OMT SOLUTIONS
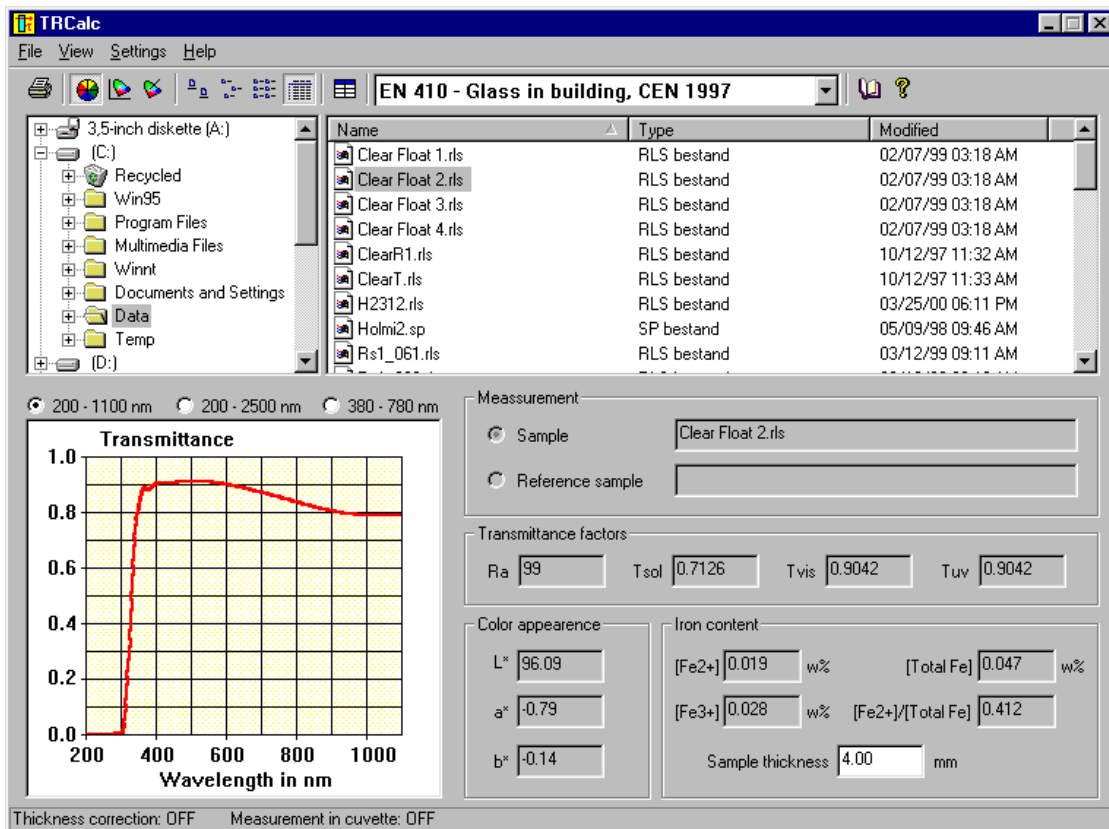
TRCalc

a user friendly point-and-click software application for the glass and glazing industry

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Introduction

TRCalc is a user-friendly point-and-click software application designed to meet the needs of a modern quality control laboratory in the glass and glazing industry.

It allows users of UV/VIS spectrophotometers to use optical measurement data (reflectance and transmittance spectra) to calculate material properties and product specifications of glass, glazing products and transparent plastics.

Spectral transmittance is measured using a spectrophotometer and stored in a spectral data file. In the data file browser on the main dialog of TRCalc this data file is selected with the mouse cursor and the calculations starts automatically.

Properties calculated by TRCalc

- UV transmittance
- visible light transmittance
- solar energy transmittance
- color rendering index of transmitted light
- CIELAB L* a* b* color coordinates
- xy chromaticity

- dominant wavelength
- excitation purity
- brightness
- Yellowness index (transparent plastics)
- Fe3+ and Fe2+ ion content (glass samples)
- Redox state (glass samples)

Calculations are performed according to procedures prescribed by international standards (ISO, CEN, DIN, NEN, ASTM, CIE, etc.). The main window contains a drop-down list with predefined standards. New standards can be implemented and existing standards can be changed or deleted using the Standards dialog.

Special features of TRCalc

- The user can implement future standards for calculation.
- Reference spectra can be specified by the user (customizing standards).
- Calculation for a different sample thickness (build-in thickness correction).
- Calculation results can be presented for total transmittance or internal transmittance.
- Systematic errors in the input data can be corrected using reference sample data.
- Spectral data is automatically adapted to the format used by TRCalc.
- -A standard report can be printed with the name of the analyst, date, sample info and calculation results.
- Settings (for calculations, data format, standards etc) can be protected with a password.

