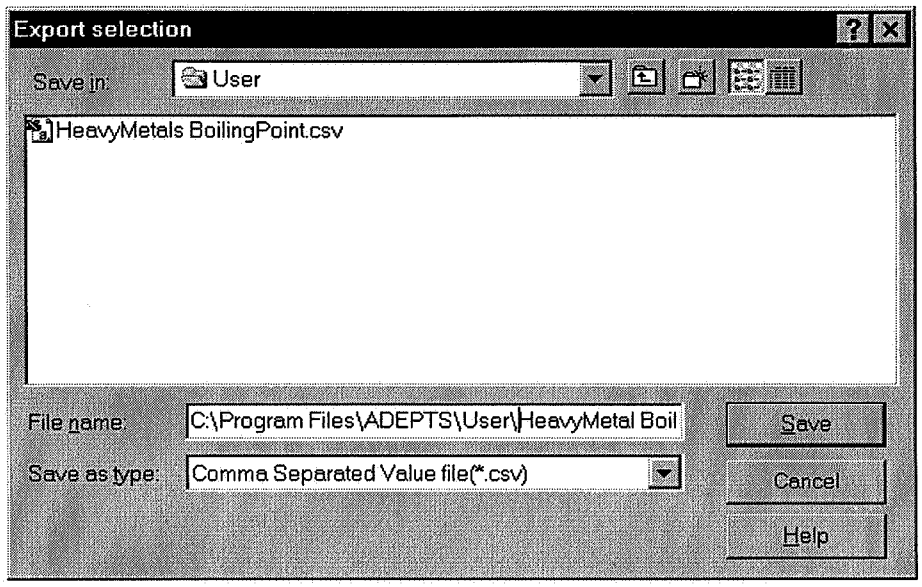
This window allows you to set constraints for a Selection. The Selection you are working with is displayed in the title of the window. More information about setting constraints can be found in *Setting constraints for a column (see page 21)*, how to hide or display columns is explained in *Show or Hide columns (see page 19)*.

The width is given in millimetres.

Constraints may be up to 1000 characters long.

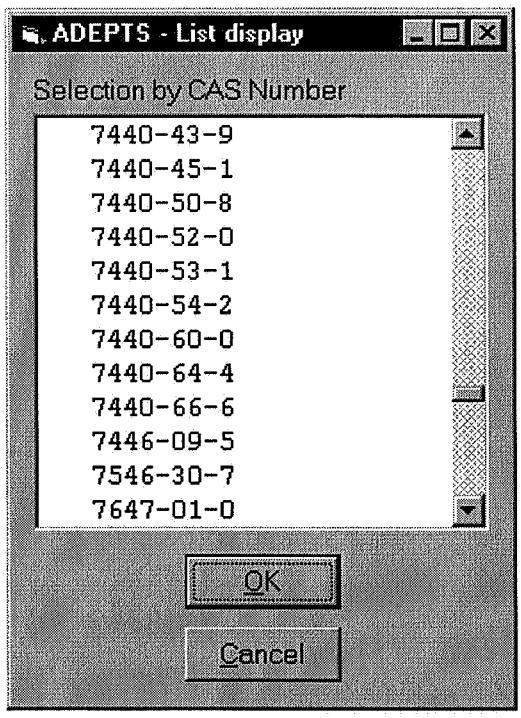
In the format field you may enter the format to use for columns. E.g. "0.00" will display numeric values with 2 digits after the decimal point (and as many before the decimal point as needed). "<" will display text fields in lowercase and ">" will display text fields in uppercase. Formats for the substance columns are ignored. The format may be up to twelve characters long.

Export dialog



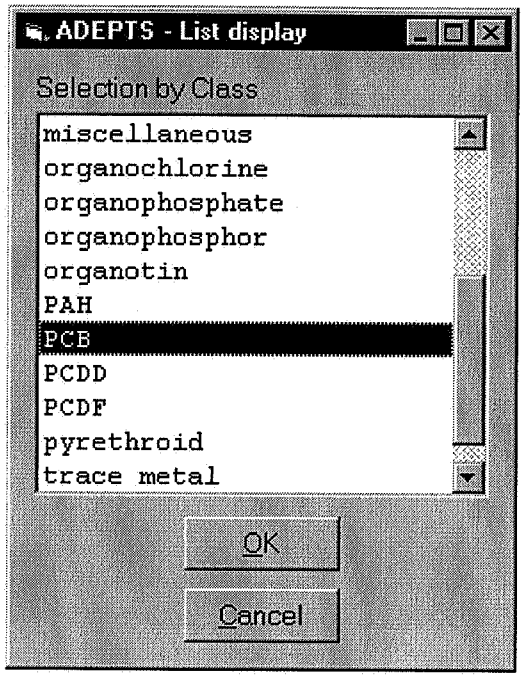
In this windows *Save as dialog* you can enter the name for the export file.

List display CAS numbers



This dialog shows all CAS numbers for the substances on the relevant side of the *Substances window (see page 40)*. The procedure where this dialog is used is described in "*Select substances by CAS number (see page 15)*".

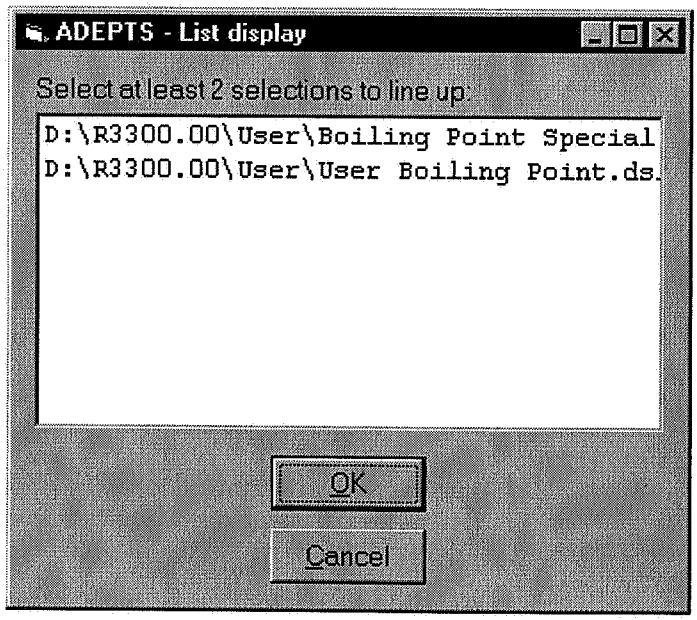
List display classes



This dialog shows all classes for the substances on the relevant side of the *Substances window (see page 40)*. The procedure where this dialog is used is described in "*Select substances by class (see page 13)*".

List display lineup

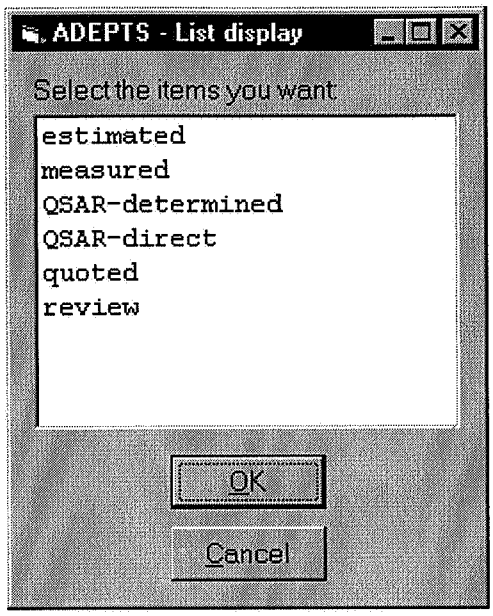
This window shows all Selections that are on the screen. You may select two or more Selections to line-up by clicking on them with the mousepointer while at the same time holding down the Ctrl-key.



