CpFit program

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Contents

Chapter 1

Thermodynamic Model

CpFit program implements thermodynamic model of heat capacity and other thermodynamic functions based on usage of Einstein-Plank functions sum and empirical parameters. The used approach has been developed by Voronin et al. [1].

All thermodynamic functions (e.g. heat capacity, entropy and enthalpy) are represented as sums of Einstein-Plank terms:

$$C_p(T) = \sum_{i=1}^{m} \alpha_i C_{\mathrm{E}} \left(\frac{\theta_i}{T} \right); \ \frac{C_{\mathrm{E}}(x)}{R} = \frac{3x^2 e^x}{(e^x - 1)^2} \tag{1.1}$$

$$S(T) - S(0) = \sum_{i=1}^{m} \alpha_i S_{\mathrm{E}} \left(\frac{\theta_i}{T} \right); \ \frac{S_{\mathrm{E}}(x)}{R} = 3 \left[\frac{x}{e^x - 1} - \ln\left(1 - e^{-x}\right) \right] \tag{1.2}$$

$$H(T) - H(0) = \sum_{i=1}^{m} \alpha_i \left[U_{\mathrm{E}} \left(\frac{\theta_i}{T} \right) - U_0 \right]; \ \frac{U_{\mathrm{E}}(x) - U_0}{RT} = \frac{3x}{e^x - 1} \tag{1.3}$$

where α_i and θ_i are adjustable (usually by means of the least squares method) model parameters. They can be estimated from experimental data using least squares method. A universal gas constant value $R = 8.3144598\ \mathrm{J \cdot mol^{-1}K^{-1}}$ from CODATA 2014 is used in the CpFit program. In eq 1.1, 1.2 and 1.3 α_i values are dimensionless and θ_i values are expressed in K.

The thermodynamic model of heat capacity based on Einstein-Plank functions allows to approximate $C_p(T)$, $S(T) - S(0)$ and $H(T) - H(0)$ in a wide temperature range using a unified set of parameters. Also unlike polynomial models it can give a physically correct extrapolation to a wider temperature range.

Implementation of this model in CpFit hides all analytical expressions and technical details and allow to use it as an ordinary statistical package for a nonlinear regression.

Chapter 2

Optimization Procedure

2.1 Theory

In CpFit program α_i and θ_i parameters are found by the least squares method using the next sum of squares χ^2:

$$\chi^2(\beta) = \sum_{i-1}^{n} W_i^2 \left[C_{p,i}^{\text{calc}}(\beta) - C_{p,i}^{\text{exp}}\right]^2 \tag{2.1}$$

where $W_i = \omega_i$ for the case of absolute deviation or $W_i = \omega_i \left(C_{p,i}^{\text{exp}}\right)^{-1}$ for the case of relative deviation where ω_i are user-defined statistical weights (default values are $\omega_i = 1$) and β is generalized notation for the α_i and θ_i model parameters. To minimize χ^2 value Levenberg-Marquardt algorithm implementation from `levmar` library [2] are used.

Standard deviations of the α_i and θ_i parameters are calculated using the next formula:

$$s_\beta^2 = \hat{\sigma}^2 \text{diag}\left[\left(J^\top J\right)^{-1}\right];\ J_{ij} = \frac{\partial c_p(T_i)}{\partial \beta_j};\ \hat{\sigma}^2 = \frac{\chi^2}{n - 2m} \tag{2.2}$$

where J is Jacobian, n is number of experimental points, m is number of terms (and $2m$ is number of parameters respectively), $\hat{\sigma}^2$ is the model standard error. Parameters confidence intervals can be estimated as:

$$\Delta\beta = s_\beta \cdot t_{p,f};\ f = n - 2m \tag{2.3}$$

where $t_{p,f}$ is t-distribution two-sided quantile with probability p (CpFit uses $p = 0.95$ for 95 % confidence intervals), $f = n - 2m$ is number of freedom degrees. Usually $t_{\alpha,f} \approx 2 \div 3$.