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TRCalc main dialog

TRCalc main dialog

TRCalc opens with its main dialog that contains the menu and tool bar for setting the main features of TRCalc. The top half of the main dialog consists of a spectrum data file browser. Selecting a spectrum data file initiates a series of calculations resulting in the values of the transmittance factors and other coefficients listed in the bottom half of the main dialog.
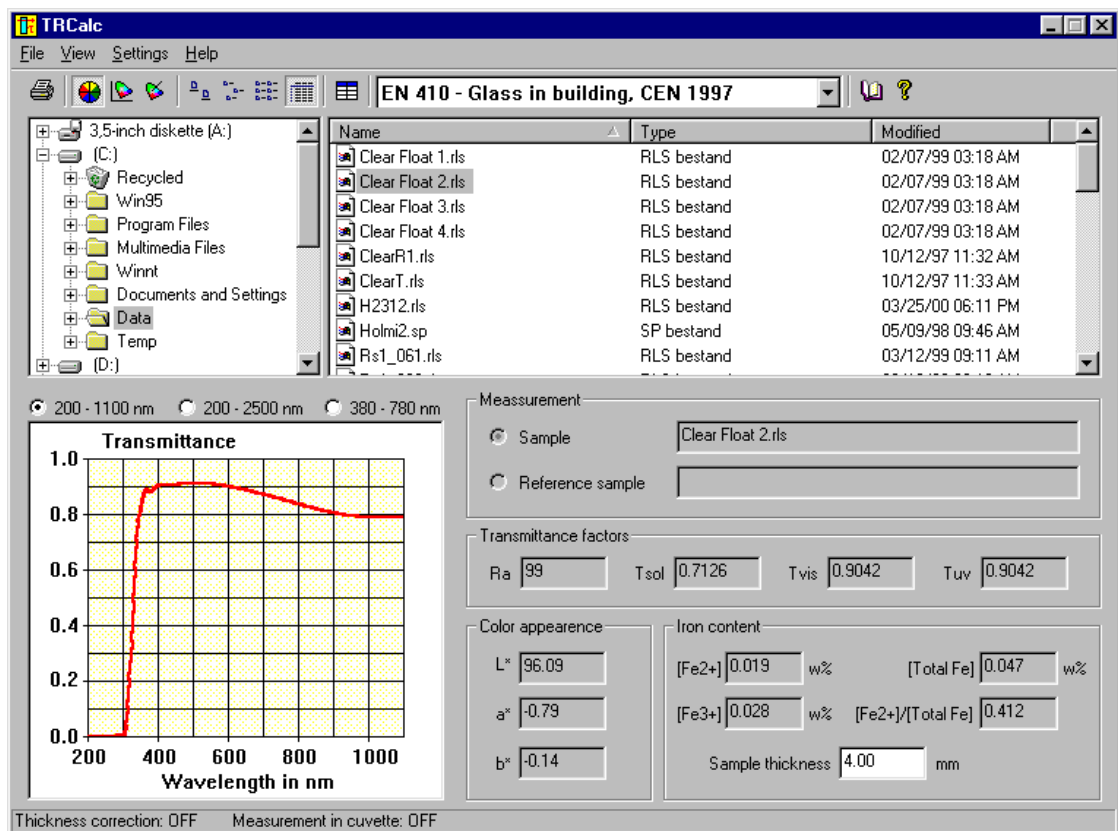
The calculation results as presented on the main dialog are obtained according to the Standard that is selected from the "Standards" drop-down list, which is located in the toolbar of the main dialog.

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The file browser

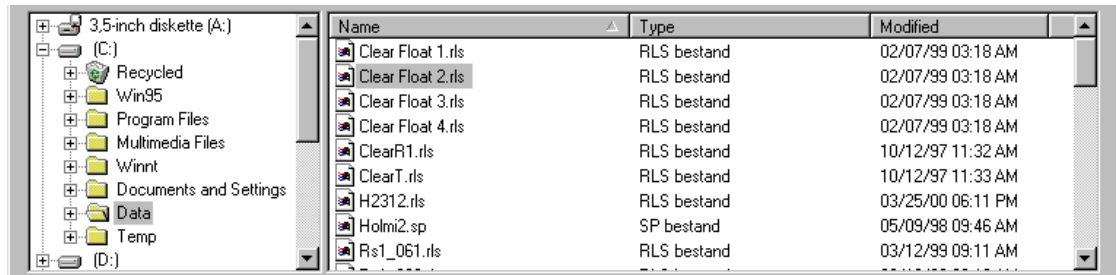The main dialog of TRCalc contains a Windows Explorer look-a-like file browser. This file browser consists of two panes, a folder tree pane on the left and a file list pane on the right.


The files in the file list pane can be sorted on name, type and date. For example, to sort the files on name, click on the button labeled "Name" on the top of the file list pane. Clicking again on this button will switch the sorting form ascending to descending or back. The little arrow on the button shows whether the sorting is ascending (arrow points upward) or descending (arrow points downward).

If changes are made, outside TRCalc, (files are added, deleted or modified) to the active folder, TRCalc will detect these changes and reloads automatically the files in the file list pane.

The graph

The main dialog of TRCalc contains a graph that shows you the spectrum of the input data from file. The graph can be set to three different ranges, 200 - 1100 nm, 200 - 2500 nm and 380 - 780 nm. To change the range of the graph, just select the proper radio button above the graph.
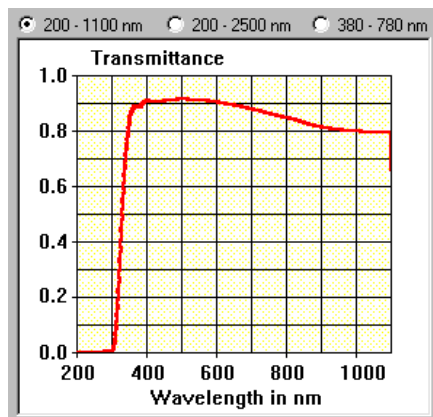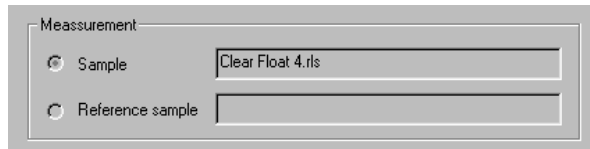
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Selecting a spectrum data file