After pressing the OK button, the selected Selections will be lined-up. See: *Line-up selections (see page 22)* for more information.

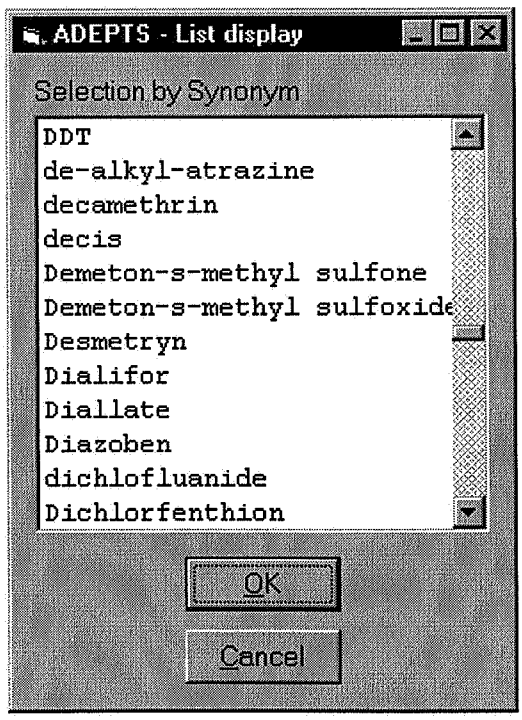
List display possible values

This window shows all possible values for this field. You may select two or more values by clicking on them with the mousepointer while at the same time holding down the Ctrl-key.



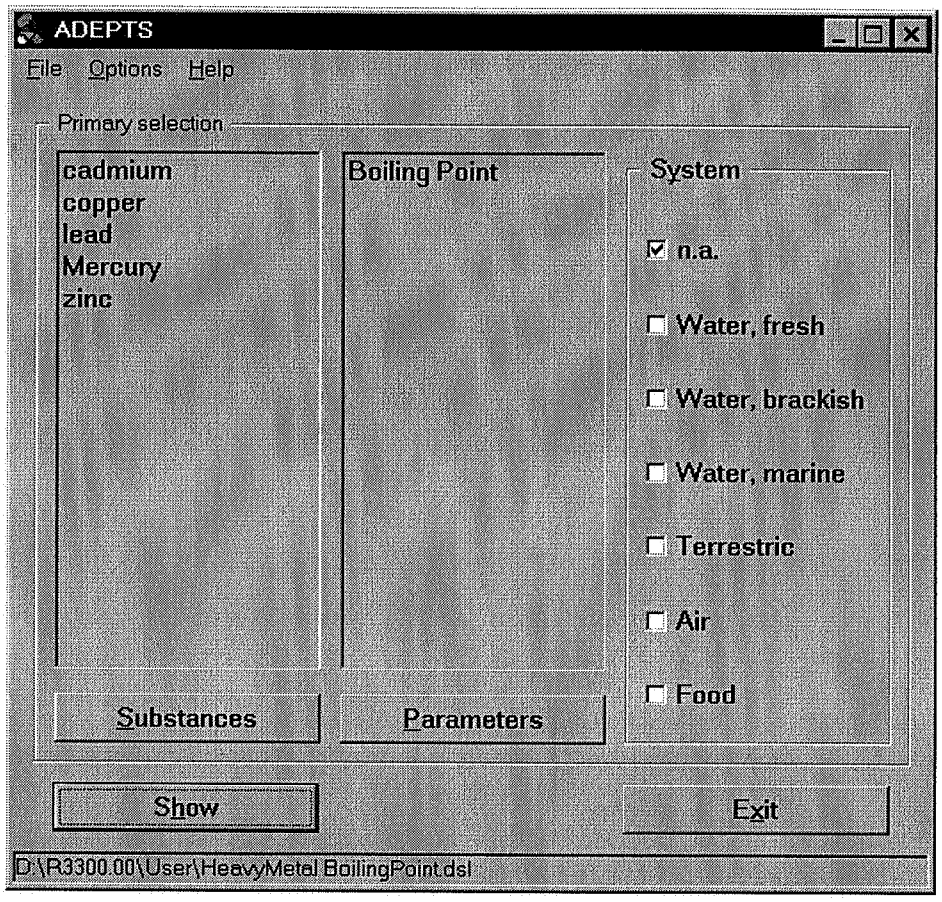
After pressing the OK button, a constraint will be made from the selected values. See: *Setting constraints for a column (see page 21)* for more information.

List display synonyms



This dialog shows all synonyms for the substances on the relevant side of the *Substances window (see page 40)*. The procedure where this dialog is used is described in "*Select substances by synonym (see page 14)*".

Main window



In the Main window you have an overview of the three principal elements of a Selection: the substances, parameters and environmental systems. The name of the current Selection is given in the status bar at the bottom of the window, while the menu's allow you to open and save files, set options and give access to the online-help.

This window has the following menu's

File	New selection			: Starts a new Selection.
	Open Selection...			: Open an existing Selection (see page 33) .
	Save selection			: Save the current Selection.
	Save selection as...			: Save the current Selection to a new file (see page 36) .
	Open profile...			: Open an existing Profile (see page 33) .
	Save profile			: Save the Profile, leaving out the substances, parameters or systems (if one or more are undetermined or as indicated by the menu Options / Preferences / Undetermined in Profile). The name of the file is the same as the name of the Selection file, with the extension replaced by .dpr.
	Save profile as...			: Save the current Profile (see page 36) to a new file.
	Exit			: End the application.
Options	Preferences	Undetermined in profile	Substances	: Leave the substances out of a profile if a Selection is saved as a Profile.
			Parameters	: Leave the parameters out of a profile if a Selection is saved as a Profile.
			Systems	: Leave the systems out of a profile if a Selection is saved as a Profile.
	Language	English		: Choose English as the language for the User Interface.
		Nederlands		: Choose Dutch as the language for the User

			Interface.
	Font Size	Extra small	: Use an extra small font for the User Interface.
		Small	: Use a small font for the User Interface.
		Normal	: Use a normal font for the User Interface.
		Large	: Use a large font for the User Interface.
		Extra large	: Use an extra large font for the User Interface.
Help	Contents		: Show this helpfile.
	Search		: Show the Search tab for this helpfile.
	About ADEPTS...		: Show the Aboutbox (see page 25) .

