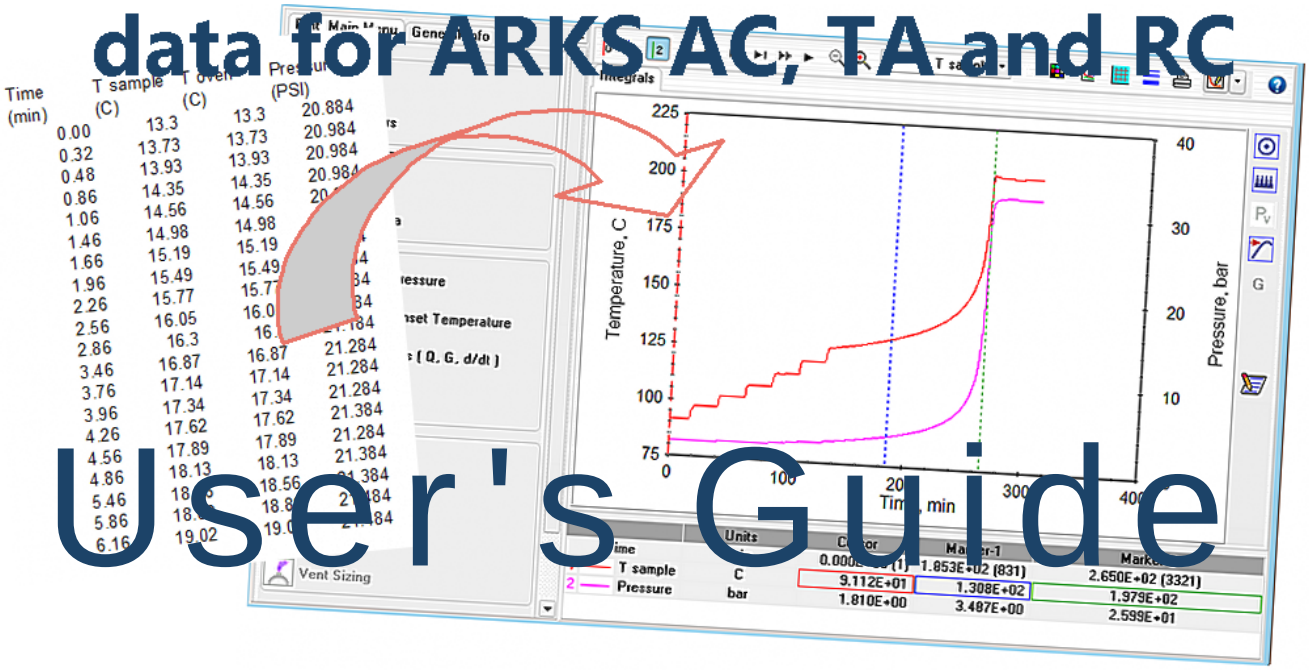
TSS-ARKS

Thermal Safety Series - Advanced Reaction Kinetics Simulation Software

ARKS Data Processing Suite

DConv

Data Converter - preparing data for ARKS AC, TA and RC



User's Guide

Saint-Petersburg, 2021

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1 OverView

A wide variety of thermal analysis instruments, adiabatic and reaction calorimeters are used for investigation of chemical reactions' kinetics. Each instrument has the computer-based system for experiment's automation, data sampling and storing. Unfortunately there isn't any common file format for experimental data storage. As it is often necessary to process the experimental data with some third-party software, the problem of data exchange and compatibility arises.

The solution to this problem is in using some auxiliary converting program (*Data Converter). Data Converter* (further simply *Converter or DConv)* works with a rather free-form ASCII file and Excel sheets. It allows loading a file, analyzing it and choosing the necessary information. In addition you can make some elementary data processing (e.g. changing units to the standard ones). The *Converter* output files are used directly by the ARKS programs ARKS AC, TA and RC of the CISP Data processing suit of Thermal Safety Series - Advanced Kinetics Simulation software- TSS-ARKS™, and by their predecessors ***ADaExpert***, ***TDPro*** *or* ***RCPro*** from the TSS line. The use of the templates allows saving the method of structural analysis for the particular data type. If data are loaded from the files then the template will be associated with the file extension. Afterwards this saved template will be automatically loaded whenever you load the file with the appropriate extension and all the parsing will be made automatically.

Comments

***ARKS AC** (ADaExpert) program is used for comprehensive processing of results of pseudoadiabatic calorimetry (ARC, VSP, RSST, DEWAR and others) and preparing them for further kinetic analysis by the ARKS FK/CK and ForK/DesK.*

***ARKS TA** (TDPro) program is used for comprehensive processing of results of thermoanalitical experiments (DSC, TG, DSC-TG, DTA) and preparing them for further kinetic analysis by the ARKS IK/FK/CK and Isokin/ForK/DesK..*

***ARKS RC** and predecessor IsoKin are flexible and easy-to-use program packages for creation of the model-free kinetics; useful for preliminary analysis of DSC data and data of isothermal calorimetry. They also provide simulation of chemical processes proceeding in well stirred reactors.*

***ARKS IK**, **ARKS FK** and **ARKS CK** and predecessors IsoKin, ForK and DesK are the powerful program packages for creation of model-free (IK) and model-based (FK and CK) kinetics of chemical reactions and simulation of chemical processes proceeding in well stirred reactors.*

How to get ARKS DConv program

Just download the setup here then extract the setup file from the archive and follow the instructions.

How to convert data

The following sequence presents the typical steps you should implement to convert data.

1. Open an ASCII file of MS Excel book containing original data or paste them from the Clipboard
2. Converter will analyse data, find and mark the first and last lines of the data table; if by some reasons automatic analysis fails then you have to mark the first and last lines of the data table manually

Note

If your data contain several separates data tables then the Converter will recognize and select the firs table only, therefore you should combine these separate tables into one continuous table beforehand

3. Select the suitable experiment type. If you run Converter from under one of the above mentioned programs the corresponding experiment type will be set automatically.
4. In the HEADER dialog, enter necessary parameters and complementary information (see Preparing a header)
5. In the TEMPLATE EDITOR dialog, define the new template or select and load the appropriate existing one (see Preparing a template)

6. After completion of data conversion in the OUTPUT FILE dialog save the resultant data (if you use Converter in autonomous mode) or click on the RETURN to the MAIN PROGRAM button (see **Creating an output file**)

How to run Converter

The general method of running the Converter is to launch it from the main data processing program. DConv will be run in the spawned mode and the data type to be converted will be automatically assigned. After you convert data they will be transferred directly into this main program and DConv will be closed automatically.

If necessary DConv can be run as an independent program. You can find it along the path C: \users\[usermame\CISP\Dconv\dconv.exe.

In this case the converted data should be saved in a separate binary file. Depending on the data type you have chosen this file will have one of the following extensions: *.tdp - for thermoanalytical data; *.adp - for adiabatic data, and *.rcp - for data of reaction calorimetry.

2 Using Converter

The software interface is designed as Wizard for more convenient and consecutive procedure of data conversion.

The **Main** window consists of the **Toolbar** at the top of it and the **Back and Next buttons** for navigation between consecutive conversion stages at the bottom.

The set of buttons of the **Toolbar** and the appearance of the Main window change in accordance with the chosen pane (conversion stage).

The conversion chain is shown below the **Back/Next** buttons. It consists of the following stages:

{Q} Input - to input data from file;

Header - to prepare a header ;

{Q}Template - to prepare a template;

{C} Input - to input concentrations data (for reaction calorimetry experiments)

{C} Template - to prepare a template for reaction calorimetry experiments data;

Output File - to create an output file.

Note

{C} Input and {C} Template stages become available if Reaction calorimetry experiment type is chosen in data input pane.

The current stage is marked.

To quit Converter press the  button.

Necessary data

Necessary responses for ARKS AC and ADaExpert are:

- t - time, s;
- Ts - sample temperature, K;

Optional responses:

- To - oven temperature, K;
- P - pressure, bar;
- dTs/dt - self heating rate; K/s;
- dP/dt - rate of pressure variation, bar/s.

If you are going to process non-adiabatic data with ADaExpert you should load one of the following additional responses::

- dQ/dt - heat production rate, mW or/and
- Q – heat production, J.

Necessary responses for ARKS TA and TDPro are:

- t-time, s;
- derivative response dQ/dt, mW; or/and mass loss response M, ;
- Ts - sample temperature, K, or heating table which defines dependency of a reference temperature on time in tabular form.

Necessary responses for ARKS RC and RCPro are:

- t-time, s;
- dQ/dt - heat production rate, mW
- Ts - temperature, K, heating table which defines dependency of a reference temperature on time in tabular form.

Optional responses:

- P - pressure
- C - species concentrations, mass fractions
- dC/dT - rate of species concentrations variation

How to convert data

The following sequence presents the typical steps you should implement to convert data.

1. Open an ASCII file of MS Excel data sheet containing original data or paste them from the Clipboard
2. Converter will analyse data, find and mark the first and last lines of the data table ***automatically***; if by some reasons automatic analysis fails then you have to mark the first and last lines of the data table manually

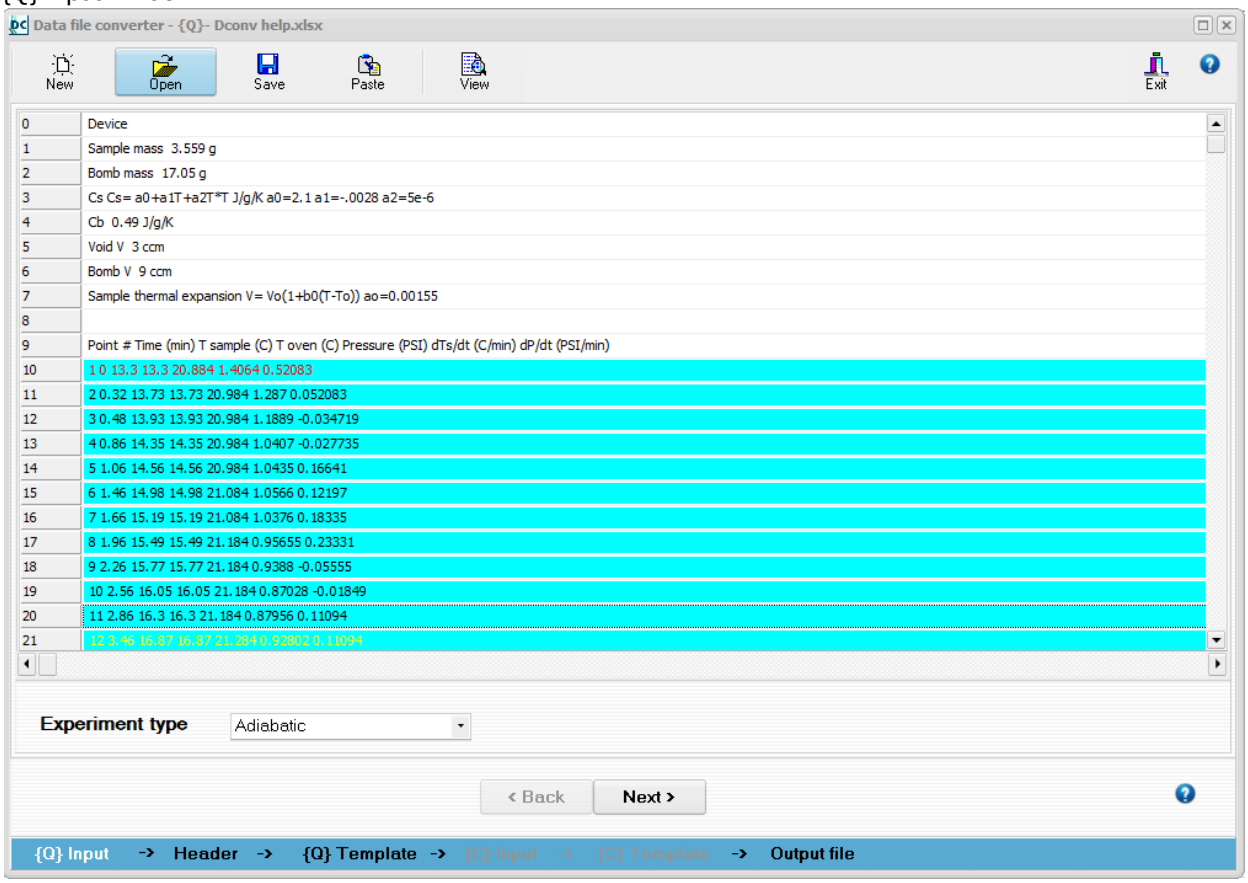
Note

If your data contain several separates data tables then the Converter will recognize and select the firs table only, therefore you should combine these separate tables into one continuous table beforehand

3. Select the suitable experiment 's type. If you run Converter from under one of the data processing programs the corresponding experiment's type will be set automatically.
4. In the HEADER pane, enter necessary parameters and complementary information (see Preparing a header)
5. In the TEMPLATE EDITOR pane, define the new template or select the appropriate one from the list of existing templates
(see Preparing a template); *don't forget to save the newly created template for further use!*
6. If the **reaction calorimetry** is set as the experiment type - open an ASCII file or MS Excel sheet containing concentrations data or paste them from the Clipboard (see Loading species concentrations data)
7. If the **reaction calorimetry** is set as the experiment type - in C-Template editor pane, define the template for concentrations data or select the appropriate one from the list of existing templates (see Preparing the {C} template).
8. After completion of data conversion in the OUTPUT FILE dialog save the resultant data (if you use Converter in autonomous mode) or click on the **Save & Exit** button (see Creating an output file)

3 Data input

{Q} Input window:



Opening a data file

To open a data file press the button. The **Open** dialog box will appear

Choose necessary file and press the **OK** button. File can be of text type or created by MS Excel.
The file will be shown in the main window with the lines numbers.