CpFit also can estimate standard deviations of thermodynamic functions that can be used to estimate their confidence intervals (don't mix with prediction intervals!) using the next formula:

$$s_{C_p}(T) = \sqrt{J_x^\top C J_x} = \hat{\sigma}\sqrt{J_x^\top \left(J^\top J\right)^{-1} J_x} \tag{2.4}$$

where C is covariance matrix, $J_x = J_x(T)$ is column vector that has the next layout:

$$J_x(T) = \begin{pmatrix} \frac{\partial C_p(T)}{\partial \beta_1} \\ \vdots \\ \frac{\partial C_p(T)}{\partial \beta_{2m}} \end{pmatrix} = \begin{pmatrix} \frac{\partial C_p(T)}{\partial \alpha_1} \\ \frac{\partial C_p(T)}{\partial \theta_1} \\ \vdots \\ \frac{\partial C_p(T)}{\partial \alpha_m} \\ \frac{\partial C_p(T)}{\partial \theta_m} \end{pmatrix} \tag{2.5}$$

Confidence intervals of the $C_p(T)$ function at the point (T) can be calculated using the next relationship similar to eq 2.3:

$$\Delta C_p = s_{C_p} \cdot t_{p,f};\ f = n - 2m \tag{2.6}$$

2.2 Practical Tips

The goal of the optimization process is to minimize the model standard error $\hat{\sigma}^2$. However during increasing the number of parameters there is a risk to obtain an ill-conditioned task and not reliable values set. To avoid it you can follow the next tips:

1. Begin the optimization for 2–3 terms (or 4–6 parameters) and gradually increase it using previous results as initial approximations
2. Avoid statistically not significant coefficients (i.e. the conditions $\alpha_i \geq \Delta\alpha_i \approx 2s_{\alpha_i}$ and $\theta_i \geq \Delta\theta_i \approx 2s_{\theta_i}$ should be satisfied). CpFit program will automatically highlight in red statistically not significant coefficients (see Figure 4.2).
3. Both α_i and θ_i must be positive numbers (automatically controlled by the CpFit optimization engine).

You can also use evaluations procedures with automatic selection of terms number (see Chapter 4.2). They use iterative addition of new terms and control of statistical significance of them using t-criterion. However they sometimes can give number of terms less than can be obtained by manual selection of initial approximations.

Chapter 3

File Formats

3.1 Experimental data file format

Input data can be supplied in human readable text files with `.dat` extension. A description of the format is present in Table 3.1.

The main features of the format are:

- .dat file is an ordinary ASCII text file
- Dot (and only dot) is used as a decimal separator
- Both DOS/Windows and UNIX line endings are supported
- Numbers are separated by either spaces or tabs (one or multiple)
- Empty lines in the data set are ignored without warning

3.2 Model parameters file format

Files with model parameters can be either exported from the Results Window or imported to the Main Window. That files have `.csv` format, semicolon `;` is used as a separator and dot `.` is used as a decimal point sign. An example of the `.csv` file with model parameters is given below:

```
alpha;dalpha;salpha;theta;dtheta;stheta
14.0168725905787;0.914895;0.457827;3583.8945135367;151.031;75.5782
6.26905917915019;0.401292;0.200813;1393.30718925711;88.5056;44.2895
7.3042223855265;0.350348;0.175319;688.948063566627;41.8236;20.9292
5.69813172425687;0.238324;0.119261;306.421049769356;20.2346;10.1257
2.86883301382133;0.329537;0.164905;145.550553624711;12.1593;6.0847
0.289410000831521;0.171896;0.0860195;66.9793881821218;12.0881;6.04905
```

The first row contains columns description and can contain the next values:

- `alpha` — α_i model parameter, dimensionless.
- `dalpha` — $\Delta\alpha_i$, 95 % confidence interval (using two-sided t-distribution quantile) for the model parameter α_i.

Table 3.1: .dat file format used by CpFit

Line number	**Example**	**String content**

1–3	`Heat capacity (ScF3)`
	`Temperature`
	`Cp`
		Arbitrary text information

4	`539`	Number of dots
5	`0`	Reserved and should be equal to zero (intended to be a number of dots to be ignored at the end of file but it is not used now)

6–k	`303.35 82.806`
	`302.98 82.421  0  1`
	`303.01 82.417  1  0.85`
		Experimental data. Either T–C_p lines or T-C_p–rf–ω lines where ω are statistical weights from eq 2.1 and rf is "use relative deviation" flag (can be either 0 or 1). If ω or rf are omitted their default values will be used for this line ($\omega = 1$ and $rf = 0$).