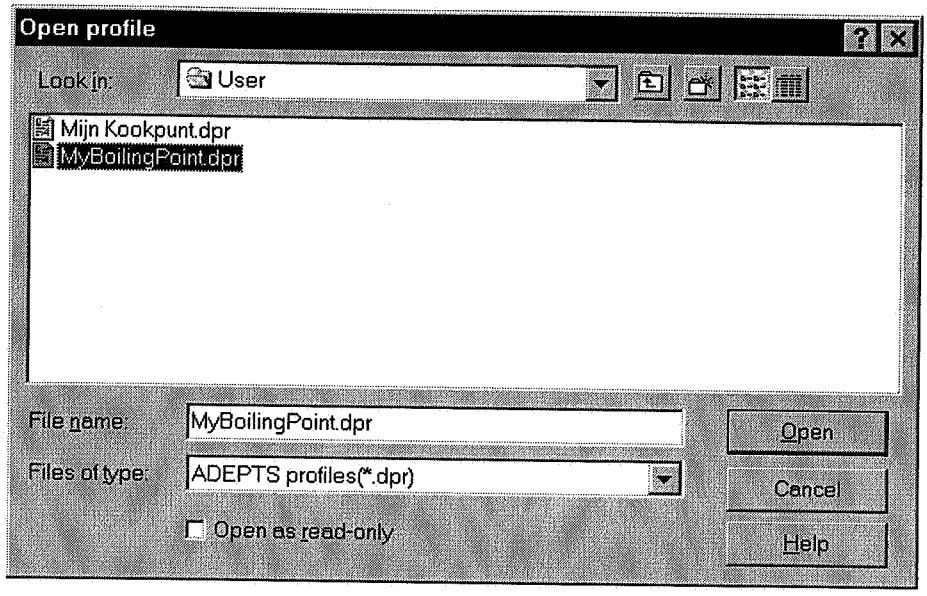
Menu's may be selected by clicking on them with the mousepointer, or pressing the Alt-key simultaneously with the underlined key. Besides the menu's you will find four large buttons:

- ***Substances*** to add substances to the Selection or to remove substances from the selection in the *Substances window (see page 40)*.
- ***Parameters*** to add parameters to the Selection or to remove parameters from the selection in the *Parameters window (see page 34)*.
- ***Show*** to show the *Selection window (see page 37)*.
- ***Exit*** to end the application.

Open ASCII import dialog

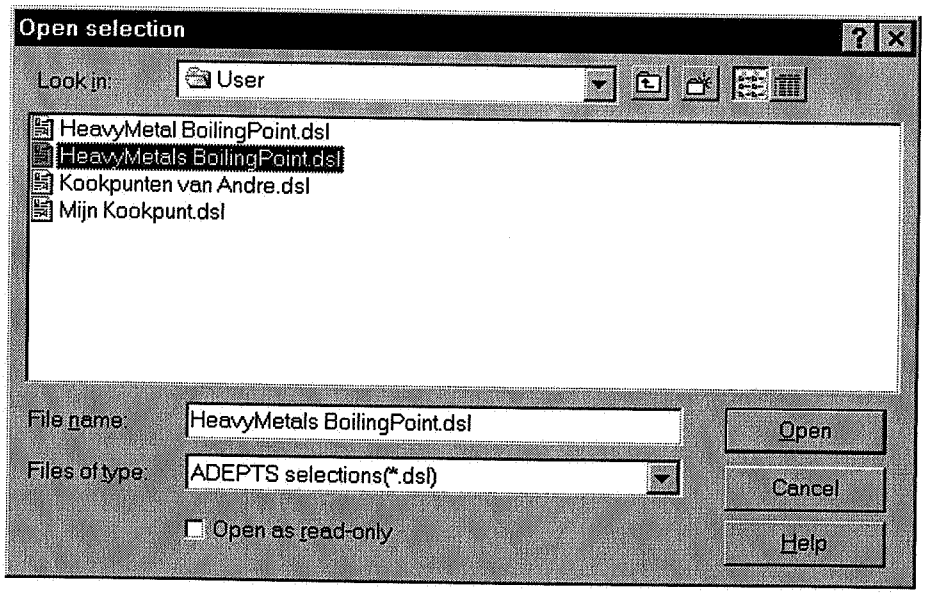
This standard windows 'file open' dialog asks for the name of an ASCII file (text file) containing CAS numbers. After pressing OK the application will open the file and select all names in the left list of the *Substances window (see page 40)* that have a CAS number equal to a number in the file. For more information see: how to *import CAS numbers (see page 17)*.

Open Profile dialog



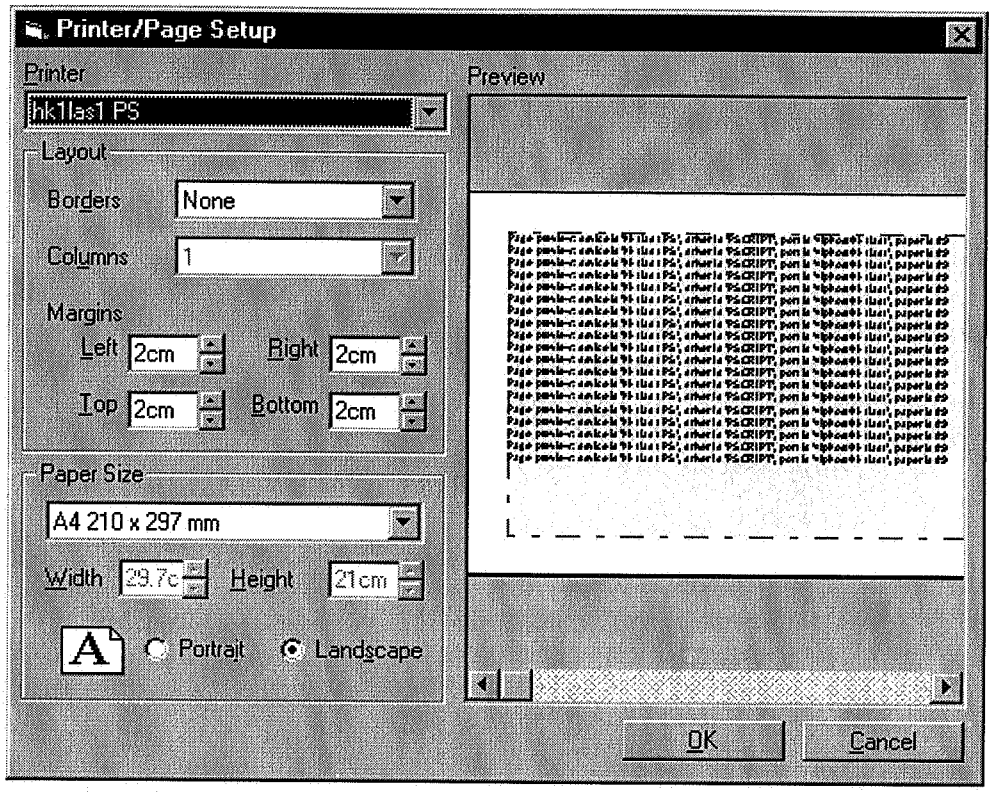
This dialog prompts you for the name of a file containing a Profile. Profile files have the extension `.dpr` by default, files with other extensions can be found by setting *Files of type* to 'All files'. The initial folder for the dialog is the 'user folder' as specified in the *ADEPTS ini file (see page 42)*.

Open Selection dialog



This dialog prompts you for the name of a file containing a Selection. Selection files have the extension .dsl by default, files with other extensions can be found by setting *Files of type* to 'All files'. The initial folder for the dialog is the 'user folder' as specified in the *ADEPTS ini file (see page 42)*.