In the case that data represents true (calibrated) transmittance data (see page 7: **Correcting (Calibrating) measurement data**) only one file has to be selected in the file browser. Its name will appear in the measurement field, for example:
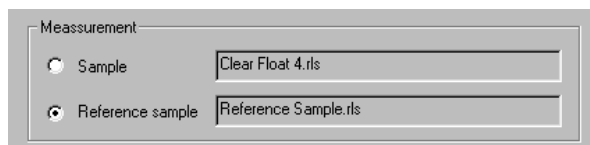
A graph of the corresponding transmittance (red curve) appears on the main window:
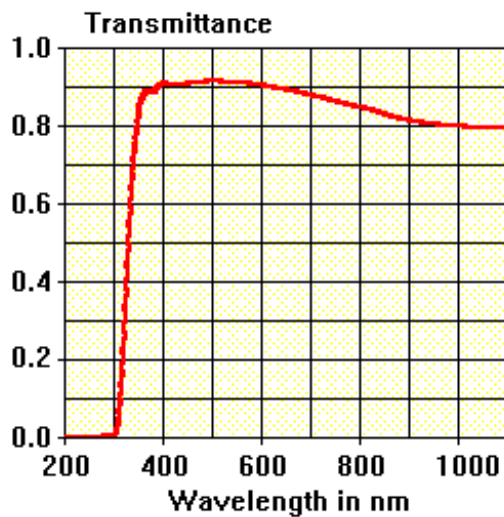
In the case that data represents raw measurement data (uncalibrated), the true transmittance of the sample is corrected using the measurements performed on a standard reference sample (see page 7: **correcting (calibrating) measurement data** for the correct setting). To select the data file of this reference sample first select the appropriate radio button in the measurement field. After selecting the reference sample data file its name will also appear in the measurement field:

An additional spectrum (blue curve) representing the reference sample data will appear:

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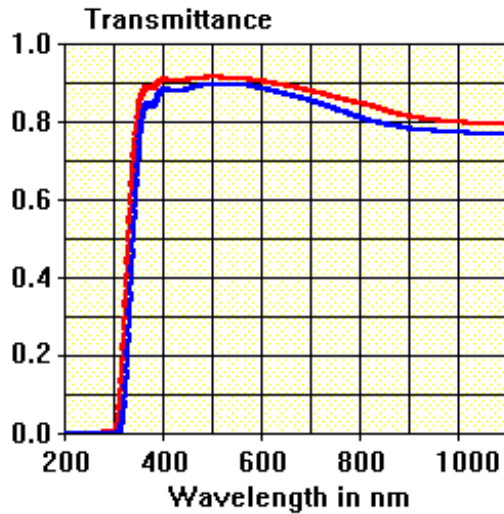
Correcting (calibrating) measurement data

In the case that the data files contain raw (uncalibrated) data, TRCalc can perform the calibration by multiplying the measured data obtained on a sample with the ratio of respectively the certified (calibrated) and the measured transmittance of a reference sample.

Selecting the option "Data correction" in the submenu "Data Handling" of the menu "Settings" enables the calibration.

Using the Data correction file dialog the user can select the name of the file that contains the certified (true) transmittance values of the reference sample. The format of this file should be according to the default data file format used by TRCalc

The table of certified values can be at an <u>arbitrary number of arbitrary wavelengths</u> within the spectral range of 200 nm - 2500 nm.

Selecting the submenu "Data Handling" in the menu "Settings" and then selecting the option "Data correction file…" initiate the "Data correction file" dialog.
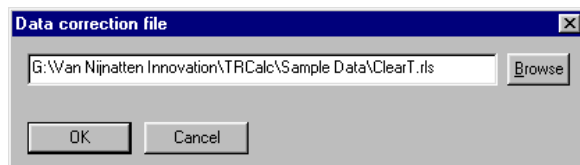
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Selecting a color system

The color appearance can be represented on the main dialog by one of three color systems:

CIELAB L*a*b* color coordinates

Selecting the 🌈 button in the toolbar on the main dialog or the option "CIE L*, a*, b*" in the submenu "Color System" of the menu "View" on the main dialog will show the CIELAB L*a*b* color coordinates:

```
┌─ Color appearence ──────┐
│                         │
│   L*   [ 96.27  ]       │
│                         │
│   a*   [ -0.72  ]       │
│                         │
│   b*   [ 0.01   ]       │
│                         │
└─────────────────────────┘
```

x y chromaticity coordinates

Selecting the 📊 button in the toolbar on the main dialog or the option "CIE x, y" in the submenu "Color System" of the menu "View" on the main dialog will show the x y chromaticity coordinates:
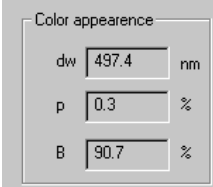
```
┌─ Color appearence ──────┐
│                         │
│   x   [ 0.3118  ]       │
│                         │
│   y   [ 0.3296  ]       │
│                         │
└─────────────────────────┘
```

Combination of dominant wavelength, excitation purity and brightness

(used for quality control of packaging glass)

Selecting the 🌈 button in the toolbar on the main dialog or the option "dw, p, B" in the submenu "Color System" of the menu "View" on the main dialog will show the dominant wavelength (dw), excitation purity (p) and brightness (B):

```
┌─ Color appearence ──────┐
│                         │
│   dw  [ 497.4  ]  nm     │
│                         │
│   p   [ 0.3    ]  %      │
│                         │
│   B   [ 90.7   ]  %      │
│                         │
└─────────────────────────┘
```
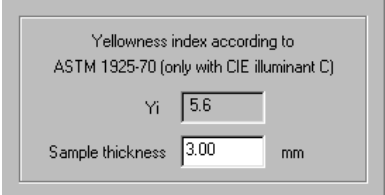
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Yellowness index and iron content

The user can set TRCalc to calculate either the Iron Content (in the case of coated glass samples only) or the Yellowness Index (mostly for plastics). Selecting the option "Iron content" or "Yellowness index" in the menu "View" on the main dialog does this setting.