- `salpha` — $s\left(\alpha_i\right)$ standard deviation for the model parameter α_i.
- `theta` — θ_i model parameter, K.
- `dtheta` — $\Delta\theta_i$, 95 % confidence interval (using two-sided t-distribution quantile) for the model parameter θ_i.
- `stheta` — $s\left(\theta_i\right)$, standard deviation for the model parameter θ_i.

Export from the Results Window (see Figure 4.2) gives all six columns. Import to the Main Window uses only two columns `alpha` and `theta`.

Chapter 4

User interface

4.1 Installation

CpFit program has the next system requirements:

- Microsoft Windows XP/Vista/7/8/8.1/10 (32-bit or 64-bit)
- 256 Mb of RAM
- 5 Mb of free disk space
- SVGA with 1024x768 resolution or higher

The program doesn't require any installation. You can just unpack an archive with the program and begin the work.

If you want to make the program from the source code (that is not required) you will need:

- GCC C++ compiler 4.5.2 or higher and MinGW environment
- wxWidgets 3.0.2 or higher
- levmar 2.6 or higher
- Doxygen is not required but highly recommended (to generate documentation about the source code)

More detailed information about compilation and linking is given in the source code.

4.2 Main window

Main window (see Figure 4.1) allows to load, save and edit experimental data and manage the parameters optimization process.

A menu of the main window contains the next items:

- **File** — Contains operations for loading and saving experimental data from and to files.
  - **New** — Clear all data in the window.

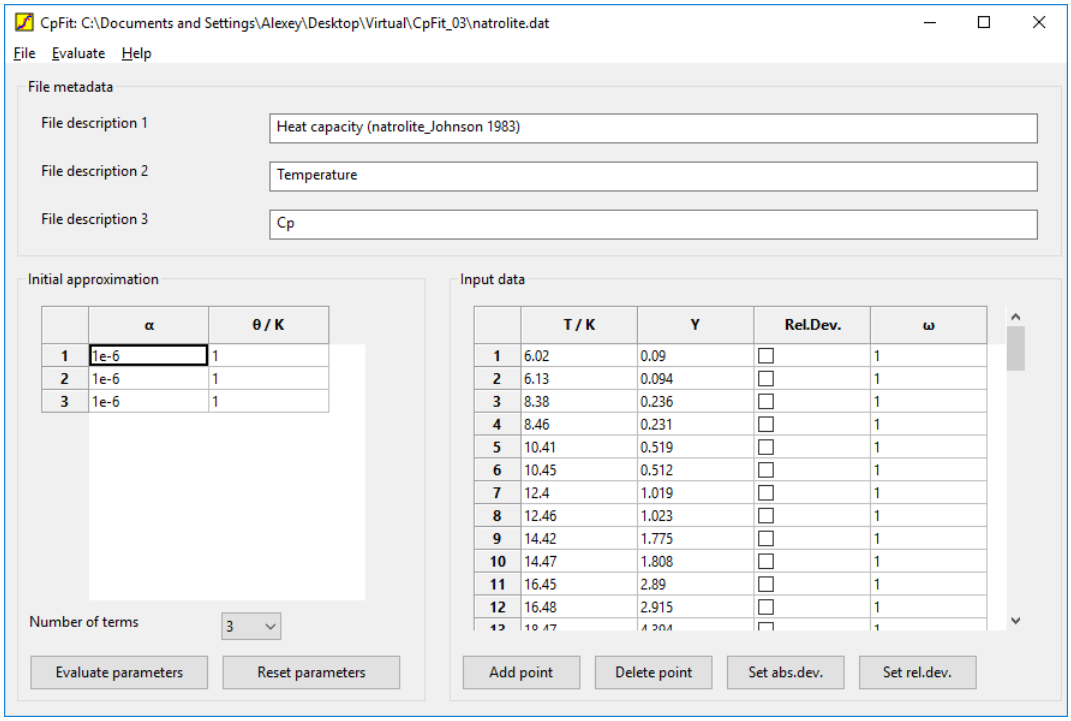

Figure 4.1: CpFit program main window

  - **Open** — Open `.dat` file with C_p data.
  - **Save as** — Save current data set into `.dat` file.
  - **Load parameters** — Loads parameters (i.e. initial approximation) from `.csv` file and puts them into an initial approximation table.
  - **Exit** — Close the main window and exit from the program.