Note

DConv can handle multi-sheet EXCEL books but only data from the first sheet can be loaded. There are two ways how to retrieve data form a multi-sheet EXCEL book:

1. ***To split the multi-sheet book into several one-sheet books and then open necessary child-book***
2. ***To open the book in a usual way by the MS Excel, shift necessary sheet to the first place, save the book and then open it by DConv.***

In case you would like to clear the contents of the window press the button. The currently loaded data will be removed.

Usually Converter will not have problems working with common data files produced by the appropriate equipment. Still we draw your attention to the following rules:

The data file must have the uniform data through the columns, i.e., the format of numbers in a column must be the same for all numbers.

Also the number of data points in the columns must be the same for all of them.

Inserting Data From A Clipboard

You may copy some data lines from another application (for example Excel) and then paste them by using the  button.

Viewing Loaded Data

After loading a data file, you may want to view its contents.

To view the loaded file at any stage of the conversion process, use the  and then vertical and horizontal Scroll Bars.

Marking A Data Area

To convert data from an input file, a data area must be marked. Converter implements this step automatically. Nevertheless it may happen that automatic data analysis fails or you are interested in certain part of data table (e.g. from the beginning to the middle of the table or from certain data row till the end of the table).

In this cases you have to mark necessary part of the data area manually by using the right mouse button.

To mark a data area do the following:

1. Click the left button at the necessary line.

2. Click the right button. The pop-up menu will appear. Choose the First Data Line or the End Of Data menu item accordingly.

You can see now the data area of the file highlighted. Now, you are ready for the next operations.

Selecting An Experiment Type

At the bottom there is the Experiment type drop-down list box.

You can select one of the following experiment types:

- Adiabatic;
- DSC;
- DTA;
- Reaction Calorimetry.

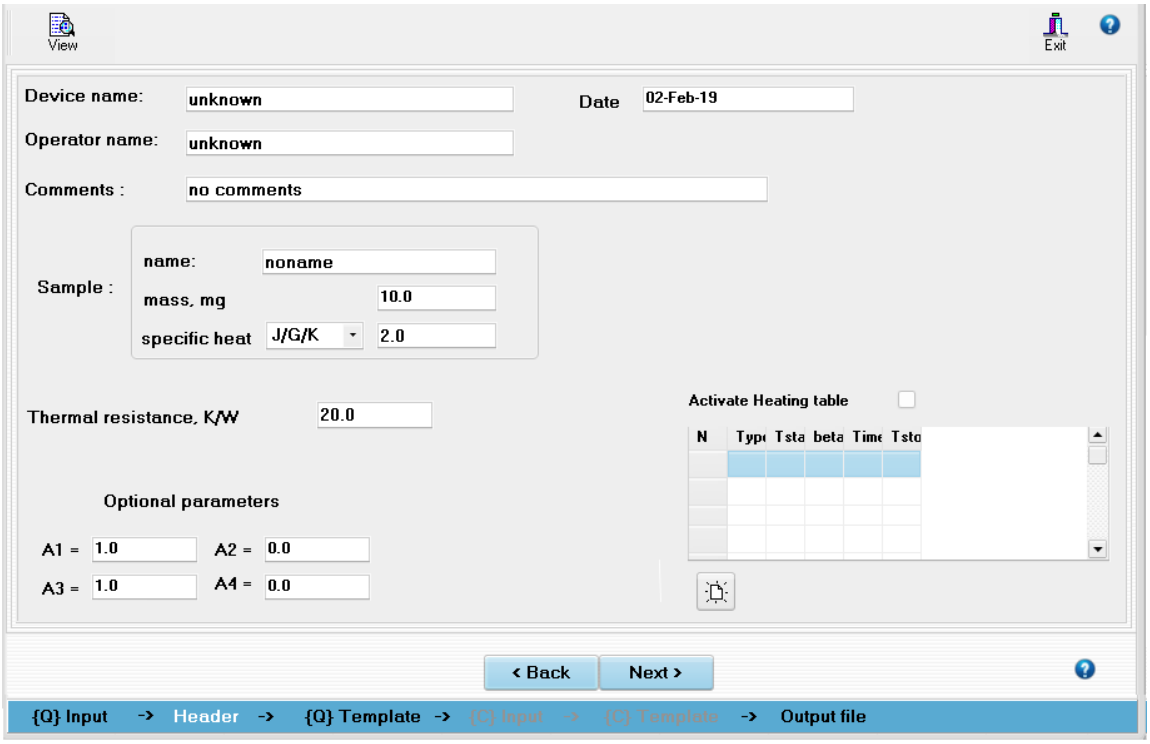
Saving A Data File

If original data were pasted into the DConv from the Clipboard you may wish to save them into a data file. Press the  button. A common windows Save dialog panel will appear.

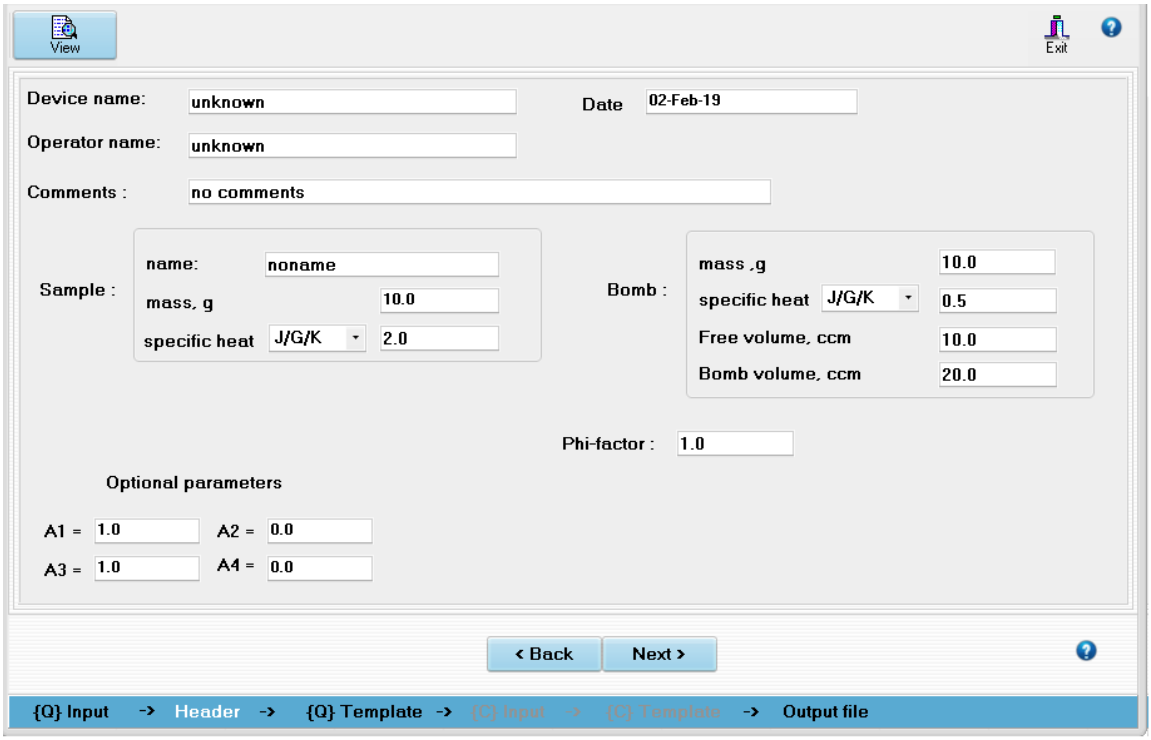
After all, click the **Next** button to go to the next stage. (See Using Converter)

4 Preparing a Header

To manage data header, choose the **Header** stage using the Back or Next button (the current conversion stage is marked in the conversion process chain). One of the dialog panels will appear in accord with the type of experiment (chosen in the **Data Input pane**) . Note that these headers are identical in the upper part and differ only in the bottom part.



Header dialog for DSC/DTA experiments



Header dialog for adiabatic experiments

The following table reminds what data must be entered for a particular type of experiment (excluding the

reaction calorimetry experiments).

Table -1. Header parameters.

	Sample mass	Sample specific heat	Thermal resistance	Heat transfer coefficient	Heating table	Bomb mass & specific heat	Phi factor	Free volume	Bomb volume
Adiabatic	+	+				+	+	+	+
DSC	+	+	+		+				
TG	+				+				
DSC+TG	+	+	+		+				
DTA	+	+		+	+				

You can choose the appropriate units for specific heats by using the corresponding drop-down box.

Notes

1. ***If some obligatory parameter is missing, DConv will give you a corresponding note when attempting to go to the next stage in conversion process chain.***
2. ***Measuring units of some parameters can be changed. To do this, click on units name (next to parameter value) and choose desired units in the list appeared.***
3. ***The Time constant parameter defines distortion of the calorimetric signal due to thermal inertia of the calorimetric cell. Usually the calorimetric response corresponds to the heat flow from/to the cell whereas part of the heat released by the reaction is accumulated by the cell. This very rate of heat release is of interest therefore time constant will be used by the ARKS TA/RC programs to reconstruct the heat rate response from measured heat flow one.***
4. ***The Thermal resistance parameter describes the conditions of heat exchange between calorimetric cell and the furnace. It will be used by the ARKS TA/RC program to reconstruct the real sample temperature if it is not measured directly.***

Using optional parameters

In some cases it may be necessary to define some transformations of data (for instance shift or scale data). It can be done when defining the columns (see Columns definition). In many cases such transformation requires additional constants that can de assigned in the Header. The four edit boxes for the a1 – a4 parameters are available. By default a1 = a3; a2 =a4 = 0

Note

One specific case when transformation may be required is converting of DTA data. See the example of Converting DTA data

Using A Heating Table

To activate a heating table check the **Activate Heating Table** check box. Now you can input the heating table. Position the mouse cursor on the first line of it and press left mouse button. The **Heat Table Item Definition** edit box will appear Type the values describing the appropriate linear segment of the heating table. You have a choice between two segment types: **Isothermal (ISO) or Dynamic (DYN)**

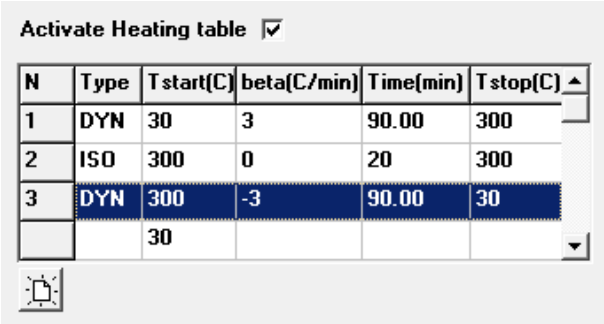
To input the **Isothermal** segment you need to type the following data:

- Initial temperature of the segment, [Tstart]=C
- time duration of the segment, [t]=minutes.

To input the **Dynamic** segment you need to type the following values:

- Initial temperature of the segment, [Tstart]=C
- Last temperature of the segment, [Tstop]=C.
- Heating rate B, C/min
- Time duration of the dynamic segment is calculated automatically: t=(Tstop - Tstart)/B.