Yellowness index

Yellowness index according to
ASTM 1925-70 (only with CIE illuminant C)

Yi 5.6

Sample thickness 3.00 mm

The Yellowness index Yi indicates the degree of departure of an object color from colorless, or from a preferred white, toward yellow. Yi is determined according to ASTM 1925-70 by
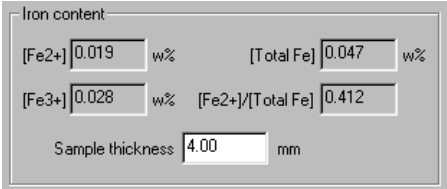
$$Yi = 100 \; \frac{1.277 \, X \; - \; 1.059 \, Z}{Y}$$

in which X, Y en Z are the chromaticity coordinates (calculated according to the selected standard!).

The user can specify Yi for a given reference thickness which is different from the thickness of the sample by using the thickness correction (see page 13). This requires the true thickness to be entered in the "sample thickness" field on the main dialog.

Note: according to ASTM 1925-70 illuminant C should be selected as reference light source for calculating color appearance.

Iron content

Iron content

[Fe2+] 0.019 w%   [Total Fe] 0.047 w%

[Fe3+] 0.028 w%   [Fe2+]/[Total Fe] 0.412

Sample thickness 4.00 mm

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Iron is present in glass as a multivalent ion that can be found in the Fe2+ and Fe3+ states. These two ions are the cause of absorption bands at approximate wavelengths of respectively 1050 nm and 385 nm. The ratio of the weight concentrations of these ions is used as a measure for the redox state of the glass melt.

TRCalc contains four different methods for calculating the Fe2+ and Fe3+ concentrations. The user should select the method that gives the best results for his specific glass composition. Sometimes this requires some experimenting at first.

Bamford & Hudson

This method proposed by C.R. Bamford and E. J. Hudson (*Proc. 7th Int. Congr. Glass, Brussels, Vol. 1. Paper 6 Pp. 1-11.*) is based on Beer's law.

The Fe2+ content is calculated according to

$$[Fe2+] = \frac{\log^{10}\left|T_{o,1050}/T_{1050}\right|}{E_{1050}\,t} \qquad \text{in weight\% } Fe_2O_3,$$

where t is the thickness of the sample in mm (as specified by the user in the "sample thickness" field on the main dialog), E is the extinction coefficient of the glass at the particular wavelength and To is the transmittance the glass would have if no iron was present (zero iron transmittance). The subscript 1050 refers to a central wavelength of 1050 nm (position of the absorption band).

The fraction Fe2+ is calculated in a similar manner using the equation:

$$[Fe3+] = \frac{\log^{10}\left|T_{o,385}/T_{385}\right|}{E_{385}\,t} \qquad \text{in weight\% } Fe_2O_3,$$

where the subscript now refers to the wavelength of 385 nm.

The position of the central wavelengths can be adapted to a specific glass composition!

Cable & Hulme

This method proposed by M. Cable and R. Hulme (*Glass Technology Vol. 26 No. 4 August 1985*) is also based on Beer's law and measurements used in the visible region only (380 nm - 780 nm).

The Fe2+ content is calculated according to

$$[Fe2+] = a1 + a2 \; Abs(700\,nm) \qquad \text{in weight\% } Fe_2O_3,$$

$$\text{where } Abs(700\,nm) = -\frac{1}{t}\log^{10}\left|T_{700}\right|$$

and t is the thickness of the sample in mm (as specified by the user in the "sample thickness" field on the main dialog).

The Fe3+ content is calculated from [Fe2+] and the [Fe2+]/[Fe3+] ratio according to

$$\frac{\left[\text{Fe2}+\right]}{\left[\text{Fe3}+\right]} = \text{b1} \frac{\text{Abs}(700\,\text{nm}) - \text{b2}}{\text{Abs}(380\,\text{nm}) - \text{b3}} \qquad .$$

The coefficients a1, a2 and b1 - b3 are determined by the glass composition.

Daneo et. al.

This method has been proposed by A Daneo, P. Polato, M.L. Scandellari and M. Verita.

The Fe2+ content is calculated according to

$$\left[\text{Fe2}+\right] = \text{a1} + \text{a2}\,\left[\text{Abs}(1050\,\text{nm}) - \text{Abs}(\lambda_{\text{MIN}})\right] \qquad \text{in weight\% Fe}_2\text{O}_3 ,$$

In which the minimum absorbance at λ_{MIN} is substracted from the absorbance at 1050 nm.

The Fe3+ content is calculated from the fourth derivative of absorptance to

$$\left[\text{Fe3}+\right] = \text{b1} + \text{b2} \cdot \text{h} \qquad \text{in weight\% Fe}_2\text{O}_3 ,$$

where h is the maximum of the fourth derivative curve referred to a baseline which connects the two neighboring minima.

The coefficients a1, a2 and b1, b2 are determined by the glass composition.

Traverse et. al.

This method has been proposed by J. P. Traverse, T. Toganidis and C. Ades (*Glastech. Ber. 65 (1992) Nr. 8*). Their calculation of the Fe2+ content is based on Beer's law, according to

$$\left[\text{Fe2}+\right] = \text{e} \cdot \text{Abs}(1060\,\text{nm}) \qquad \text{in weight\% Fe}_2\text{O}_3 ,$$

The Fe3+ content is calculated from the [Fe2+] and the total iron content according to

$$\left[\text{total Fe}\right] = \text{f} \cdot \exp\left\{\text{p}\,\lambda^{-1} + \text{q}\right\} \qquad \text{in weight\% Fe}_2\text{O}_3 ,$$

where the straight line describes by the exponent represents the UV absorption edge. For calculating the total iron content the wavelength is taken to 325 nm

The coefficients e and f are determined by the glass composition.