- **Evaluate** — Different variants of the model parameters evaluation.
  - **Parameters values** — Evaluate only values, number of terms is fixed (similar to "evaluate parameters" button).
  - **Parameters set (don't use init.approx.)** — Evaluation of both number of terms and parameters values without using of an initial approximation given by a user.
  - **Parameters set (use init.approx.)** — Evaluation of both number of terms and parameters values with using of an initial approximation given by a user.
  - **Evaluate without optimization** — Creates results window with parameters given as initial approximation by a user but doesn't run any optimization process. Can be used without any experimental data. If experimental data are given the program will evaluate deviations and parameters confidence intervals.

- **Help** — Contains information about the program.
  - **About** — Show the window with a brief information about the program.

All evaluation methods that evaluate number of terms use the next algorithm:

1. Set initial approximation. CpFit can use either user-defined initial approximation (see Figure 4.1) or set it automatically. In the case of automatic selection one term with $\alpha_1 = 0.1$, $\theta_1 = 1$ will be used.

2. Run optimization for a given initial approximation and test an obtained set of parameters for statistical significance (using t-test with two-sided 95 % confidence intervals, see eq. 2.3).

3. If all parameters are statistically significant — add new term with $\alpha_i = 10^{-3}$ and $\theta = 1$ and go to the Step 2. If some parameters are statistically not significant — take the previous result of optimization and return it.

Such algorithm allows to obtain reasonable results in most cases. However in some cases it can give less model terms than possible and manual setting of an initial approximation consisting from several terms may be beneficial.

The main window contains three areas: file metadata area, initial approximation area and input data area.

File metadata area contains three arbitrary text strings that are used to describe a content of the data set. It is recommended to use the first line for data series description and leave default values in the second and in the third line.

Initial approximation area contains tools for setting initial values of model parameters and number of terms in eq 1.1, 1.2 and 1.3.

- *Table* — This table contains values for the model parameters. Each row correspond to the model term, α and θ / `K` columns correspond to α_i and θ_i parameters respectively. Note that the content of this table can be modified by results window (by means of transferring results into initial approximation area).

- *Number of terms* combo box — Use this combo box to select a desired number of terms.

- *Evaluate parameters* button — Runs a proces of the parameters optimization. Results window will be opened.

- *Reset parameters* button — Sets each α_i and each θ_i value in the table to 10^{-6} and 1 respectively.

Input data area contains the data set that will be used for model parameters optimization. It contains the next elements:

- *Table* — Contains the used data set and contains four columns. `T / K` is for temperature in K, `Y` is for C_p in $\mathrm{J} \cdot \mathrm{mol} \cdot \mathrm{K}^{-1}$, `Rel.dev.` is for absolute/relative deviation selection, ω is for statistical weights ω_i from eq 2.1.

- *Add point* button — Adds a new point into the table.

- *Delete point* button — Removes selected rows from the table.

- *Set abs.dev.* button — Sets all deviations for all points as absolute (i.e. unselects all checkboxes in the third row)

- *Set rel.dev.* button — Sets all deviations for all points as relative (i.e. selects all checkboxes in the third row)