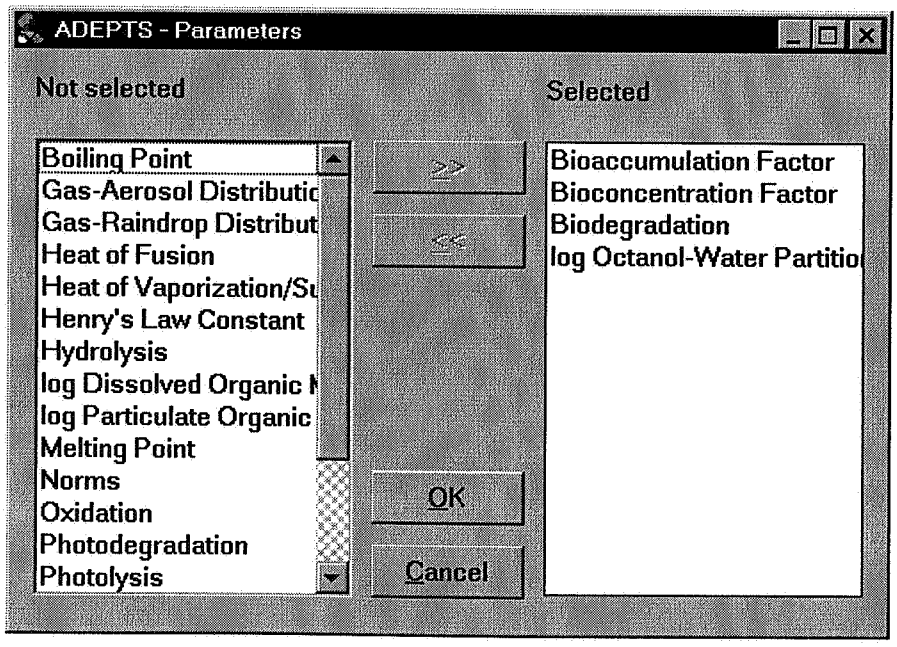
Page Setup window



In this window you can select various aspects of the print setup, like the printer to use, the orientation of the paper and the margins.

Parameter window

In this window two lists are displayed. The list on the left side of the window contains the parameters that are **not** part of the Selection (or Profile), the list on the right contains the parameters that **are** part of the Selection.



In each of these two lists you can select one or more names.

By pressing the button with the arrows pointing to the right (>>, located between the two lists), all names that are selected in the left list, will be removed from the left list and added to the right list (and thus become part of the Selection).

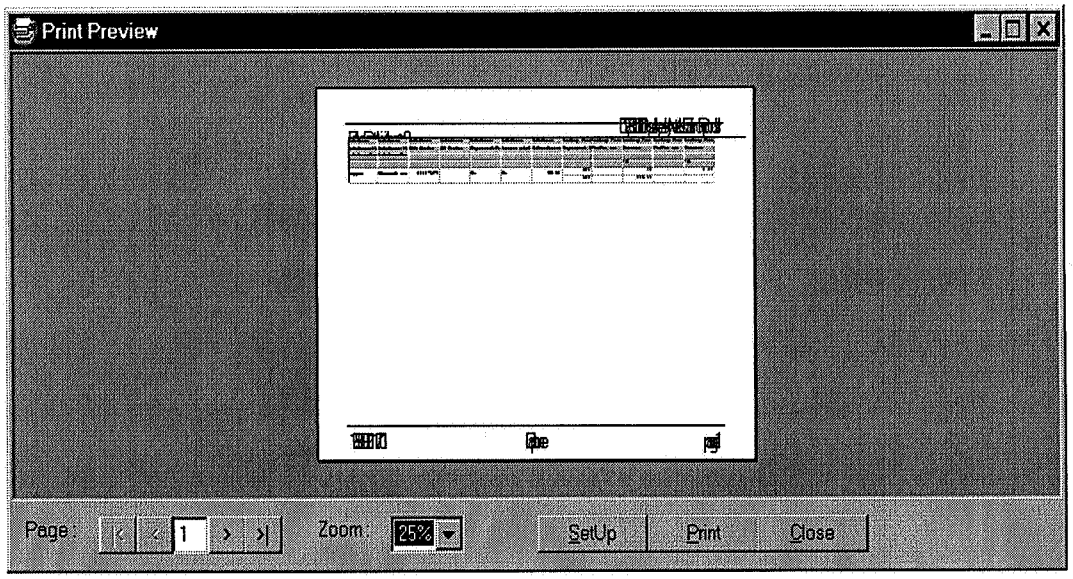
By pressing the button with the arrows to the left (<<), all names that are selected in the right list, will be removed from the right list and added to the left list. Changes to the selection become effective as soon as you press the "OK" button. This button also closes the window. If you press the "Cancel" button, you go back to the Main window and any changes will be discarded.

By double clicking on a parameter in one of the two lists, the help-item from this helpfile for that parameter will be shown.

The *database administrator* may add parameters to ADEPTS, these will not be present in this helpfile. How to add these parameters is explained in a separate manual.

See also: how to *Select parameters (see page 17)*.

Print Preview window



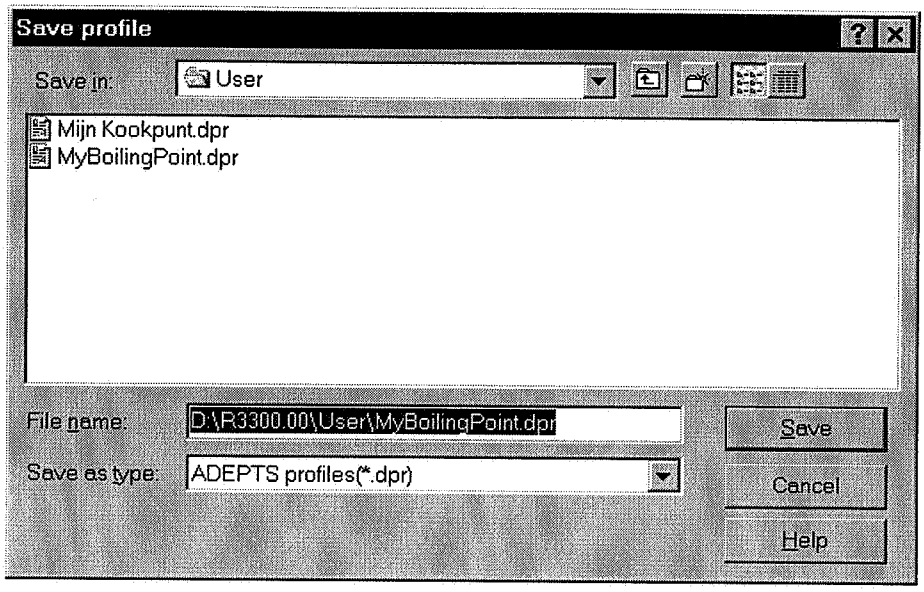
This window shows a preview of the printed output. The rows and columns are printed as they are laid out on the screen at that moment.

You can use the four *page buttons* or enter a page number in the textbox to select a particular page for previewing.

By selecting a zoomlevel from the *zoom combobox*, you can determine the level of detail for the preview. Lower levels, like 25% or 50%, give a reasonable overview of the page lay-out, details like the placement of the headers and footers are better viewed at larger magnifications.