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Redox settings

Redox state

Two commonly used representations of the redox state are $[Fe^{2+}]/[total\ Fe]$ and $[Fe^{2+}]/[Fe^{3+}]$. The user can select one of these representations through the submenu "Redox" in the menu "Settings"

Redox method

One of the methods for calculating the iron content can be selected through the submenu "Redox" in the menu "Settings"

Redox parameters

The Redox parameters dialog is used to set the coefficients used in the calculations of iron content. Selecting the submenu "Redox" in the menu "Settings" and then selecting the option "Parameters…" initiate the "Redox parameters" dialog.
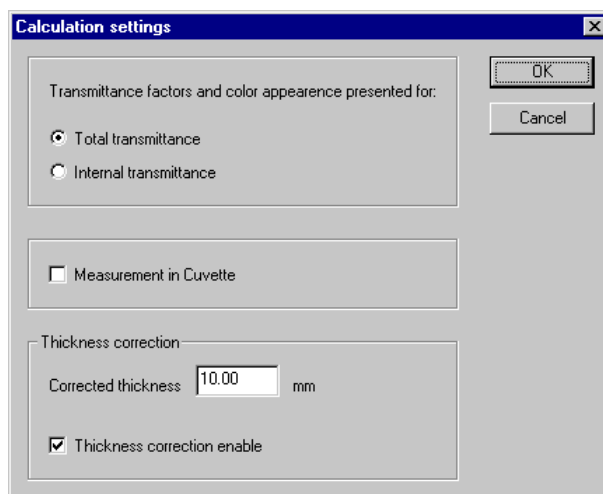
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TRCalc has a number of build-in procedures which perform the necessary corrections for different measurement and sample conditions.

Selecting the submenu "Data Handling" in the menu "Settings" and then selecting the option "Calculations …" initiate the "Calculation settings" dialog.

Sample thickness correction

For some applications, for instance when calculating the UV transmittance and color properties of packaging glass, it is necessary to calculate these properties for a reference thickness which is different from the true sample thickness.

In the thickness correction field of the "calculation settings" dialog you can enable the thickness correction and fill in the reference thickness for which the calculations have to be performed. If the thickness correction is enabled and the reference thickness differs from the true sample thickness filled in on the main dialog, all properties (except for the Iron content) calculated by TRCalc will be for a sample having the corrected thickness.

The status bar on the main dialog shows whether the thickness correction is enabled:

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Sample measured in a cuvette

Measurement of samples with a complex shape or rough surfaces can cause systematic errors due to deflection or scattering of the measurement beam. To avoid these problems some procedures require the use of a cuvette in which the sample is submerged in a liquid with matching refractive index. In order to make the appropriate corrections (see 'Total versus internal transmittance'), TRCalc needs to take this fact into account.

In the "calculation settings" dialog you can inform TRCalc that a cuvette is being used. The status bar on the main dialog shows whether the use of a cuvette is enabled.

Total versus internal transmittance

TRCalc can present the calculation results (transmittance factors and color properties) for total transmittance (sample in air) as well as for internal transmittance (sample in a cuvette). The choice can be made in the "calculation settings" dialog.

This setting is useful in the case where measurements have been performed without cuvette but the result of the calculations has to be specified for measurements with cuvette. In this case, by selecting 'internal transmittance', TRCalc makes the appropriate correction.

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TRCalc performs its calculations according to procedures (Standards) prescribed by standardization organizations. These procedures use reference tables which represent source energy distributions, detector sensitivity curves and spectral data of prescribed test surfaces. These tables are implemented in reference table files in the "references" directory of TRCalc.

Two drop-down-lists can by found on the Standards dialog:

1. The list "Standard name" is equal to the Standards drop-down-list on the toolbar of the main dialog.

2. The list "Name" in the field "Standard reference table" gives a list of reference tables (see also page 25: **Reference table files**).
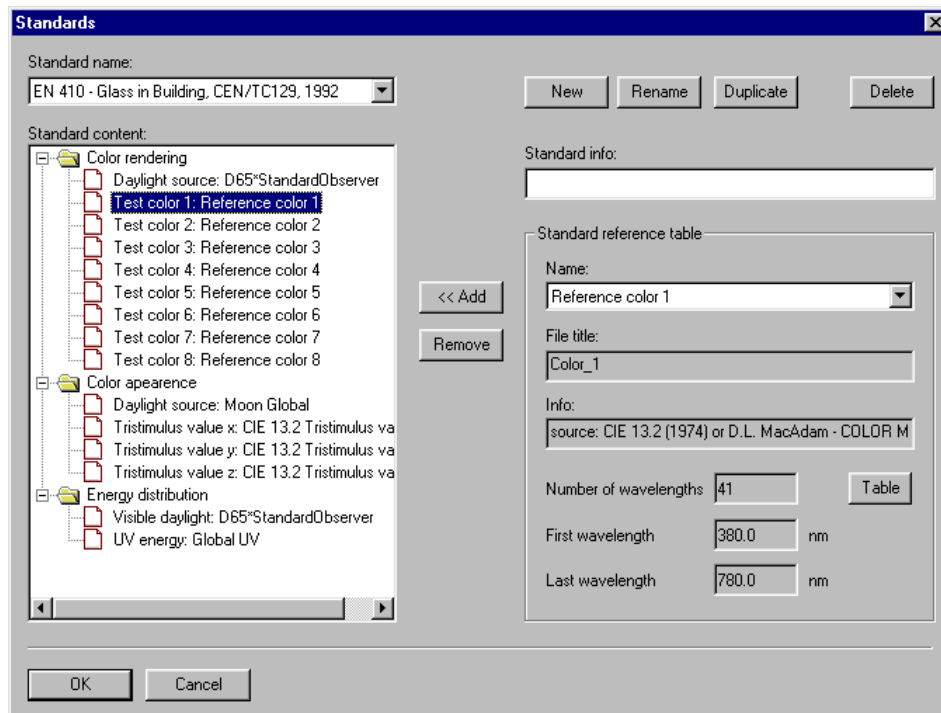
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The "Standard content" tree-list on the left half of the dialog shows which reference tables are connected to the selected standard, sorted by category:

- Color rendering
- Color appearance
- Energy distribution

The contents of each reference table can be inspected using the "Standard reference table" field in the right half of the dialog using the "Name" drop-down-list to select the reference table.