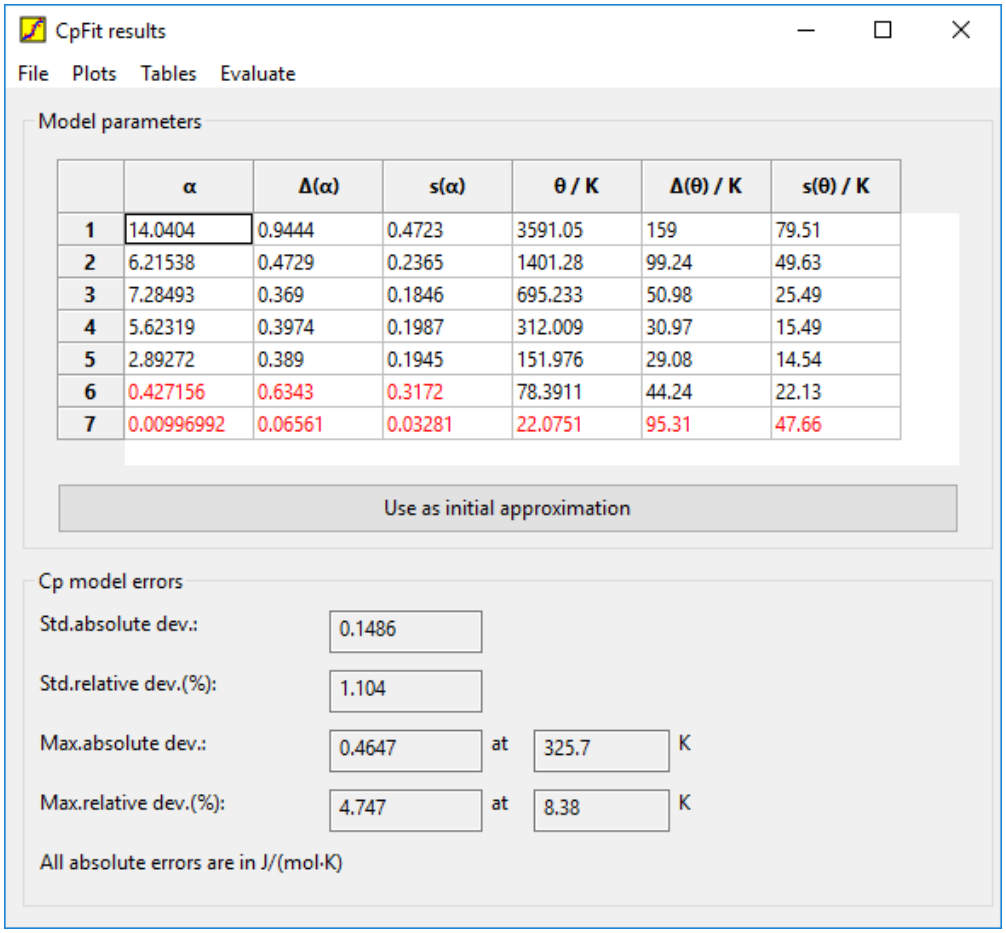

Figure 4.2: CpFit results window

4.3 Results window

Results window (see Figure 4.2) contains an optimized set of parameters. It allows to create reports, draw 2D plots and different tables using the optimized parameters.

A menu of the main window contains the next items:

- **File** — File input-output (exporting parameters to files)
  - **Save as CSV** — Exports optimized parameters into `.csv` file readable by MS Excel and another programs.
  - **Save as HTML** — Exports optimized parameters and model errors into `.html` file that can be considered as a report suitable for printing.
- **Plots** — Creation of plots (thermodynamic functions, absolute deviations, relative deviations). Every new plot will be opened in a separate window.
  - **Cp function** — Plots for the $C_p(T)$ function.
  - **Cp/T function** — Plots for the $C_p(T)/T$ function.
  - **H function** — Plots for the $H(T) - H_0$ function.

  - **S function** — Plots for the $S(T)$ function.

- **Tables** — Creation of tables with thermodynamic data in separate windows. All tables can be exported into `.csv` files.

  - **Thermodynamic functions** — Customizable table with tabulated thermodynamic functions values (and their confidence intervals). $C_p(T)$, $H(T) - H(0)$ and $S(T)$ functions are supported.
  - **Residuals** — Table with absolute and relative residuals for each experimental $C_p(T)$ point.

- **Evaluate** — Evaluates some extra properties and values useful for management of optimization procedure.

  - **Low-T S correction** — Allows to evaluate deviation of isobaric heat capacity $C_p(T)$ from Debye function at low temperatures. Such estimation can be used for correction of entropy values.

Results window contains two areas: model parameters area and Cp model errors area.

Model parameters area contains the optimized parameters of the model (α and θ), their standard deviations ($s(\alpha)$ and $s(\theta)$) and 95 % confidence intervals ($\Delta\alpha$ and $\Delta\theta$) calculated using eq 2.2 and eq 2.3 respectively. Each row correspond to one model term. Statistically not significant terms are automatically highlighted in red colour.

Cp model errors area contains information about accuracy of the optimized parameters data set present in the window. Note that all deviations are calculated without taking statistical weights ω_i from 2.1 into account (however they were used during the optimization).

4.3.1 Debye function

Evaluate — Low-T S correction menu item of *Results window* uses Debye model. In Debye model heat capacity is approximated by means of the next formula:

$$\frac{C_p^D(T)}{3NRT} = 4D\left(\frac{T_D}{T}\right) - \frac{3\frac{T_D}{T}}{\exp\left(\frac{T_D}{T}\right) - 1} \tag{4.1}$$

where N is the number of atoms in the compound, T_D is Debye temperature, $D(x)$ is Debye function:

$$D(x) = \frac{3}{x}\int_0^x \frac{y^3}{e^y - 1}\,dy \tag{4.2}$$

The next algorithm of entropy correction calculation is used:

- Get the lowest trusted point T_0 and $C_p(T_0)$ at the curve (i.e. Einstein-Plank model). T_0 is manually set by user and usually is 5–30 K. The user also must give N (number of atoms) value.
- Calculate T_D value by solving $C_p^D(T_0) = Cp(T_0)$ equation.
- Calculate $S^D(T_0)$ value using eq. 4.1.