Figure below shows the Heating table that defines linear heating from 30 to 300 C with the rate 3 C/min followed by the isothermal 20 min plateau and cooling till the start temperature at 3 C/min.



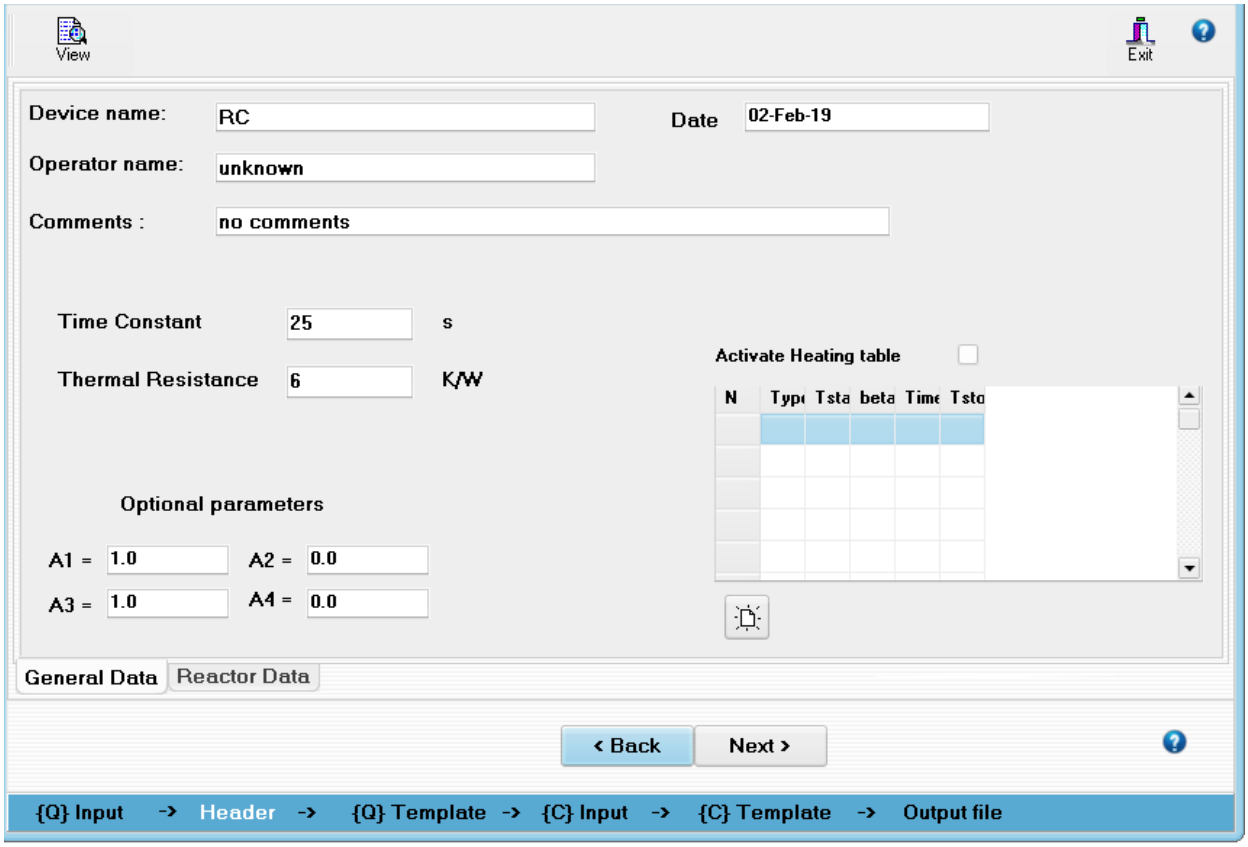
Working with data of reaction calorimetry

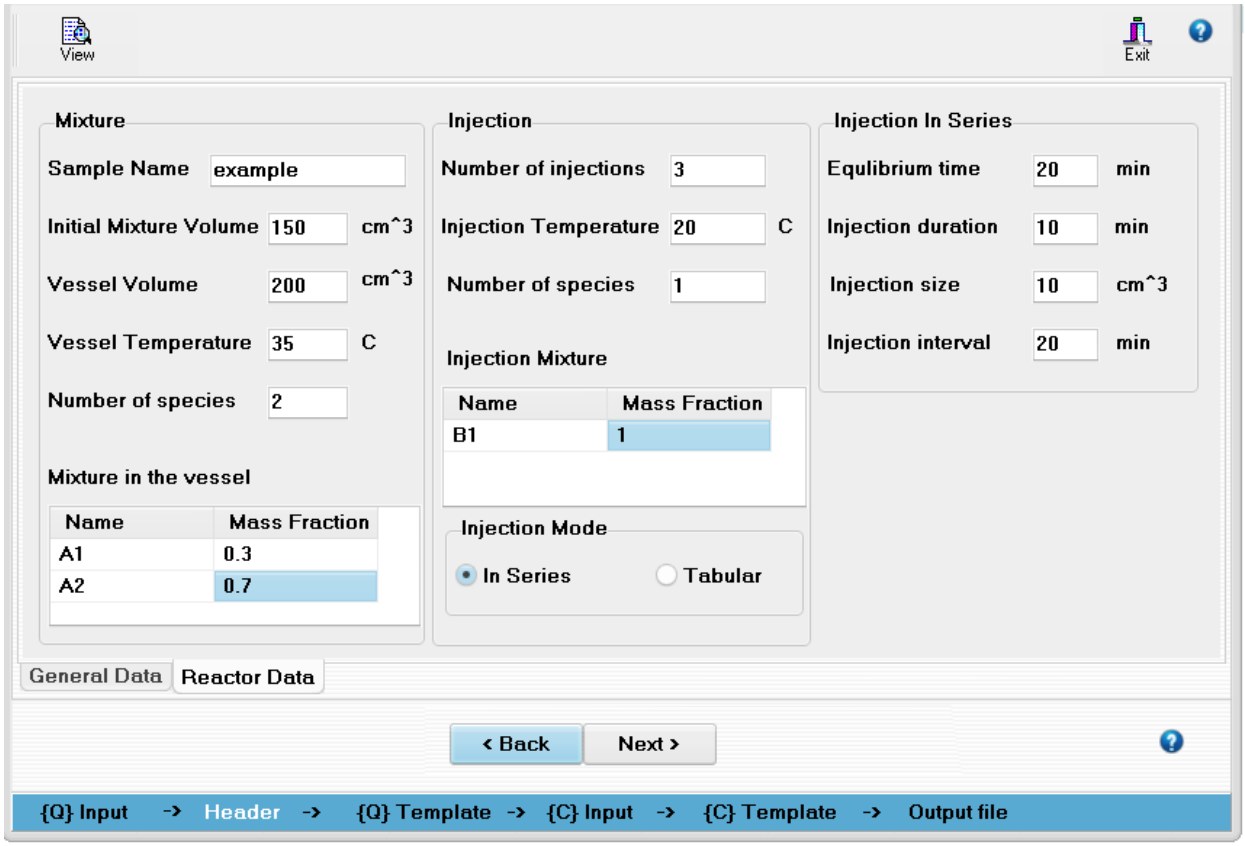
Note for ARKS μRC Package Users

If you are working with ARKS μRC Package and converting data stored in THT *.tit, *.sca, and *.col formats DConv will automatically retrieve and paste most part of information described below, including compositions of vial and injection mixtures and the parameters of injections.

Nevertheless we strongly recommend to check whether this information has been transferred correctly.

The header for converting this type of data contains more information to be defined, therefore the header consists of two tabs - General data and Reactor data:





The Reactor data tab contains 3 specialized panels - Mixture, Injection and Injection in series/Tabular injections

Obligatory parameters are:

- Initial mixture volume;
- Vessel volume;
- Number of species;
- Species mass fractions.

Mixture

This panel serves for defining the parameters of the reactor (vial) and initial conditions of the mixture initially loaded. Most of the parameters are self-evident. Some comments regarding several particular parameters are given below.

Number of species . As soon as number of species in the mixture is defined the **Mixture in the vessel** table is expanded so that the number of rows will correspond to the number of species.

Mixture in the Vessel. For every species the alias and mass fraction should be defined. Program checks whether the sum of mass fractions equals 1 and requests to correct the values if the sum is different.

Injection

This group is optional; it is used in the case of semi-batch mode. The mixture injected may comprise several species; its composition must be defined similarly to defining mixture in the vessel.

Note

In the case of multiply injections it is always supposed that the same mixture is injected

Injection mode. If several injections are made during the experiment one should choose whether each injection has unique parameters or series of identical injections was applied. In the first case select the **Tabular** radio button otherwise select the **In Series** one.

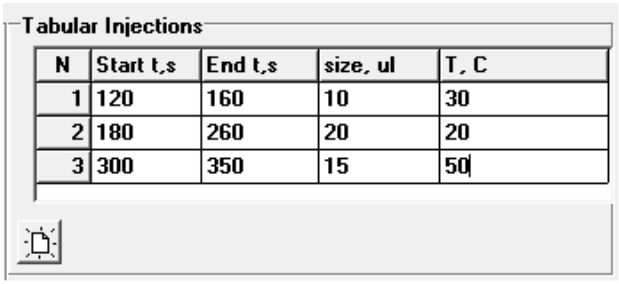
Injections In Series. In this case one should define the parameters of an injection (see the Injections in

series group)

- *Equilibrium time* - waiting period before start of the first injection
- *Injection duration* - time interval during which injection continues
- *Injection size* - volume of mixture injected
- *Injection interval* - duration of the pause between two adjoining injections

For the **Tabular** type of injections the **Injections In Series** group will be replaced with the **Tabular injection** table:

Tabular injection table contains the number of rows equal to the number of injections.



Note

You can switch from Injections in Series to Tabular injection only after defining the number of injections

For every injection one should define the start and the end time instants, injection volume (in micro liters) and temperature

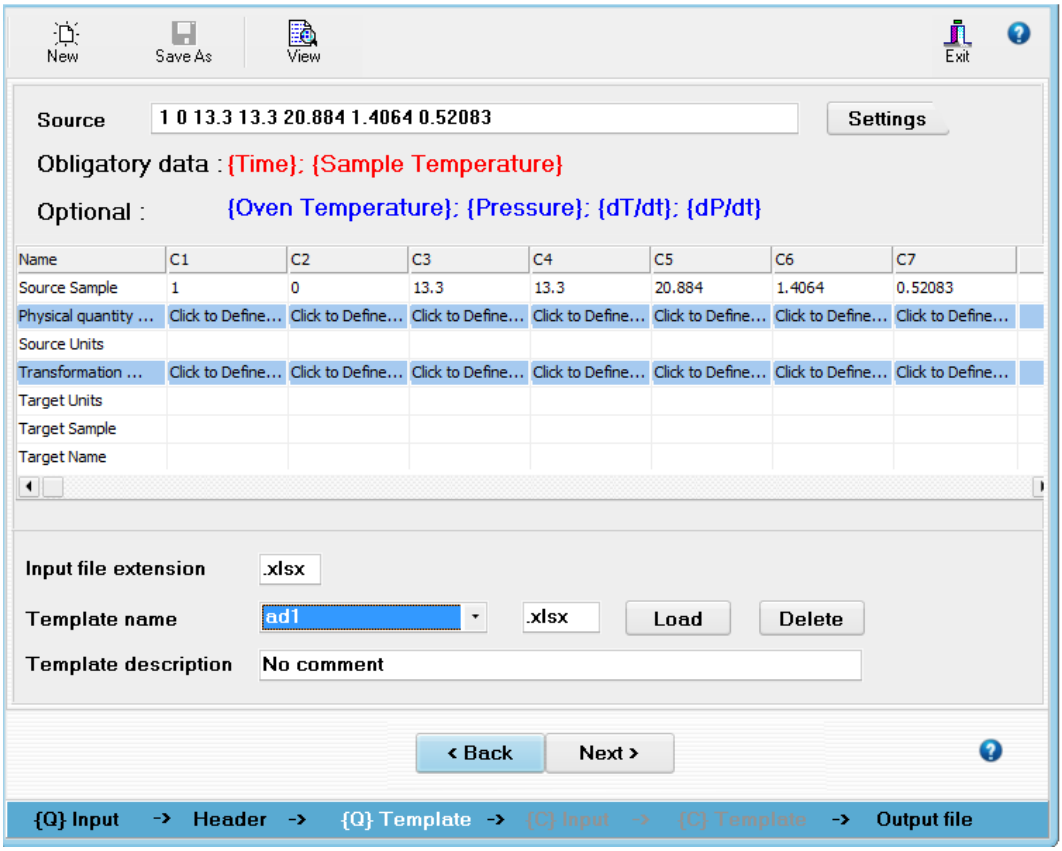
After all, click the **Next** button to go to the next stage.