Selecting the option "Standards …" in the menu "Settings" initiate the "Standards" dialog.

Modifying a standard

After selecting a standard using the "Standard name" drop-down-list in the Standards dialog, this standard can be modified by the user:

- The standard can be completely removed from the list by selecting the button "Delete"
- The name of the standard can be changed after selecting the button "rename"
- The text in the field "Standard info" can be changed
- A link to a reference table in the content list can be changed by selecting the reference table in the content list, then selecting the new table in the reference table "name" drop-down-list and selecting the button "<< Add"
- A link to a reference table in the content list can be removed by selecting the reference table in the content list and then selecting the button "Remove"

Implementing a new standard

The easiest way for implementing a new standard in TRCalc is by first duplicating an existing standard and then modifying its name and contents using the procedure given in "Modifying a standard'.

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In TRCalc the user can print a standard report of the calculated results. Selecting the option "Print Results…" in the menu "File" initiate the "Print results" dialog.
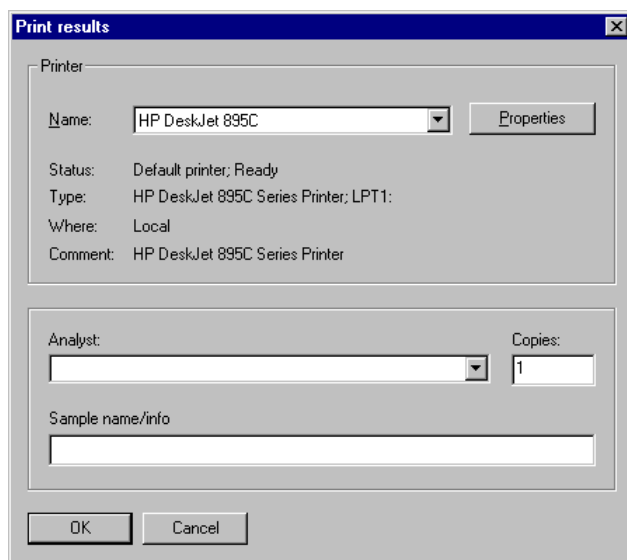
On the "Print results" dialog the printer can be selected and the name of the analyst and additional information regarding the sample can be inserted in the printed report.

After closing the dialog with the "OK' button, de printing of the report starts.
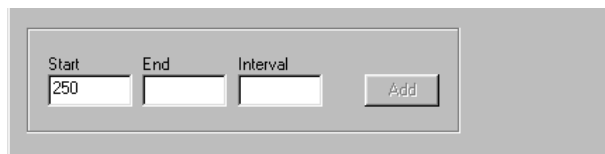
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Changing the data format in TRCalc

The data format dialog is used to set the wavelengths at which data is collected from the spectrum data files. The wavelength range is split-up into different ranges with different wavelength intervals.

Selecting the option "Data Format…" in the menu "Settings" initiate the "data format" dialog.
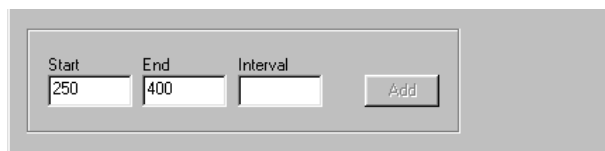
The following step-by-step procedure shows you how to specify a data format:

1. Clear the list by clicking the "Reset" button

2. Type the lowest wavelength in the "Start" field (not lower than 200 nm), for example 250 nm.
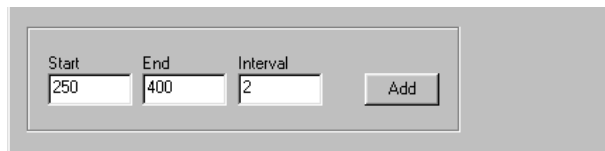
```
Start        End          Interval
250                                    Add
```

3. Type the highest wavelength of the first interval in the "End" field (not higher than 1100 nm), for example 400 nm.

```
Start        End          Interval
250          400                       Add
```

4. Type the size of the wavelength interval in the "Interval" field, for example 2 nm

```
Start        End          Interval
250          400          2           Add
```