The *Setup button* gives access to the *Page Setup window (see page 34)*, the *Print button* prints the Selection on the selected printer and the *Close button* closes this window.

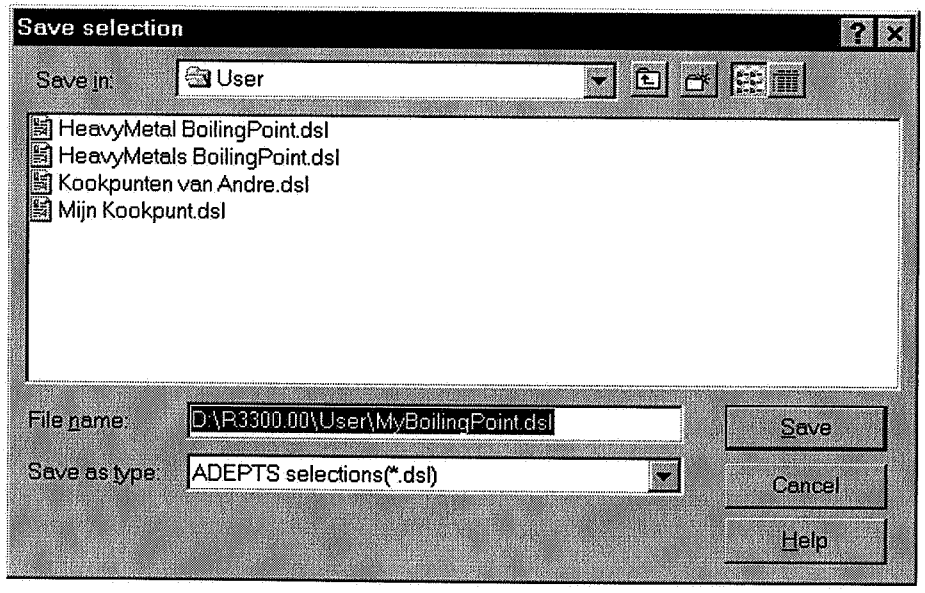
Save Profile dialog



This dialog prompts you for the new name of a file containing a Profile. Profile files have the extension `.dpr` by default, files with other extensions can be saved by setting *Files of type* to 'All files'. The initial folder for the dialog is the 'user folder' as specified in the *ADEPTS ini file (see page 42)*. When saving a Selection, which is complete, as a Profile, which by definition is incomplete, at least on of the three main elements of a Selection is left out. Which element is left out is determined by the menu *Options / Preferences / Undetermined in Profile* in the *Main window (see page 30)*.

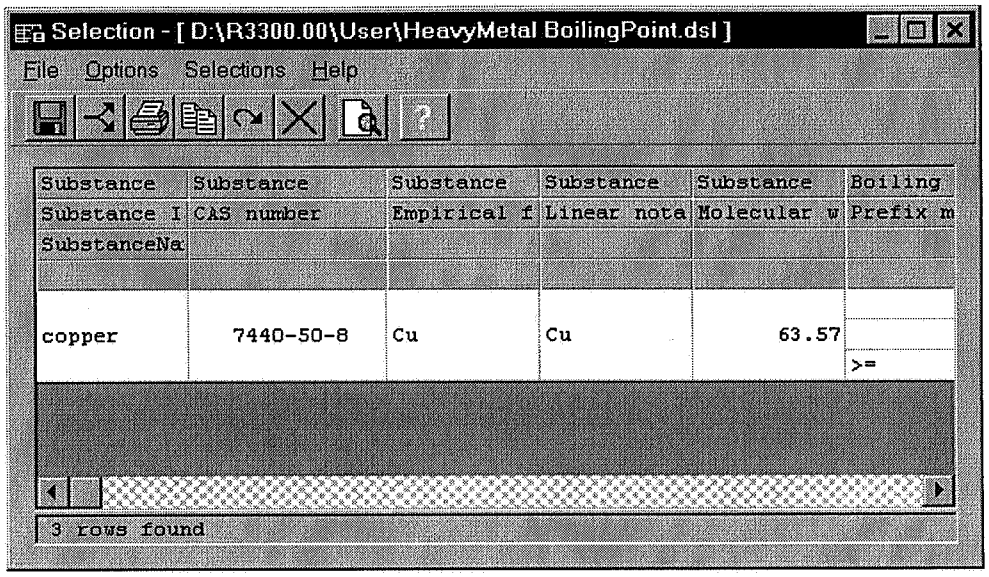
See also: *Selections and Profiles (see page 7)*.

Save Selection dialog



This dialog prompts you for a new name of the file containing the current Selection. Selection files have the extension `.dsl` by default, files with other extensions can be saved by setting *Files of type* to 'All files'. The initial folder for the dialog is the 'user folder' as specified in the *ADEPTS ini file (see page 42)*. From Windows™ 95 on, you can use long filenames, which allow meaningful naming of the file.

Selection window



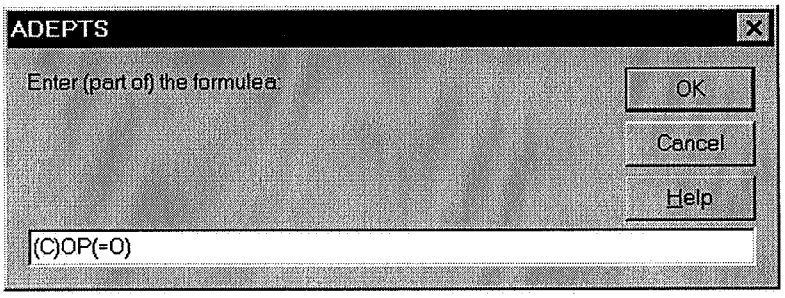
This window displays a grid with the Selection. It has the following menu's and a toolbar with buttons that serve as a shortcut for popular menu-items:

File	Save selection		:	Save the current Selection.
	Save selection as...		:	Save the current Selection to a new file (see page 36) .
	Clone selection		:	Make a copy of the current selection.
	Print		:	Open the Print Preview Window. (see page 35)
	Export		:	Export the current Selection (see page 23) to a csv file.
	Close		:	Close the window. The menu and the button with the red cross will close the window, if this Selection is not the same as in the Main window, you will be prompted if you want to loose the changes. The button with the arrow will make the Selection in the Main window the same as the one you are closing, so changes are preserved.
Options	Toolbar visible		:	Make the toolbar visible or invisible.
	Language	English	:	Choose English as the language for the User Interface.
		Nederlands	:	Choose Dutch as the language for the User Interface.
	Constraints		:	Display the Constraints window (see page 26) .
	Column options	Sort Descending	:	Sort the active column in descending order.
		Sort Ascending	:	Sort the active column in ascending order.
		Hide	:	Hide the active column.
Selections	Cascade		:	Order all Selection windows by cascading them.
	Tile		:	Order all Selection windows by Tiling them. Up to 5 windows are tiled horizontally, from 6 to 8 windows are tiled in two columns, and 9 windows are tiled in 3 columns. Tiling fails if more then 9 windows are active.
	Line up		:	Line up two or more Selections. See: Lining up Selections (see page 22) .
Help	Contents		:	Show this helpfile.

Search	:	Show the Search tab for this helpfile.
About ADEPTS...	:	Show the Aboutbox (see page 25) .