5 Preparing a template

Note for ARKS μRC Package Users

If you are working with ARKS μRC Package and converting data stored in THT *.tit, *.sca, and *.col formats DConv will use pre-defined template therefore you can omit this step. Nevertheless we strongly recommend to check whether the template is valid.

To prepare a template for the main data, choose the {Q}**Template** stage by pressing the Back or Next button (the current conversion stage is marked in the conversion process chain). The pane is available in case you have defined a data area.



Template Editor pane contains all necessary controls for preparing the template.

The **Source** line displays the exemplary (first) line of data.

The **Settings** button allows Adjusting source line format if necessary.

Note

The Setting option is used if the source data file utilizes formatting that differs from the settings of current template, specifically different column separators or decimal delimiter are used. In this case when you enter the Template page you will get the warning Some items are not numerical, invalid decimal symbol, invalid column separator

Two lines remind you the **Obligatory** set of data for the chosen type of an experiment and **Optional** data that can be also converted.

The main part of the dialog is occupied by the interactive table for easy defining source data (physical quantity, units, necessary transformations). The number of columns (numbered as C1, C2, etc.) in the Source panel coincides with the number of columns in data table (the selected line reminds its structure). The active cells of this table are highlighted in blue.

The main purpose is to choose the necessary columns from the input file, combining them with necessary transformations (see for example preparing data of DTA experiment) and producing columns of the output

file

Managing templates

The pane below the Source data table contains the tools for Managing templates: storing a template, selecting it from the template library, loading a template, deleting it from the library.

Creating A New Template

To create a new template press the **New Template** button. Proceed as described in the next section.

Editing An Existing Template

At first you need to definite physical quantity and units to the data of each column.

1. In the **Physical quantity** raw, place the mouse cursor in the Click to define cell of any source column and click left mouse button. The **Input column definition** dialog box will appear.
2. Select in the Physical quantity drop-down list box an appropriate physical meaning and in the Units box an appropriate physical units.
3. Select OK or Cancel button.
4. The **Source units**, **Transformation**, **Target units, Target sample** and **Target name** cells are filled automatically. By default the Target name (the response name) coincides with Physical quantity. This is perfectly suitable for the individual responses of different quantity (e.g. Temperature, Heat production rate, Pressure, etc.) but it may be confusing in the case of concentration responses as all of them are of the same physical quantity. In such the cases the possibility to change **Target names** will be very helpful. This can be done by applying **Transformation.**
5. By default the **Transformation** cells show that the source data in the basic units will be transferred into target data. If some additional transformation is required including renaming, place the the mouse cursor in the *Click to define* cell and click left mouse button. The **Output column definition** dialog will appear. This dialog panel looks like and works also like simple calculator. All you need is to enter new target name and define the expression which can contain the arguments c1, c2,… referring the columns of the source file, a1 - a4 parameters, and numbers.
6. If you want to clear the column definition go to the **Input column definition** dialog and select **None** from the Physical quantity drop-down list box.

Notes

1. ***As soon as a source data column has been defined the Transformation cell must contain at least the name of a column (e.g. C1), you cannot make it empty while working with the Output column definition dialog.***
2. ***If the expression should include references to several source columns all these columns must be defined beforehand otherwise they won't be available in the Output column definition dialog***

The following figure demonstrates an example of defining part of source data

Name	C1	C2	C3	C4	C5	C6	C7
Source Sample	1	0	13.3	13.3	20.884	1.4064	0.52083
Physical quantity ...	Click to Define...	Time	Temperature	Click to Define...	Pressure	Click to Define...	Click to Define...
Source Units		Minute	Celsius		pound per square inch		
Transformation ...	Click to Define...	C2	C3	Click to Define...	C5	Click to Define...	Click to Define...
Target Units		Second	Kelvin		bar		
Target Sample		0.00000E+0	2.86450E+2		1.43990E+0		
Target Name		Time	Temperature		Pressure		

Data from the first column were just converted to basic units and transferred into the target data array.

Data from the second column were converted to basic units and shifted - the Transformation cell shows the expression used for transformation.

Data from the third column were converted to basic units and renamed.

Saving A Template

To save a template press the **Save As Template** button. See Managing templates for the details. If the template with the same name already exists the warning will appear.

After all, click the **Next** button to go to the next stage. (See Using Converter)

5.1 Managing templates

An Input File Extension

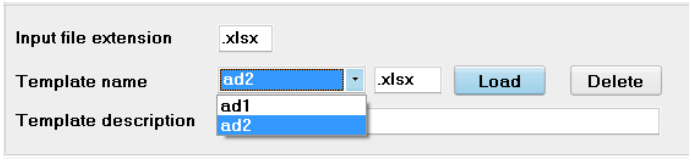
Input file extension associates the current template with the file's type; in the future the first template from the list of templates associated with the particular file extension will be indicated in the **Template name** combo box right after you loaded data from such a file..

Note

If original data have been pasted from the clipboard you cannot associate them with any file extension. Nevertheless you can save the template and then select the appropriate template from the list of the created ones to convert data pasted provided that these data have the same structure as those used for template creation.

Selecting and loading A Template

You can load any template by selecting its name in the drop-down list box. The drop-down list box contains the names of those templates that correspond to the selected experiment type. Select the template you think is appropriate and press the **Load** button.



The Source data table will be filled with the data definitions and, possibly, transformation rules; you should carefully check whether the template matches data.

Note that the button label changes from **Load** to Ready and becomes disabled.

Attention!

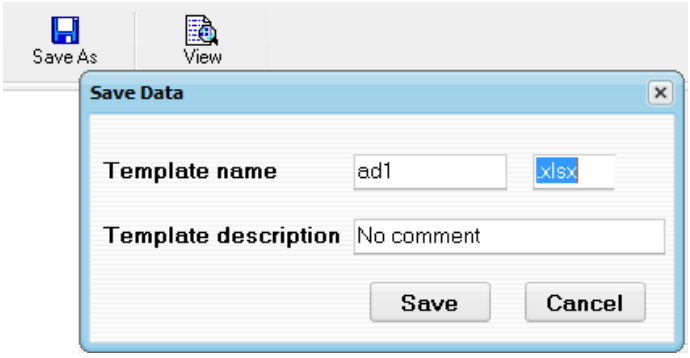
It may happen that several different templates have been created and saved for files with the same extension but with different structure of data (e.g for *.txt files or *xlsx files or data pasted from the clipboard without any extension). The Template list will contain all the templates that are associated with this file extension. The first template from the list will be loaded automatically. Check carefully whether the template suits data. The Converter can only check automatically the discrepancy between the number of columns in the data table and number of columns defined in the template. DConv verifies whether number of columns in the template exceeds number of columns in the data table and warns that the template doesn't match data if this discrepancy has been detected. You will have to choose another template.

Deleting A Template from the library

If you want to delete a template from the library created for certain experiment just select it from the listbox and press the **Delete** button. You will be asked to confirm the action.

Saving A Template

After the template was created or edited it can be saved (added to the Template library) for further use. Press the Save as button from the main toolbar. In the dialog displayed define the template name, add comment and press the **Save** button.



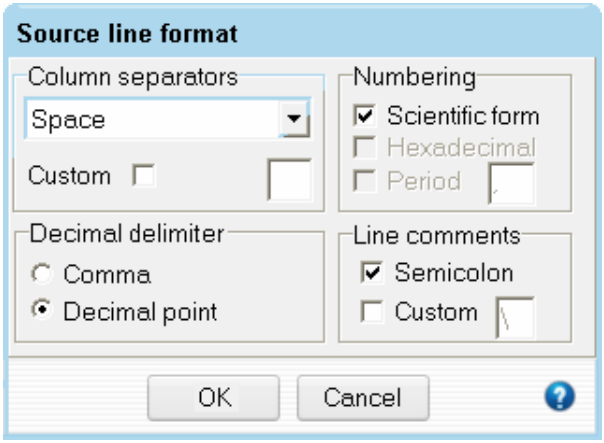
Note

Don't forget to define the file extension for new template on the right of the name box!

If the template with the same name already exists you will be warned that existing template will be overwritten. Confirm or Cancel

5.2 Adjusting source line format

This dialog suggests to choose the set of formatting options which will be used while parsing files with the current template. The options are divided into 4 groups. All the options are explained further.



Column Separator

This group defines the symbols that are used as columns' separators in a file. By default the **Space** symbol is used. Tabulation, Comma, Semicolon are the alternatives.

Select the appropriate separator from the drop-down list box

Numbering

This version assumes numbers only in a scientific notation. The Hexadecimal and Period fields are disabled.

Decimal Delimiter

The **Decimal separator** group is simple and allows selection between Point or Comma.

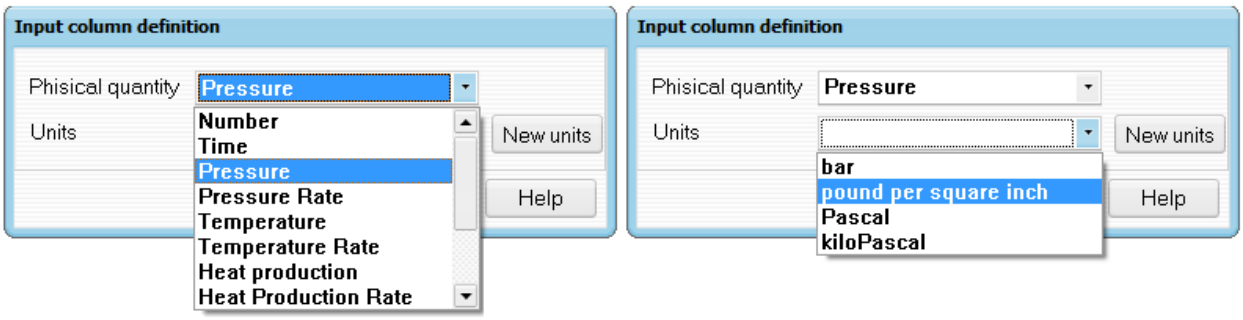
Line Comments

The lines starting from the symbols specified in this group will be considered as comments.

5.3 Columns definition

The input column definition dialog allows you to define physical quantity and units for data of a source column. It appears when you place the mouse cursor in the *Click to define* cell of the **Physical quantity** raw of any source column and click left mouse button

1. Select an appropriate physical meaning (a) in the **Physical quantity** drop-down list box and the appropriate physical unitsin the **Units** box (b).



a) b)

2. Select **OK** or **Cancel** button.

In the case you are not satisfied with the set of already available units for any of the physical quantity you can introduce the new units.

To define additional units (new units), press the NEW UNITS button next to the Units drop-down list box. The corresponding dialog will appear.

5.3.1 Defining new units

This dialog is intended for introducing of new units in the case you are not satisfied with the set of already available ones.

1. Select necessary physical quantity in the **Physical quantity** drop-down list box.
2. Enter full and short names for your units.
3. Enter appropriate coefficients to obtain values in base units from values in your units. Base units for physical quantities envisaged in TFC are as follows:

[time] – seconds
[Temperature] – K
[Pressure] – bar
[Heat Production] – J
[Mass Loss] – %
[Temperature Rate] – K/s
[Pressure Rate] – bar/s
[Heat Production Rate] – mW
[Mass Loss Rate] – %/s
[Concentration] - kmol/m3

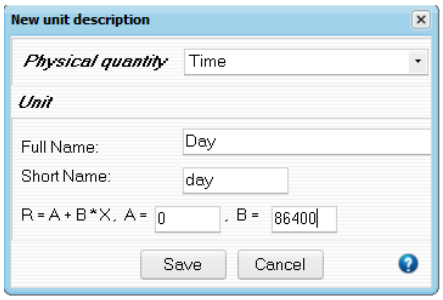
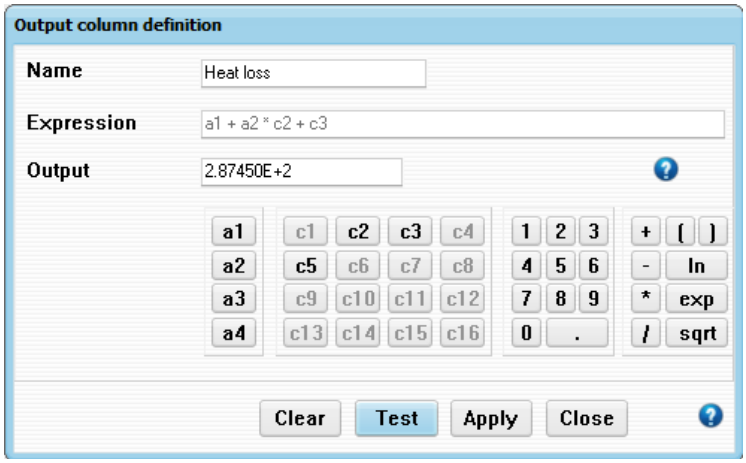


Fig. on the right shows the example of defining additional time unit - Day

5.3.2 Defining transformation

The Output column definition dialog looks like and works also like simple spreadsheet.