5. Clicking the "Add" button ads the first interval to the list so that the dialog now looks like:

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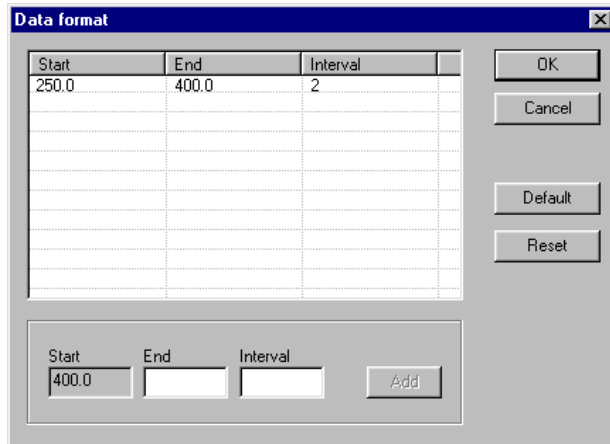
6. Fill in the "End" and "Interval" wavelengths of the next interval, for example 800 and 5 respectively
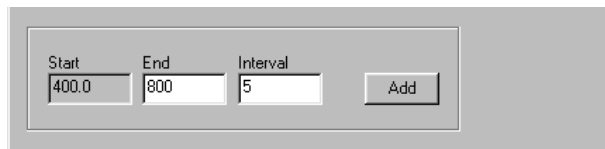
7. Clicking the "Add" button ads the second interval to the list so that the dialog now looks like
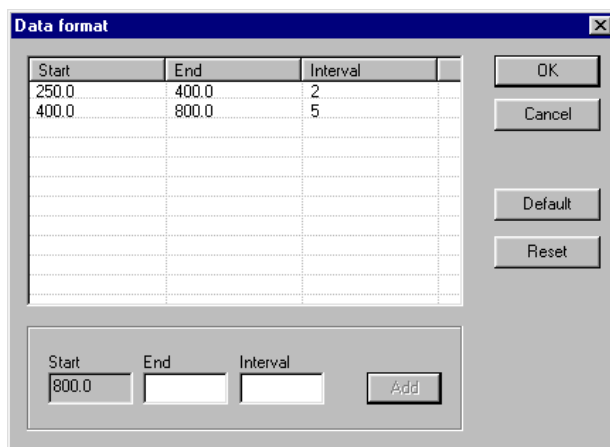
8. Now, repeat filling in the data for the following intervals and add them to the list.

9. Clicking the "OK" button saves your specified data format.

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Note: You can add as many intervals as you like.

- The minimum wavelength should not be smaller than 200 nm.
- The maximum wavelength should not be greater than 1100 nm.
- Values at wavelengths for which no data exists in the spectrum data file are determined by interpolation or extrapolation.

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Data file filters

Filters are used as an interface between the data file and TRCalc. They act as a translator to convert the data file format to a format that is recognized by the program.

Three filters are supplied with TRCalc:

1) The "Default file filter" for reading default ASSCI data files (see page 24: **File formats** for the format of the files recognized by this filter)

2) The "Sp file filter" for reading sp files.

3) The "Reference file filter" for reading reference table files. This filter normalizes the data in the reference tables by dividing each value by the maximum value found in the table. This results in a graph of the reference table on the main dialog with values always in the range 0 - 1.

Note: The calculation results obtained after selecting a reference table file as data file have no physical meaning!

Custom filters can be designed and supplied by Van Nijnatten Innovation on request.

Selecting the option "Data file filters…" in the menu "Settings" initiate the "Spectra data file filters" Dialog:

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The "available filters" drop-down list at the top of this dialog shows the available data filters. The "Properties" field gives a description and shows the file extensions which are assigned to the files to which the filter refers. Extensions can be modified or removed by selecting the appropriate button in the properties field.

Clicking the button "Add" allows a new extension to be added to the extensions list of the selected filter (for example the extension "new"):
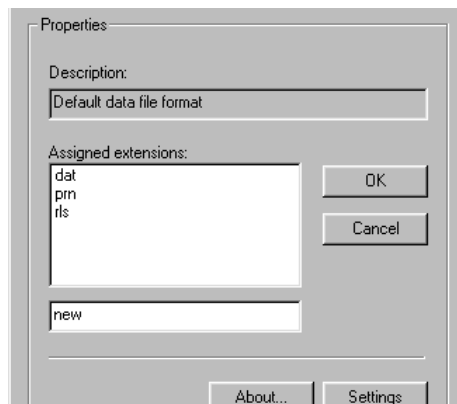
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To protect your settings with a password, select "Security" from the menu "Settings". After this, the following dialog will appear:
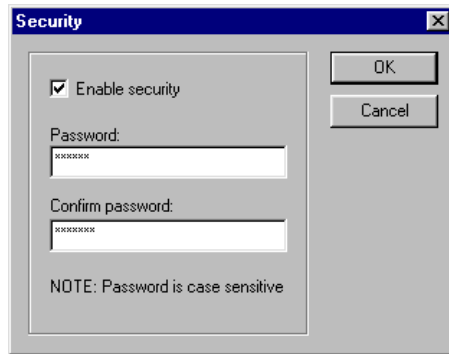
First check the "Enable security" checkbox. Then type in the "Password" field the password you want to use to protect your settings. Type again the password in the "Confirm password" field to confirm the password. After this, close the dialog with the "OK" button. Your settings are now protected with your specified password.

Note: If you already enabled security, you can disable it by uncheck the "Enable security" checkbox and closing the dialog with the "OK" button.

To access the protected settings, again select "Security" from the menu "Settings". After this, the following dialog will appear:
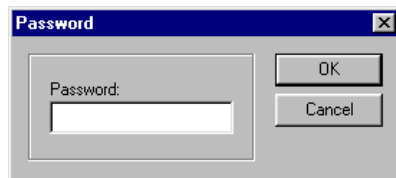
Type in the "Password" field your password and close the dialog with the "OK" button.

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Default data file format

Spectral transmittance is measured using a spectrophotometer and stored in a data file. An example of the content of a data file of the default format is as follows:

```
310     0.00139
320     0.04647
330     0.24757
340     0.52111
...     ...
...     ...
1660    0.84554
1670    0.84607
1680    0.84650
```

The first column is the wavelength in nm, the second column the transmittance.

This example shows the content of a data file in which the transmittance values are reported as values in the range 0 - 1. The "default data filter" is also capable of reading data files in which the transmittance values are reported as a percentage (values in the range 0 - 100).