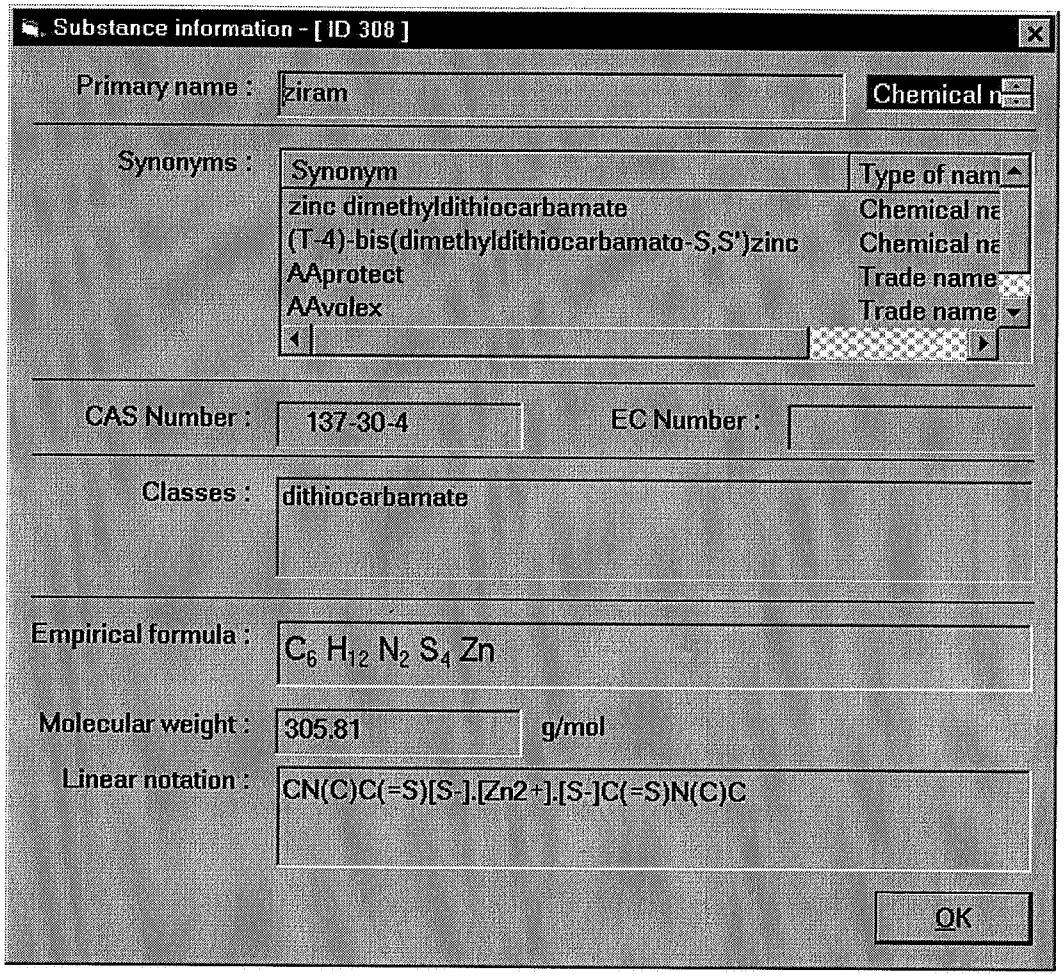
The columns may be sorted and hidden: by pressing the right mousebutton while pointing to a column a menu will pop-up. Columns may be dragged to a new position by pressing the left mousebutton while pointing to one of the four header rows: the mousepointer will change into a double horizontal arrow and the column will be moved to the location where you let the left mousebutton button go.

SMILES substring dialog



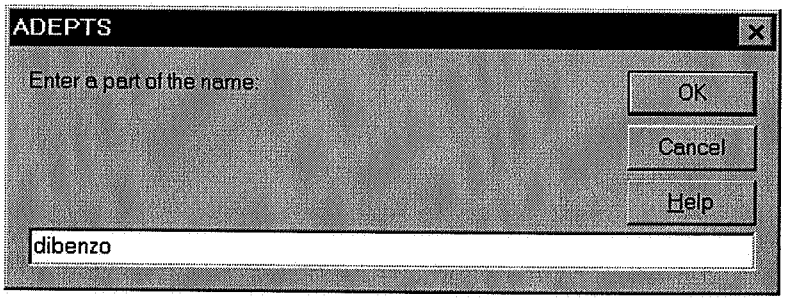
This dialog asks for a part of the linear formula (or SMILES notation) of a substance. The procedure where this dialog is used is described in "*Select substances by SMILES (see page 16)*". This comparison **is** case-sensitive (Zinc in a substance will not be found by entering "ZN" or "zn", but will be found by entering "Zn").

Substance information window



This window displays all information about the selected substance.

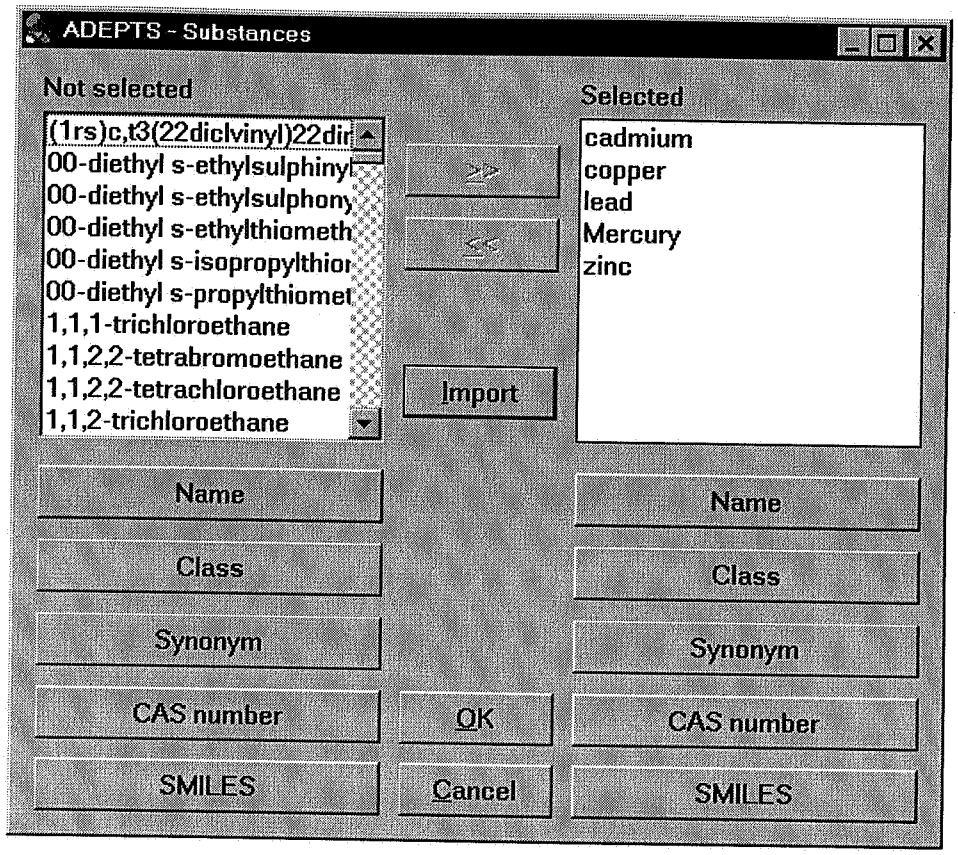
Substance name dialog



This dialog asks for a part of a substance name. The procedure where this dialog is used is described in "*Select substances by name (see page 12)*".