To define transformation enter the expression which can contain the arguments
c1, c2,… referring the columns of the source file, a1 - a4 parameters, and numbers.



The meanings of the dialog elements located at the panel are the following:

the **Name** edit shows the default name of the target which coincides with the physical quantity. Type any other name you want to assign to the target.

the **Expression** window displays a formula for the values of the target column calculation;

the **Output** window displays a result of calculations performed with the elements of the first data line in accordance with the expression. This result appears when pressing the **Test** button;
Character keypad description:

a1- a4 buttons - denote parameters defined in the Header.

c1…c16 - denote the columns from the source (input) file that were defined already.

On the character keypad only currently significant buttons are enabled.

Numeric keypad is ordinary for mathematical calculator and does not need any special explanation.

Functional buttons description:

the **Clear** button	Clears the contents of the current target column;
the **Test** button	Performs calculations on the values of the first chosen data line in accordance with the formula and displays results in the **Output** window;
the **Apply** button	Inserts definition of the current column into the template;
the **Close** button	Closes the dialog panel.

ATTENTION!

1. ***If you are going to use additional parameters while defining a target column, keep in mind that their values should be entered in a Header beforehand, otherwise default values a1=a3=1 and a2=a4=0 will be used for calculations.***
2. ***All the calculations that involve source data are implemented after they have been converted into base units. Therefore additional parameters used in arithmetic expression must also be presented in corresponding units. The list of base units is as follows:***

[time] – seconds	*[Temperature Rate] – K/s*
[Temperature] – K	*[Pressure Rate] – bar/s*
[Pressure] – bar	*[Heat Production Rate] – mW*
[Heat Production] – J	*[Mass Loss Rate] – %/s*
[Mass Loss] – %	*[Concentration] - kmol/m^3*

3. ***Template allows saving the algorithm of data transformation from source to target but not the numerical values of parameters because they may be unique for every data set. Therefore you should enter proper values of additional parameters for each data file to be converted.***

6 Loading species concentrations data

To input concentrations data, choose the **{C} Input** stage using the Back or Next button (the current conversion stage is marked in the conversion process chain). The dialog is very similar to one for input a main data. See also Converting data of reaction calorimetry

If there is no concentration data then just click the **Next** button.

Note

This stage is only available if Reaction calorimetry experiment type is chosen when preparing a {Q} Template.

7 Preparing the {C} template

To prepare a template for concentrations data, choose the **{C} Template** stage using the Back or Next button (the current conversion stage is marked in the conversion process chain). The dialog is very similar to one for preparing a template for main data. See also Converting data of reaction calorimetry

Note

This stage is only available if Reaction calorimetry experiment type is chosen when preparing a {Q} Template.

8 Creating an output file

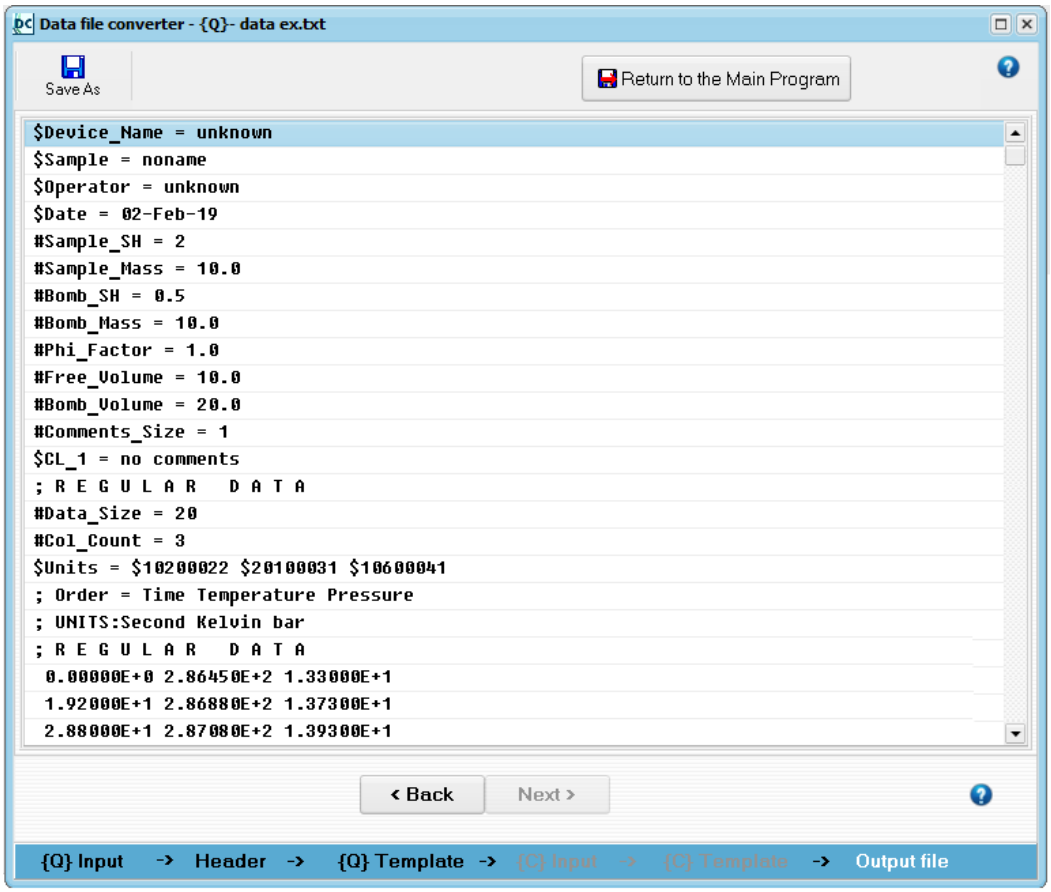
To work with an output file choose the **Output File** pane using the Next button (the current conversion stage is marked in the conversion process chain).

If Converter encounters some mistakes in input file (some obligatory data are missing, etc.), the warning message will appear. Usually this message signals about invalid items in an input data. Look it through and try to correct the values.

In the case everything had been done correctly you will be asked

Are you sure that your template matches data?.

Answer **Yes** to continue or **No** to modify something. When your answer **Yes** the program will convert data and show the output file



Saving An Output File

When the Converter has been launched as an autonomous program the toolbar contains the **Save as** button. To save the results of conversion press it. The Save dialog box will appear The suggested extension depends on the type of experiment you have set. The extension is important because it defines the software that will process the Converter output file further:

- ARKS AC/ADaExpert works with the files having an **.adp** extension.
- ARKS TA/TDpro works with the files having a **.tdp** extension.
- ARKS RC/RCPro works with the files having an **.rcp** extension.

If you launched DConv in spawned mode, i.e. launch it from the ARKS AC/TA or RC program there is no need to save data. Just press the **Return to the Main Program** button on the right of the toolbar to transfer data into the main program. DConv will be closed and you will find your converted data in the chart of the main program. Nevertheless you can save data in a separate file as in the case when DConv works in an autonomous mode.

9 Examples of Data Conversion

The following examples represent several typical cases and can help in understanding the technique of data conversion.

Three examples are included:

- conversion of DSC data when the original data don't contain all the necessary information
- conversion of DTA data when transformation of original Ts-Tr signal to heat release rate is required
- conversion of data of reaction calorimetry that contain as thermal responses as concentration responses.

9.1 Converting DSC data that don't contain time

The original DSC data contains only the {dQ/dt}, W/g, (specific DSC signal), {Q}, J/g (heat production) and {Tr} (reference temperature) arrays, heating rate, b, is defined, but time data are missing. Let us suppose that temperature data are placed in Column 1, DSC - in Column 2 and Q - in Column 3 (c1, c2 and c3 on the keypad of the Output Column Definition Form).

As heat production can be calculated later by ARKS TA we will use this column to create the target column with times.

ATTENTION !

The original data table should contain at least 3 columns. The extra column will be required for creating the time array. If the original data file contains only two columns (e.g. {dQ/dt} and {T]) you will have to add one more column with arbitrary data; you can, e.g., duplicate the {T} column. This can easily be done in MS Excel.

After data conversion we should obtain the necessary set of data: {time}; {DSC data} (absolute values instead of specific ones), and {reference temperature}. Therefore we will use the following relationships for data transformation:

$$t_i = (T_{r,i} - T_{r,o}) / \beta; \quad [dQ/dt]_{i,target} = [dQ/dt]_{i,source} \cdot M$$

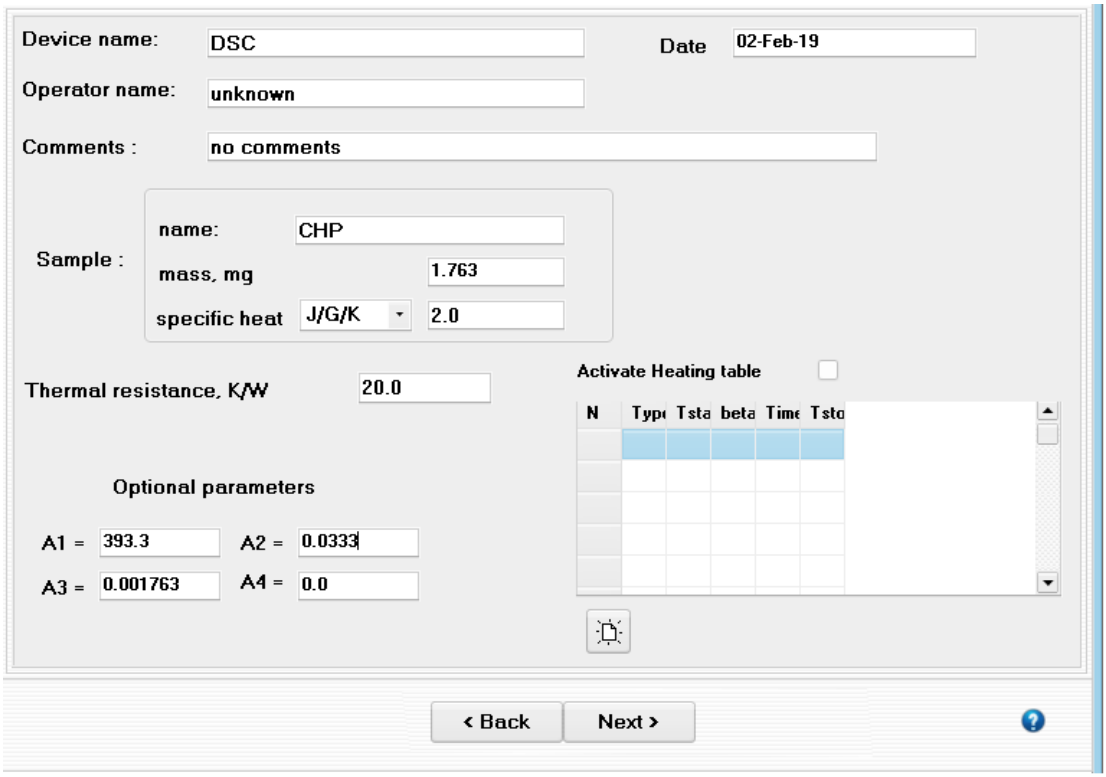
where i is the number of an experimental point; Tro is temperature for the first data point; M is sample mass; target and source indices correspond to the output and input (original) values. The formula for time calculation is used because the experiment has been carried out at linear heating, i.e. the rate of temperature raise was constant.

According to the rules of data transformation, Tro, b, and M should be defined in the Header as additional parameters. Let ***a1=Tro, a2= β, and a3 = M***.