The proper selection can be made using the "Settings" dialog which accompanies the default data filter:
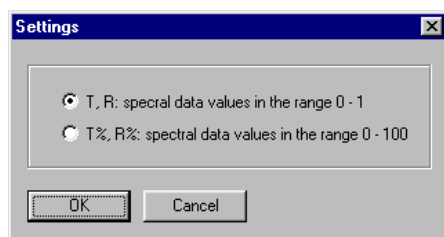
This dialog can be opened by selecting "default filter" in the "Available filters" drop-down list of the data filter dialog and then clicking the "Settings" button .

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Reference table files

TRCalc performs its calculations according to procedures (Standards) prescribed by standardization organizations. These procedures use reference tables which represent source energy distributions, detector sensitivity curves and spectral data of prescribed test surfaces. These tables are implemented in reference table files in the "references" directory of TRCalc.

The user can add new reference tables to the "references" directory which are recognized by TRCalc if the same format is used.

An example of the content of such a reference table file is given below. The actual table consists of two columns for respectively wavelength and corresponding reference value. Wavelengths must be in nm. The intervals can be chosen arbitrary. The red colored text is used by TRCalc to detect the start of the header and the table and the positions of the "Name" and "Info" texts. The latter are shown in the Standards dialog.

Example of a reference table

```
[Header]
Name = Global Solar (prEN410)
Info = Global Solar Energy distribution according to prEN 410 (Dec.
1997)
[Table]
300    0.0005
320    0.0069
340    0.0122
360    0.045
380    0.0177
...    ...
...    ...
2300   0.0066
2400   0.0041
2500   0.0006
```

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Standard terminology

ASTM
abbreviation for the American Society for Testing and Materials

Calibration
Correction for systematic errors in the instrument scale by use of measurement results obtained on a reference sample for which the true values are known.

CEN
Abbreviation referring to the Commission of European Normalization

Chromaticity
The color quality of a color stimulus definable by its chromatic coordinates, or by its dominant wavelength and its purity taken together

Chromaticity coordinates
The ratio of each of the tristimulus values of any observed light to the sum of the three (x, y, z)

Chromaticity diagram
A plane diagram in which points specified by chromatic coordinates represent color stimuli

CIE
Abbreviation of the French title of the International Commission on Illumination, Comission Internationale de l'Eclaire

CIE standard illuminant A
Colorimetric illuminant, representing the full radiator at 2855.6 K, defined by the CIE in terms of a relative spectral power distribution

CIE standard illuminant C
Colorimetric illuminant, representing daylight with a correlated color temperature of 6774 K, defined by the CIE in terms of a relative spectral power distribution

CIE standard illuminant D65
Colorimetric illuminant, representing daylight with a correlated color temperature of 6504 K, defined by the CIE in terms of a relative spectral power distribution

Color rendering
Color rendering is effect of a light source (or light from a reference source transmitted by a sample) on the color appearance of an object (or sample), compared to the color appearance under a reference light source

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Color rendering index Ra
The color rendering properties of the transmitted light are given by the general color rendering index Ra. It is calculated according to the test color method which has been established by the CIE as the recommended method of measuring and specifying color rendering properties of light sources. The reflectance spectra of the 8 test colors and the spectral energy distribution of

the illuminant which are used for the calculations are listed in the reference tables connected to the items in the folder "Color rendering" of the selected standard

Color temperature
The color temperature of a light source is the temperature (usually expressed in Kelvin) of a <u>full radiator</u> that would emit light of the same chromaticity (color) as the light source

DIN
Abbreviation referring to the German Standardization Institute: "Deutsche Industrie Normung"

Dominant wavelength
the wavelength of a spectrally pure light that, when added to a reference achromatic (white) light, will produce a combination that matches the color of a specimen light

Full radiator
a thermal radiator that completely absorbs all incident radiant flux, whatever the wavelength, direction of incidence, or polarization

ISO
Abbreviation referring to the International Standardization Organization

NEN
Abbreviation referring to Dutch standardization: "NEderlandse Normalisatie"

Spectral transmittance
Transmittance T of a planar sample as function of the wavelength, as measured by a spectrophotometer.

Transmittance factors
Single numbers quantifying a specific optical property:
Tuv =   UV transmittance.
Tvis=   Visible daylight transmittance.
Ra =   Color rendering index.

UV transmittance Tuv
Fraction of the ultra violet part of the solar radiation which is transmitted by the sample. The UV transmittance Tuv is calculated from the spectral transmittance T using the formula:

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$$Tuv = \frac{\sum_\lambda T_\lambda\, U_\lambda}{\sum_\lambda U_\lambda}$$

In which U is the spectral energy distribution of the UV part of the solar energy multiplied by the wavelength interval. U is listed in the reference table connected to the item "UV energy" in the folder "Energy distribution" of the selected standard.

Visible light transmittance Tvis
Fraction of the visible part of the solar radiation which is transmitted by the sample. The visible light transmittance Tvis is calculated from the spectral transmittance T using the formula:

$$Tvis = \frac{\sum_\lambda T_\lambda\, DV_\lambda}{\sum_\lambda DV_\lambda}$$

In which DV is the product of the spectral energy distribution of a daylight source D multiplied by a detector sensitivity curve V (human eye sensitivity or plant sensitivity) and the wavelength interval. This product is listed in the reference table connected to the item "visible daylight" in the folder "Energy distribution" of the selected standard.

Yellowness index
A number Yi determined according to ASTM 1925-70 by Yi = (127.7*x - 105.9*z) / y in which x, y en z are the chromaticity coordinates. The Yellowness index indicates the degree of departure of an object color from colorless, or from a preferred white, toward yellow. It should be calculated with CIE illuminant C as color appearance daylight source.