Substances window

In this window two lists are displayed. The list on the left side of the window contains the primary names of all substances that are **not** part of the Selection (or Profile), the list on the right contains the primary names of all substances that **are** part of the Selection.



In each of these two lists you can select one or more names. This selection may be either *directly from the lists (see page 11)*, *by name (see page 12)*, *by class (see page 13)*, *by synonym (see page 14)*, *by CAS number (see page 15)* or *by SMILES notation (see page 16)*. All these methods mark a number of strings in the left or the right list. *Import from an ASCII file (see page 17)* with CAS numbers is another way to select names in the list, but in contrast to the other methods, this only works on the left list.

By pressing the button with the arrows pointing to the right (>>, located between the two lists), all names that are selected in the left list, will be removed from the left list and added to the right list (and thus become part of the Selection).

By pressing the button with the arrows to the left (<<), all names that are selected in the right list, will be removed from the right list and added to the left list. Changes to the selection become effective as soon as you press the "OK" button. This button also closes the window. If you press the "Cancel" button, you go back to the Main window and any changes will be discarded.

By double clicking a substance name in one of the lists, the *Substance information window (see page 40)* for this substance will be shown.

See also: how to *select substances (see page 11)*.

Synonym information window

This window lets you edit the information about a synonym. It is not accessible in this release of ADEPTS.

Support files

The ADEPTS ini files

The ADEPTS application uses a so-called client/server model, and consists of several modules, each of which may use it's own initialisation file. The most important file the end-user is the initialisation file for the user-interface: `ADEPTS.ini`. The module which reads from the database (ADEPTSDC) uses it own initialisation file: `ADEPTSDC.ini`.

ADEPTS.ini

This file is located in the same folder as the user-interface executable. The location of this folder is determined during the installation. The default location is C:\Program Files\ADEPTS. Its stores general information like the location of the helpfiles and the *languagefile (see page 44)*, as well as preferences of the user, like window positions. It contains the following entry's:

Section	Key	Type of key	Example	Description
General	UserFolder	String	C:\Program Files\ADEPTS\ User	The name of user folder, the folder where Selections and Profiles are stored by default.
General	LanguageFile	String	C:\Program Files\ADEPTS\ ADEPTS.lng	The name of the language file, including the path.
General	Language	Integer	1	The number of the active language.
General	Font	String	normal	The relative fontsize. May be one of 'extra small', 'small', 'normal', 'large' or 'extra large'.
Main-Window	Left	Single	10.0	The position of the left side of the MainWindow, as percentage of the screenwidth.
Main-Window	Top	Single	10.0	The position of the top side of the MainWindow, as percentage of the screenheight.
Main-Window	Width	Single	60.0	The width of the MainWindow, as percentage of the screenwidth.
Main-Window	Height	Single	80.0	The height of the MainWindow, as percentage of the screenheight.
Main-Window	State	Integer	0	The windowstate of the MainWindow. May be 0 (normal), 1 (minimised) or 2 (maximised)
Window	Left	Single	10.0	The left position for window Window, See MainWindow for other keys that are possible and their description.

ADEPTSDC.ini

This file is located in the same folder as the data-centric executable. Depending on the set-up, this executable may be integrated with the user-interface, but may also be running on a separate computer: the 'server'. It is used to store information about the physical location of the database. It contains the following entry's:

Section	Key	Type of key	Example	Description
Database	Path	String	`C:\Program Files\ADEPTS\ ADEPTSDB.mdb`	The name of the database file, including the path.

The ADEPTS language file

This file contains translations for the user interface. It is normally present in the same folder as the executable for the user-interface, but another location may be specified in the initialisation file. It may contain the translations in up to four active languages, which then may be selected at run-time from the language menu in the *main window (see page 30)* or the *selection window (see page 37)*. This file can be edited with the WL | Delft Hydraulics application EditLang, part of the Delft Tools.

See also: *The ADEPTS INI files (see page 42).*

Parameters

Bioaccumulation Factor

The ratio of the concentration of a substance taken up from water and food in a certain organism and the dissolved concentration of this substance in water after a given duration. This ratio is used in bioaccumulation models and ecotoxicological effect models.

Unit: litres per kilogram [l/kg]

See also: *Bioconcentration Factor (see page 46)*

Bioconcentration Factor

The ratio of the concentration of a substance **directly** taken up from water in a certain organism and the dissolved concentration of this substance in water after a given duration. This ratio is used in bioaccumulation models and ecotoxicological effect models.

Unit: litres per kilogram [l/kg]

See also: *Bioaccumulation Factor (see page 46)*

Bioegradation

A set of parameters to define and quantify the process of biodegradation in water, the enzymatic degradation of a substance by micro-organisms. Main characteristic is the apparent half-time of a substance, the time required to decompose 50% of the mass of a substance, at a given temperature. Directly related to this parameter is the first-order biodegradation rate ($k = \ln(2)/t_{50\%}$), which is used in fate models.

Unit: per day [/d]

Boiling Point

Temperature at which boiling of a substance proceeds at a given pressure.

Unit: Centigrade. [C]

Gas-Aerosol Distribution Coefficient

The ratio of concentrations of a substance in (atmospheric) gas and aerosols in equilibrium at a given temperature. This ratio is used in fate models.

Unit: -

Gas-Raindrop Distribution Coefficient

The ratio of concentrations of a substance in (atmospheric) gas and rainwater in equilibrium at a given temperature. This ratio is used in fate models.

Unit: -

Heat of Fusion

Energy required for the melting of a substance at a given pressure.

Unit: kiloJoules per mol [kJ/mol]

Heat of Vaporization/Sublimation

Energy required for the vaporisation/sublimation of a substance at a given pressure.

Unit: kiloJoules per mol [kJ/mol]

Henry's Law Constant

The ratio of the vapour pressure and the concentration in water of a substance at equilibrium at a given temperature. This constant is used in fate models, either directly at an average ambient temperature or corrected for temperature, which requires a temperature coefficient.

Unit: Pascal.cubic meter per mol [Pa.m3/mol]

Hydrolysis

A set of parameters to define and quantify the process of hydrolysis in water, the decomposition of a substance by means of reaction with water. Main characteristic is the apparent half-time of a substance, the time required to decompose 50% of the mass of a substance, at a given temperature. This parameter can be derived from the second-order acid hydrolysis rate, the first-order neutral hydrolysis rate, the second-order base hydrolysis rate and the pH, which are used in fate models.

Unit: k-acid litres per mol per day [l/mol/d]
k-base litres per mol per day [l/mol/d]
k-neut per day [/d]

log Dissolved Organic Matter Partition Coefficient

The log k_{DOC}, the ratio of the concentration in dissolved organic matter (carbon) and the dissolved concentration of a substance in water at equilibrium. This coefficient or its ratio with Kpoc (= Xdoc) is used in fate models.

Unit: -

log Octanol-Water Partition Coefficient

The logarithm (base 10) of the octanol-water partition coefficient, the ratio of the equilibrium concentrations of an organic substance in an octanol-water mixture.