Note

Transformations will be implemented for data in basic units (temperature – in K, time – in s, heat production rate – in mW) therefore Tro should be given in K, b - in K/s, and M - in g.

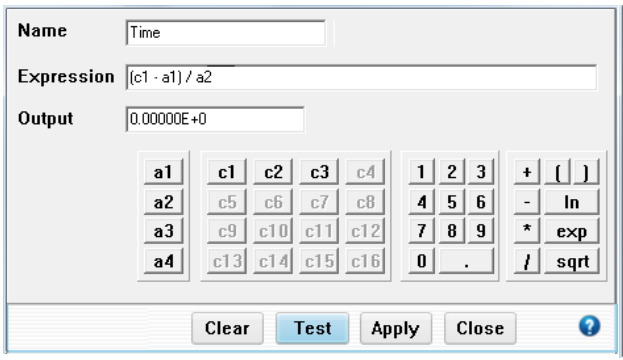
The Header window with all necessary data entered for DSC is shown below:



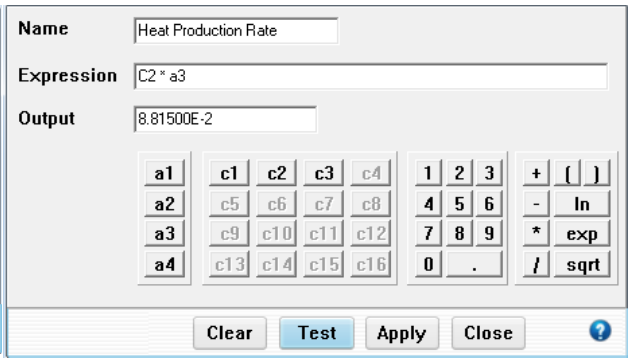
Note

Original DSC data are given in W/g. The Converter doesn't support specific values. Therefore while determining the source columns DSC units should be defined as Watt. Then DSC data will be converted to mW. As a result DSC data will be in mW/g. Hence M should be defined in grams.

In our case the Output Column Definition Forms for {time} and $[dQ/dt]_{out}$ calculation will be as follows:

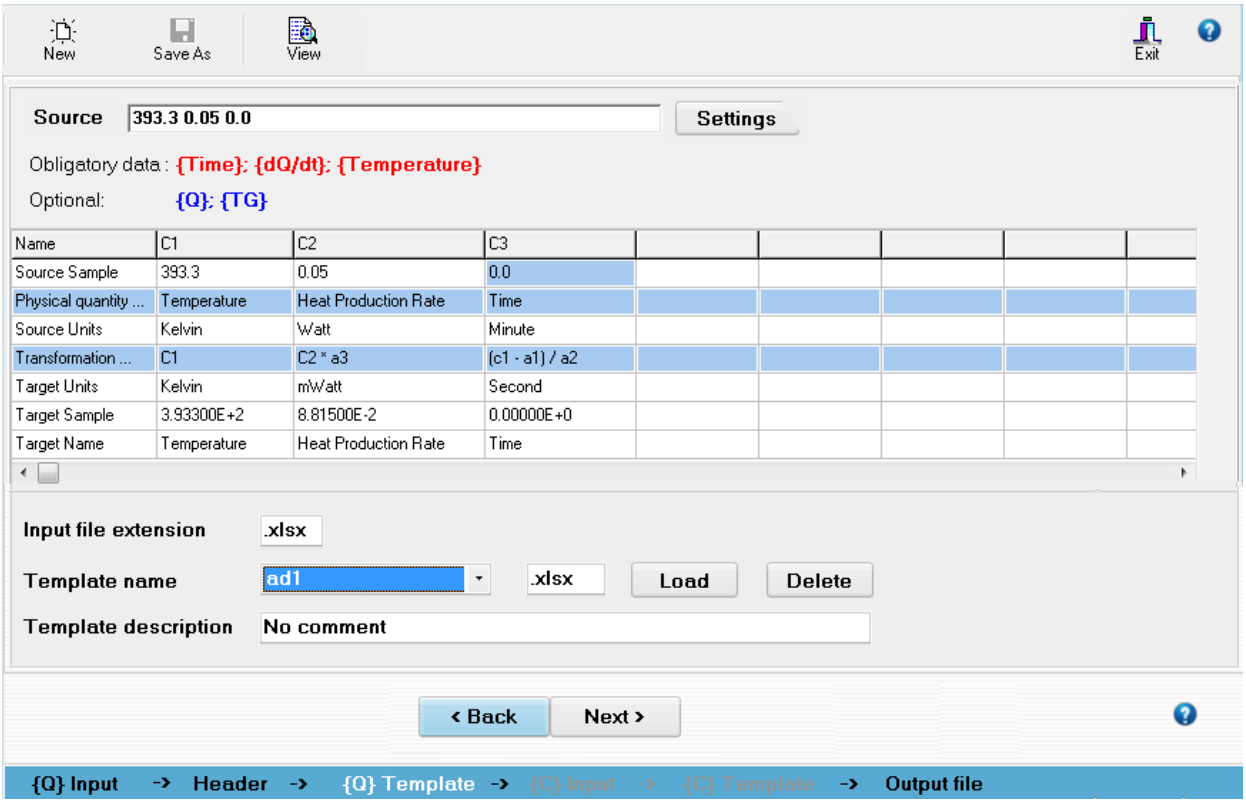


The **Output Column Definition** Form: defining Time target column



The **Output Column Definition** Form: defining dQ/dt target column .

The final content of the Template Editor window is as follows:



Notes

1. ***As it was mentioned the third source column contains heat production but we defined it as time because we need the target column with times***
2. ***The order of target columns is optional therefore there won't be any problem that the first column is Temperature instead of time which seems more natural.***

9.2 Converting DTA data

Consider now the case when DTA data are to be converted. An original file contains: {time}, {sample overheating, $\Delta T_s = T_s - T_r$ }, and {reference temperature, T_r) arrays.. Let us suppose that time, overheating and temperature data are placed in Column 1, Column 2, and Column 3 respectively (c1, c2 and c3 on the keypad of the Output Column Definition Form).

ATTENTION !

The original data table should contain at least 4 columns. The extra column will be required for creating the sample temperature array. If the original data file contains only 3 columns (e.g. {time}, {sample overheat} and {Tr]) you will have to add one more column with arbitrary data; you can, e.g., duplicate the {Tr} column. This can easily be done in MS Excel.

After data conversion we should obtain the set of data: {time}; {heat production rate, dQ/dt}, and {sample temperature, T_s}. Therefore we will use the following relationships for data transformation:

$$\frac{dQ}{dt} = (US)\Delta T_s; \quad T_s = \Delta T_s + T_r$$

where *(US)=a1+ a2* T_r* - overall heat transfer coefficient defined as a function of T_r .

Notes

1. ***As dQ/dt in output file must be presented in mW we should define overall heat transfer coefficient, (US), in mW/K.***
2. ***For DTA experiments the sample overheating may be big enough therefore the most correct method of assigning the temperature mode is to define the sample temperature rather than a heating table that describes properly furnace or reference temperature but not the sample temperature***

The Header window with all necessary data entered is presented in Fig. 1:

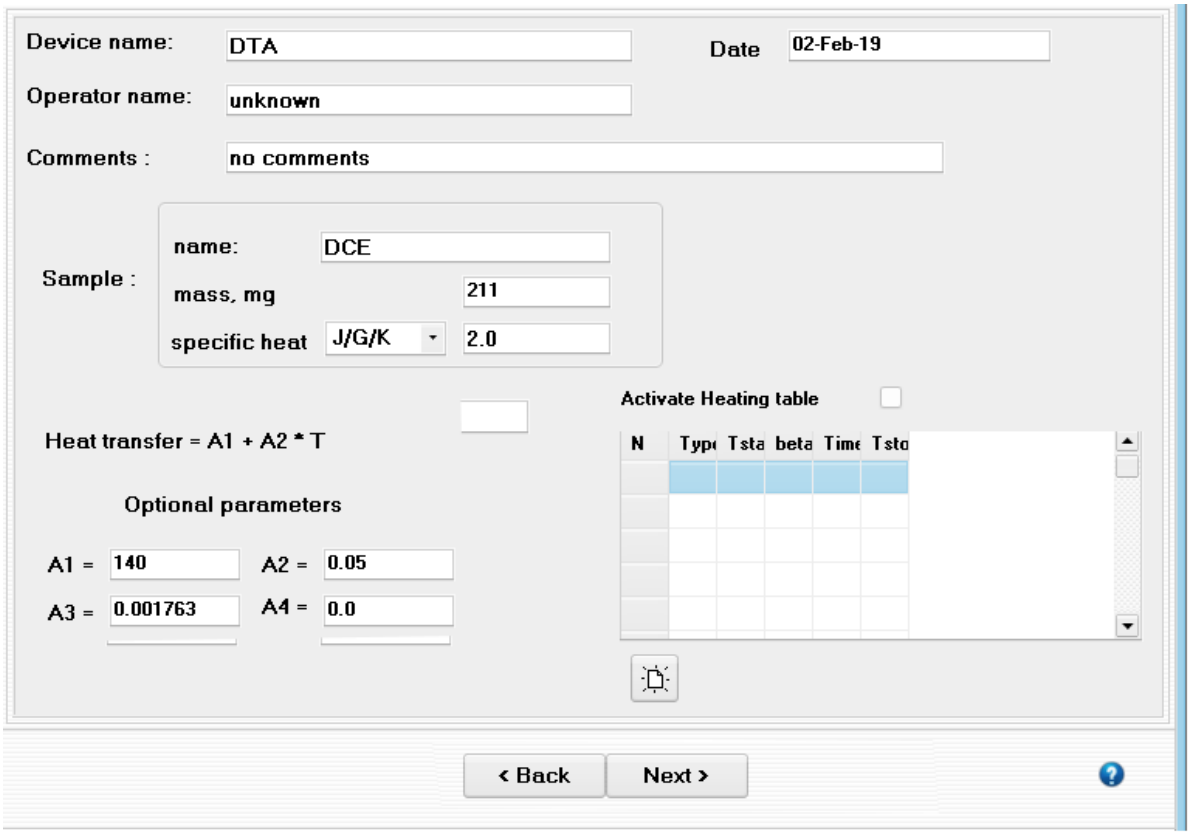


Figure 1 . The **Header** Window: data of DTA type.

In this case the Output Column Definition Forms for $[dQ/dt]_{out}$ and $\{T_s\}$ calculation will be as follows:

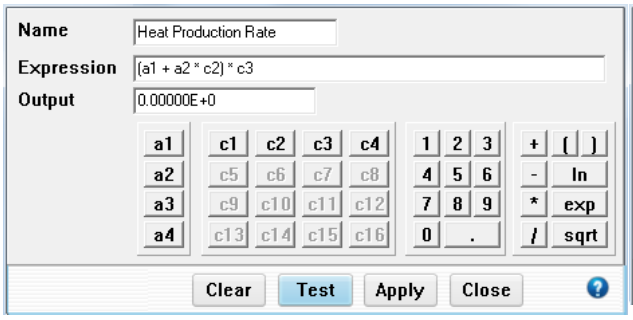


Figure 2 The **Output Column Definition** Form: defining dQ/dt target column .

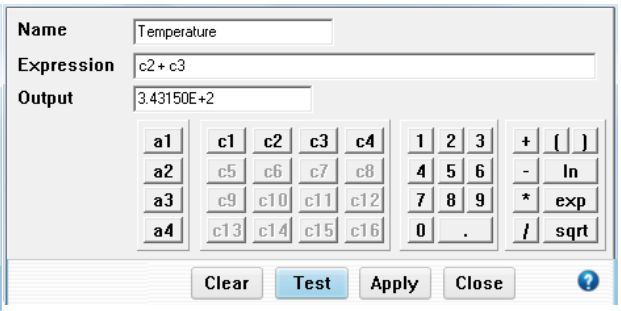


Figure 3 The **Output Column Definition** Form: defining T_s target column

The final content of the Template Editor window is shown in Fig. 4

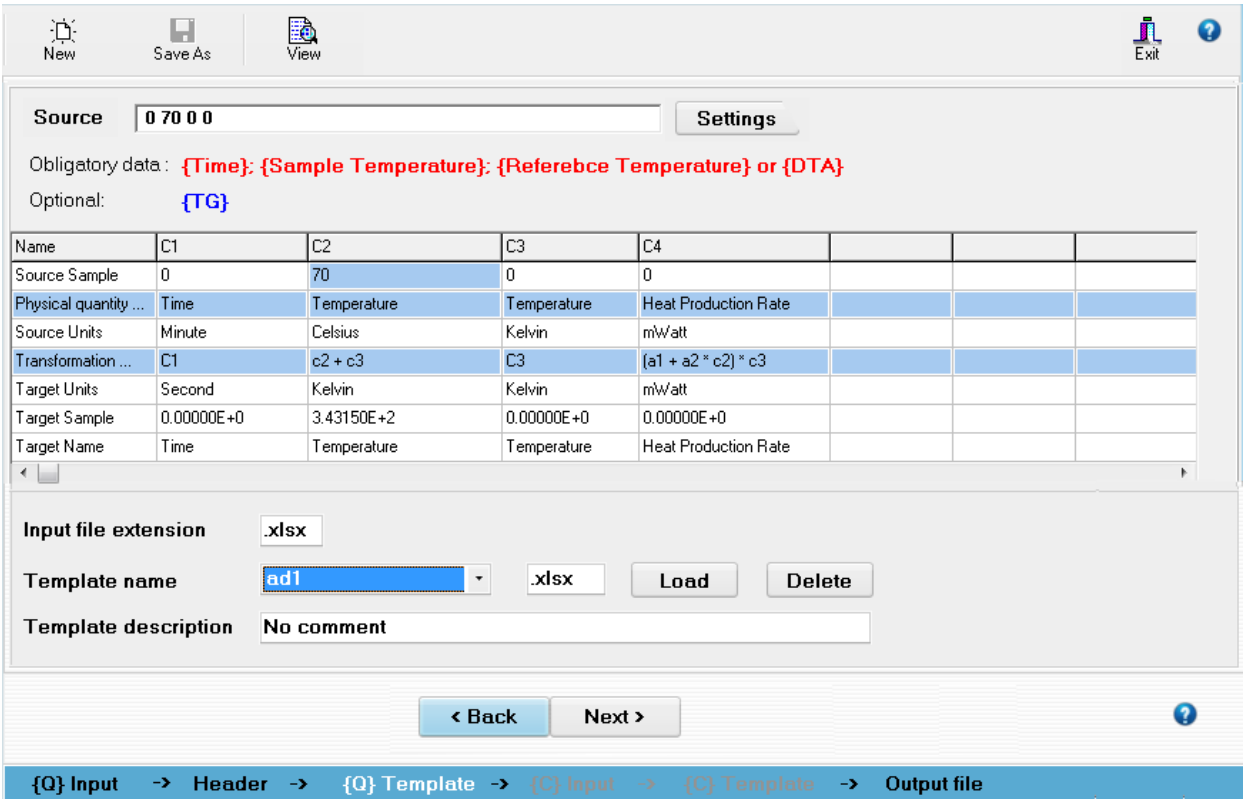


Figure 4 . The **Template Editor**: creating the template is completed.

9.3 Converting data of reaction calorimetry

Preparing data of reaction calorimetry that may include concentration responses is more complex procedure; it differs in many aspects from the methods of handling data of scanning or adiabatic calorimetry, therefore we will demonstrate it in more details.

Experimental data on esterification reaction

Isopropyl aclcohol (IP) + propionic anhydride (PA) -> isopropyl propionate (IPA) + propionic acid (Pac)

will be used as an example. The reaction calorimeter with 1 l vessel was used for investigation. Jacket temperature 70 ^{o}C was kept constant during the semi-batch experiment.

Initially the vessel was filled with 300 cm^3 of isopropyl alcohol (IP) at the same initial temperature 70 ^{o}C.

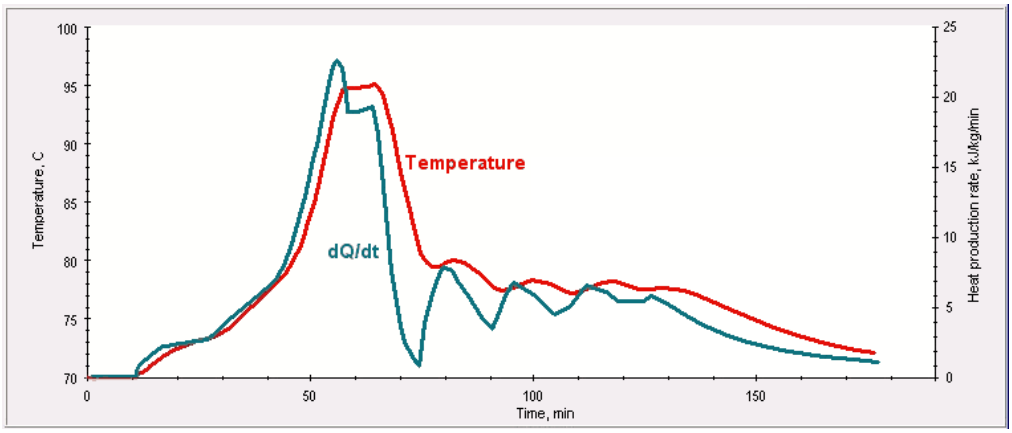
Propionic anhydride (PA) was fed in 8 portions (pulses):

- Duration of the pulse – 6 min;
- Pause between pulses – 10 min;
- Volume of the component added during 1 pulse – 60 cm^3;
- The first pulse started after a lapse of 10 min (equilibrium time).

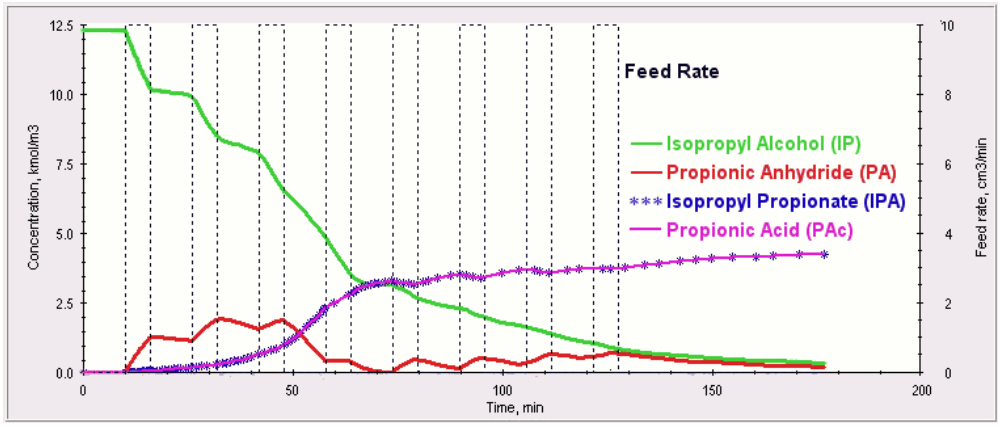
The following variables (responses) have been measured:

- Temperature of the reacting mixture Ts (in ^{o}C)
- Heat production rate dQ/dt (in J/min)
- Concentrations of IP, PA, IPA and Pac (in kmol/ m^3).

The available T, dQ/dt and concentration responses are presented in Fig. below



Temperature and heat production rate

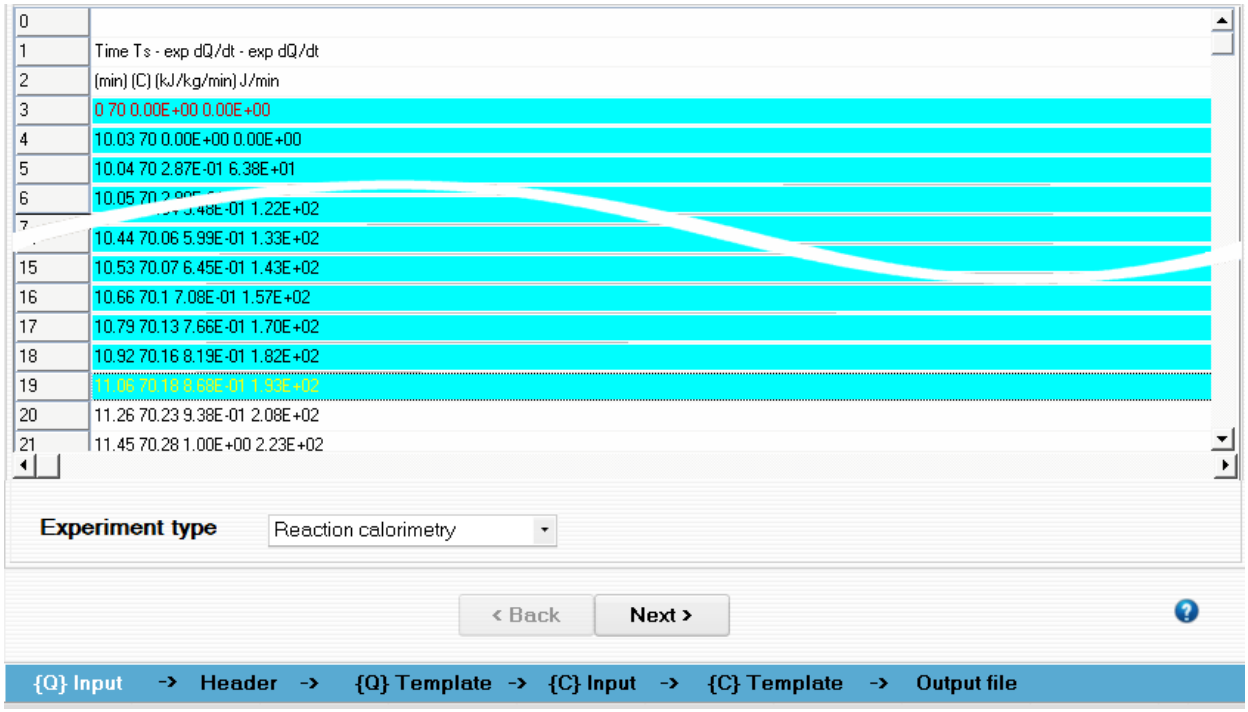


Concentration responses and feed profile

Processing data of reaction calorimetry comprises three steps – defining general data (header), preparing thermal responses and preparing concentration responses.

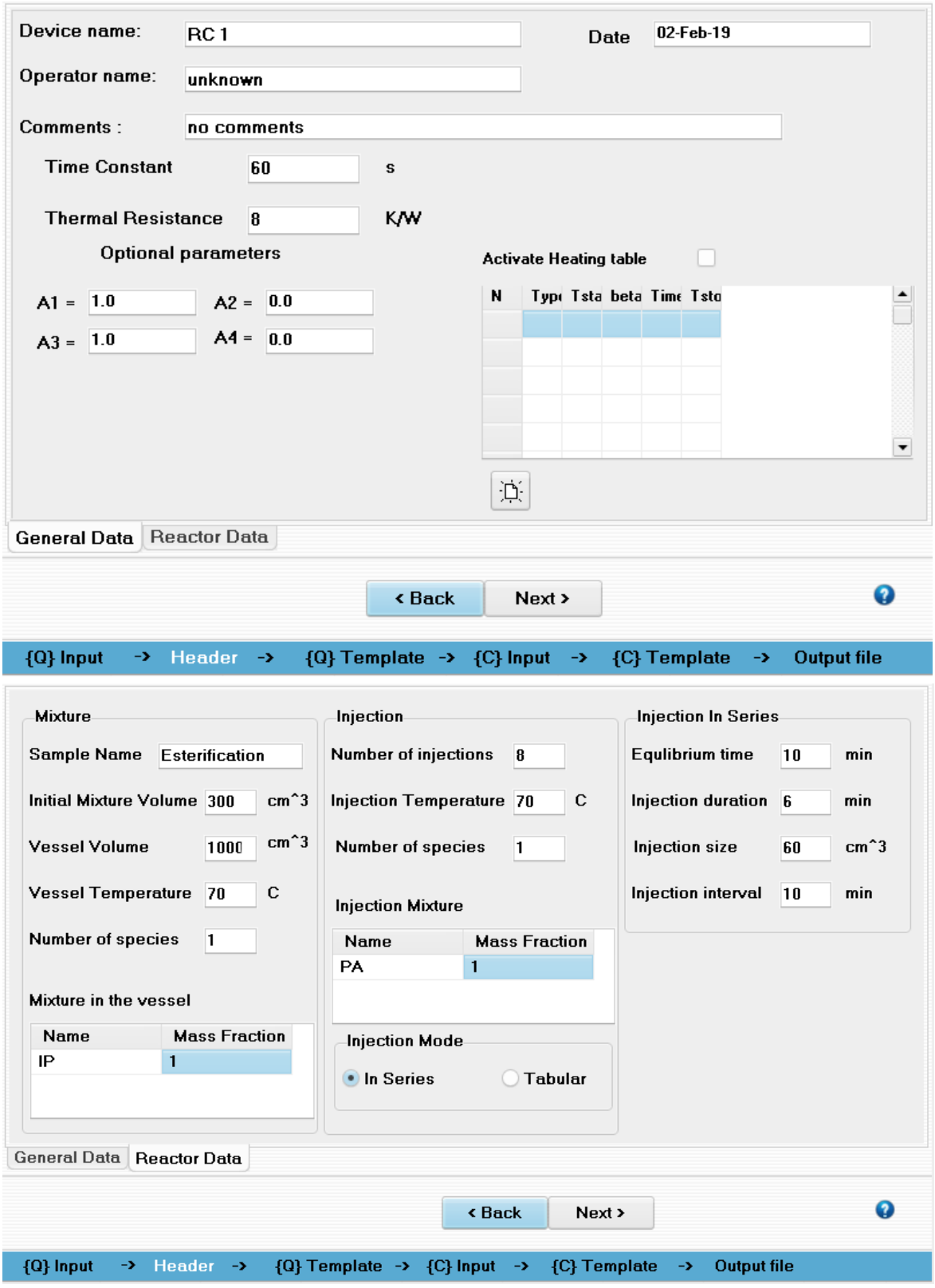
9.3.1 Preparing the header

At first thermal responses (time, temperature and heat production rate) should be loaded (or pasted from the clipboard) in a usual way using the facilities of the {Q} Input window, the first and the last lines of data table should be marked, and the appropriate experiment type should be selected:



Q-input window with thermal responses

The Header for data of reaction calorimetry requires detailed initial information about the experiment. The completed headers are presented below:



There is the set of obligatory data. It includes:

- Initial mixture volume;
- Vessel volume
- Vessel temperature (initial temperature of a mixture)

- Number of species in the initial mixture (at least one species should be defined)
- Initial composition of a mixture in the vessel

Other parameters are optional. Specifically, if the experiment is carried out in the BATCH mode one should only define number of Injections=0.

If the temperature response is unavailable the jacket or mixture temperature can be defined in the tabular form as in the case of DSC data. Check the Activate Heating table checkbox to be able to define temperature profile.

9.3.2 Preparing thermal data

Thermal data (i.e. time, heat production rate, temperature, pressure) are treated in the same way as in the case of DSC or adiabatic data. The Template window is shown in Fig. 5

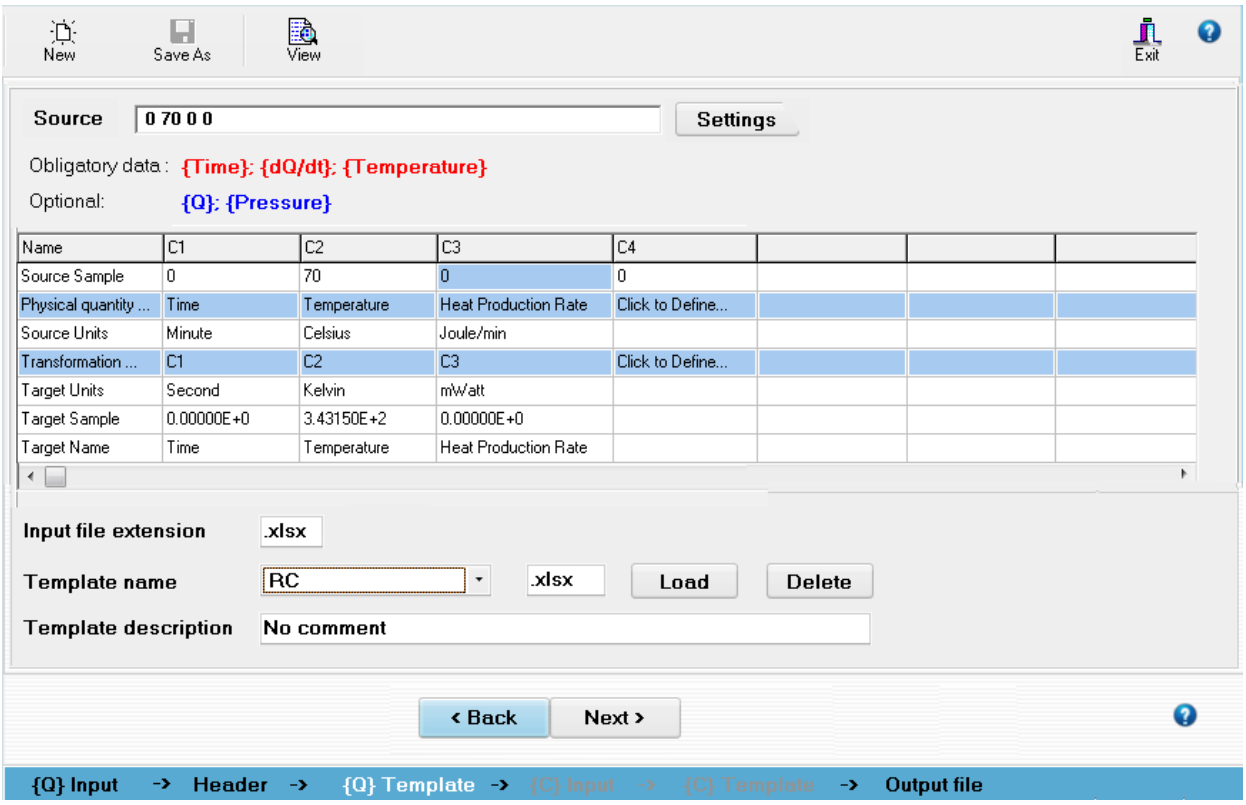


Fig. 5 The template for thermal responses

9.3.3 Preparing concentration responses

First the concentration responses should be loaded using the options of the {C} input window (Fig. 6).

Note

Concentration responses can be presented on the time grid that differs from the time grid of thermal responses. It is always assumed the time grid for all the concentration responses is the same.

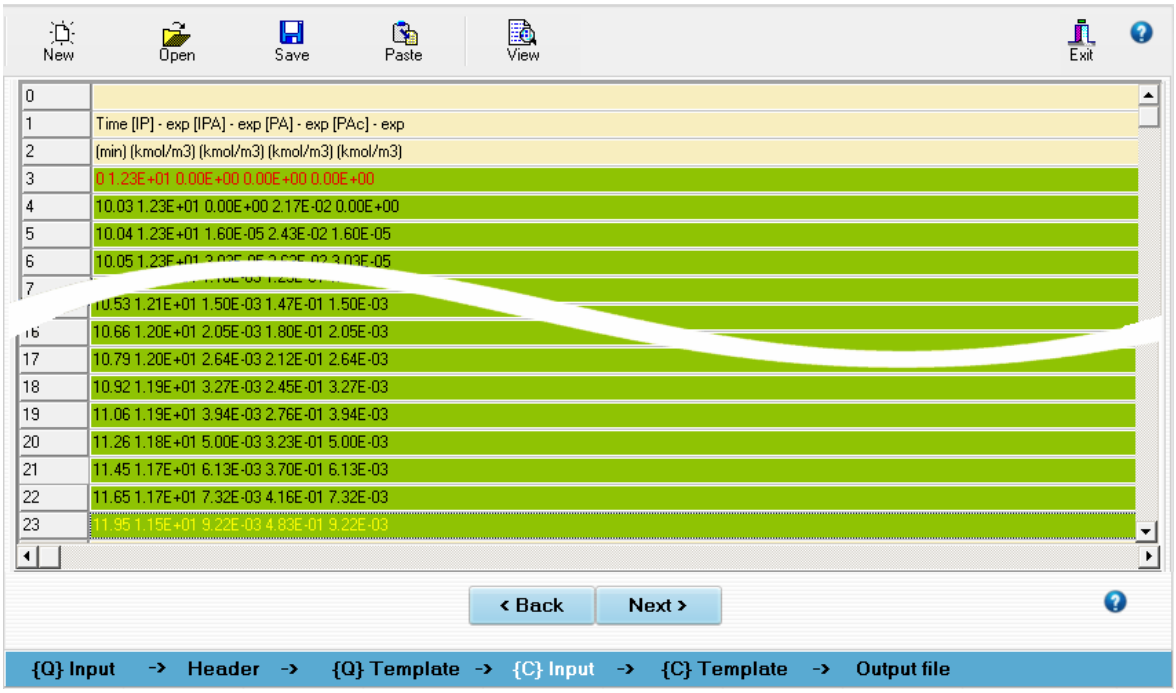


Fig. 6 The {C} Input window with the concentration responses loaded

Then the template for concentration responses should be prepared, that is the Source/Target Table should be defined (Fig. 7). The template for concentration responses can be saved separately from the template for thermal responses.

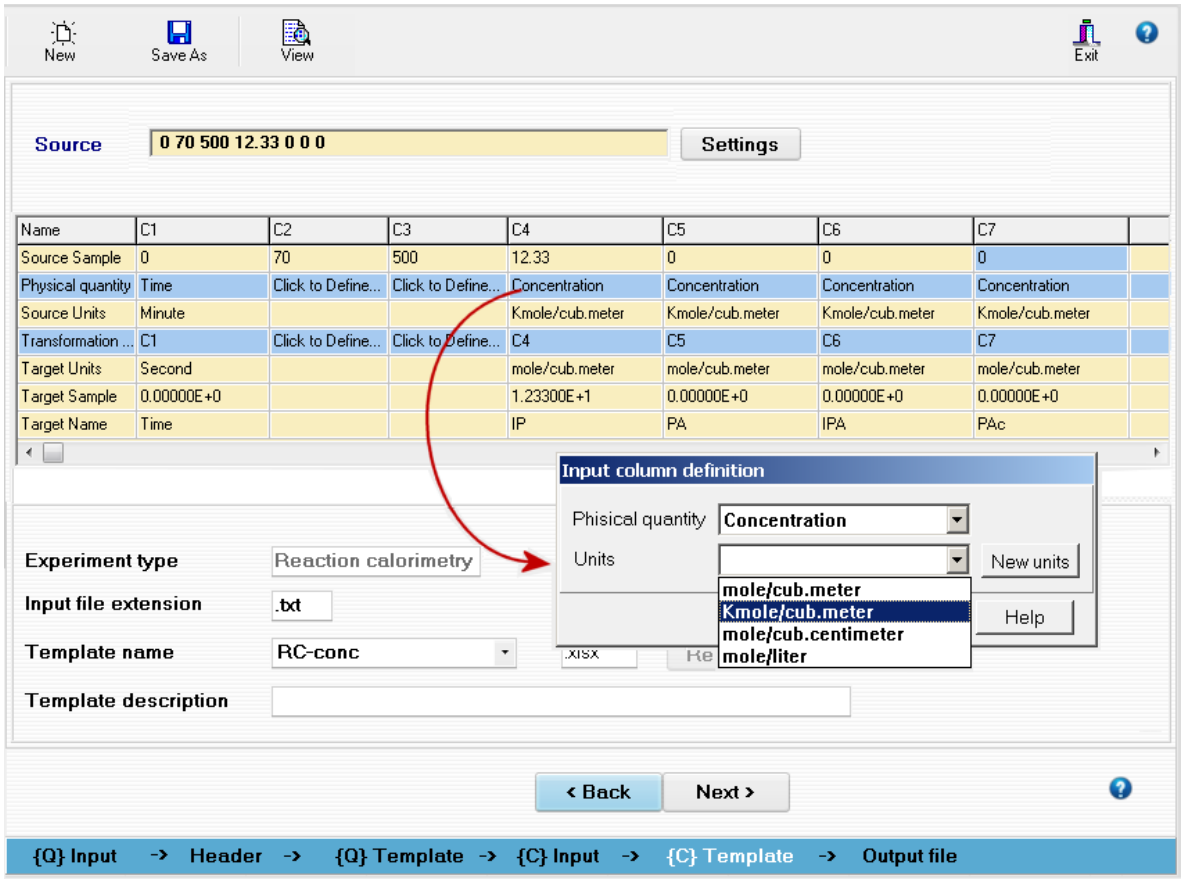


Fig. 7 Template for concentration responses. Highlighted is the list of available units for concentrations.

Now data are ready for converting and transferring into the RCPro program for further processing.

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