Unit: -

log Particulate Organic Matter Partition Coefficient

The log k_{POC}, the ratio of the particulate concentration in organic matter (carbon) and the dissolved concentration of a substance in a suspended organic matter-water mixture at equilibrium. This coefficient is used in fate models and may be derived from K_{ow} using simple linear relations.

Unit: -

Melting Point

Temperature at which melting of a substance proceeds.

Unit: Centigrade. [C]

Norms

Norms and riskphrases for a substance.

Unit: depends on norm.

Oxidation

A set of parameters to define and quantify the process of oxidation, the decomposition of a substance by means of reaction with oxygen and/or oxygen containing compounds. Main characteristic is the first-order oxidation rate of a substance at a given temperature, which is used in fate models.

Unit: litres per mol per day [l/mol/d]

Photodegradation

A set of parameters to define and quantify the process of photolysis in the atmosphere, the decomposition in air of a substance by means of reaction with photons. Main characteristic is the apparent half-time of a substance, the time required to decompose 50% of the mass of a substance. The second-order reaction rate can be derived from this parameter, using the light intensity, the quantum yield and the molar light absorption, which are used in fate models.

Unit (quantum yield): [mol/E]

See also: *Photolysis (see page 49).*

Photolysis

A set of parameters to define and quantify the process of (direct) photolysis in water, the decomposition of a substance by means of reaction with photons. Main characteristic is the apparent half-time of a substance, the time required to decompose 50% of the mass of a substance. The second-order reaction rate can be derived from this parameter, using the light intensity, the quantum yield and the molar light absorption, which are used in fate models.

Unit (quantum yield): [mol/E]

See also: *Photodegradation (see page 49).*

pKa

Negative logarithm (base 10) of the acid ionisation (equilibrium) constant of a substance in water. This constant is used in speciation models and in (some) fate models.

Unit: -

Solubility

The mass of a substance contained in water which is in equilibrium with an excess of this substance at a given temperature. This constant is used in QSAR's, for instance to predict Henry's constant.

Unit: grams per cubic meter [g/m3]

Suspended Matter Partition Coefficient

The k_d, the ratio of the particulate concentration and the dissolved concentration of a substance in a suspended matter-water mixture at equilibrium. This coefficient is used in fate models of inorganic substances (e.g. heavy metals).

Unit: litres per kilogram [l/kg]

Toxicity

The toxicity of a substance for an organism or organism group.

Unit: depends on environmental system.

Vapour Pressure

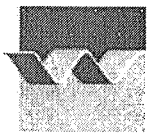
The pressure exerted when a solid or liquid is in equilibrium with its own vapour at a given temperature.

Unit: Pascal [Pa]

Problem solving

Support

For all questions concerning the use of this version of ADEPTS you may contact the ADEPTS helpdesk:



WL | Delft Hydraulics,
ADEPTS helpdesk,
c/o André Hendriks

P.O. Box 177
2600 MH Delft
The Netherlands

Telephone: +31 15 285 8492
Telefax: +31 15 285 8582
E-mail: Adepts.support@wldelft.nl

ADEPTS run-time error overview

Several error may occur while running ADEPTS. The most common have their own entry in this helpfile where the reasons for the error and possible solutions are explained. If you cannot solve the error by reading these parts of this helpfile, please contact *WL | Delft Hydraulics (see page 52)*.

Possible errors are:

- *No data for combination (see page 52).*
- *Field cannot be hidden.*
- *Constraint error: invalid constraint (see page 53).*
- *Constraint error: (alpha)numeric expected (see page 53).*
- *No substances satisfy constraints.*
- *Initialization errors (see page 53).*

No data for combination

Sometimes there is no data for a combination *parameter* and *environmental system* because the parameter is not defined for all available systems. For instance, if you select

the Environmental System **Air** and the Parameter **Toxicity**, you will get this message, because there is no information for toxicity in the air.

Constraint error: invalid constraint

The database engine detected an invalid constraint. Check that the constraint is a valid SQL-like WHERE clause for the type of field specified. See "*Set constraints for a column (see page 21)*" for examples of valid constraints.

Constraint error: (alpha)-numeric expected

The database engine detected an invalid constraint. Probably you specified an alphanumeric constraint for a numeric field or vice-versa.

Initialisation errors

While initialising a number of errors may occur. In general these have to do with errors during the installation, resulting in incorrect initialisation files and/or communication problems between the *client* (user-interface) and *server* (database). The most frequent errors and their causes are described in this helpfile, if you cannot find a solution with this information, please contact *WL | Delft Hydraulics (see page 52)*.

See also : *The ADEPTS INI files (see page 42)*

Error: INI file not found (see page 53)

Error: database file not found (see page 53)

Error: workgroup file not found (see page 54)

Error: database error (see page 54)

Error: invalid account (see page 54)

Error: INI file not found

This error occurs if the part of the application that reads the database cannot find the initialisation file `ADEPTSDC.ini`. Make sure this file is present in the correct folder.

See also: *The ADEPTS INI files (see page 42)*

Initialisation errors (see page 53)

Error: database file not found

This error occurs if the part of the application that reads the database cannot find the name of the database in the initialisation file `ADEPTSDC.ini` or if the name of the database in this file is not correct. Make sure the key `Path` in the section `Database` is correct. Your *database administrator* should be able to tell you the correct path to the database.

See also: *Initialisation errors (see page 53)*

Error: workgroup file not found

This error occurs if the *workgroup* file `system.mdw` cannot be found. This file contains information about users of the database and their permissions, and normally should be located in the same folder as the database file. This file is described in a separate manual, which your *database administrator* should have.

See also: *Initialisation errors (see page 53)*

Error: database error

This error occurs if there is some problem reading the *workgroup* file `system.mdw`. It cannot be found or contains wrong information about users of the database and their permissions. This file should be located in the same folder as the database file. This file is described in a separate manual, which your *database administrator* should have.

See also: *Initialisation errors (see page 53)*

Error: invalid account

This error occurs if the *workgroup* file `system.mdw` contains wrong information about users of the database and their permissions. This file is described in a separate manual, which your *database administrator* should have.

See also: *Initialisation errors (see page 53)*

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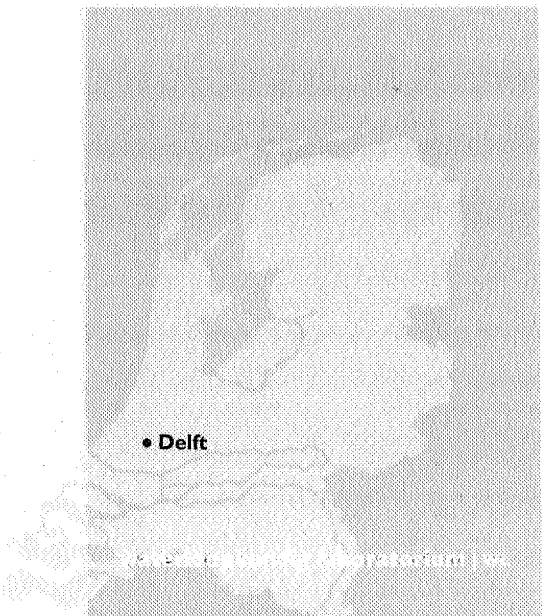

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