Table 4.1: Terms colors in the $C_p(T)/T$ function plots.

Term number	**Color**
1	Black
2	Blue
3	Green
4	Cyan
5	Red
6	Magenta
7	Brown
8	Gray

4.4 Plots

CpFit 2-dimensional plot is a resizable window that can show experimental data points, analytical functions obtained by a nonlinear regression or both of them. They can also contain plots with absolute or relative deviations. Use results window to build new plots.

A menu of any 2D plot window in the CpFit program contains the next items:

- **File** — Export of the plot into graphic files.
  - **Save as** — Export into `.png` file with screen resolution.
- **Edit** — Figure customization and clipboard operations.
  - **Copy** — Copy the plot into Clipboard (in a vector format similar to Windows Metafile)

In the case of the $C_p(T)/T$ function plot extra dashed lines of different color that correspond to the function terms (see eq 1.1) are shown. A color of the line codes the term number (see Table 4.1).

You can also zoom in/zoom out plots using mouse wheel scrolling and drag-n-drop technique to navigate inside a zoomed plot.

4.5 Tables

Two kinds of tables can be constructed by CpFit: tables with tabulated thermodynamic values and tables with comparison of calculated and experimental values. Both of them can be exported into `.csv` file format (readable by Microsoft Excel).

4.5.1 Tabulated thermodynamic functions

This kind of table contains tabulated values for $C_p(T)$, $H(T) - H(0)$ and $S(T)$ thermodynamic functions. Every new table contains rows for default T values for $T = 10 \div 1000$ K and always contains a 298.15 K row. However a user can add or delete any rows with any step.

A menu of the tabulated thermodynamic functions table window contains the next items:

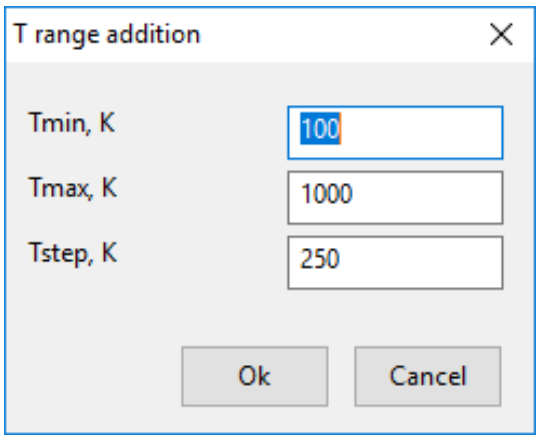

Figure 4.3: T range addition dialog

- **File** — File input-output (exporting table to files).
  - **Save as** — Export into `.csv` file.
- **Edit** — A customization of the table.
  - **Reset the table** — Removes all rows from the table.
  - **Add T range to the table** — Adds new rows for requested temperature range with requested step.

    When a user adds a new T range a special dialog shown in Figure 4.3 is opened. The user can set Tmin (minimal temperature), Tmax (maximal temperature) and Tstep (a step between new points). After the addition a table of tabulated values will be automatically sorted by the temperature.
  - **Errors estimation** — Allows to select the mode used for estimation of errors for tabulated S, H and C_p values.
    - **Standard deviation** — calculate standard deviations.
    - **95 % confidence interval** — calculate confidence intervals (95 % confidence intervals using two-sided t-distribution quantiles).

4.5.2 Calculated vs experimental

A menu of the residuals table window contains the next items:

- **File** — File input-output (exporting table to files).
  - **Save as** — Export into `.csv` file.

Chapter 5

Changelog

- 05 July 2017 — CpFit 0.4
  - Errors in columns name (`s(H-H0)` and `s(S-S0)` names mismatch) in `.csv` files containing exported tables of thermodynamic functions was fixed.
  - Some typos in the manual were fixed
  - Bibliographic references were added to examples (`natrolite.dat`), (`ScF3.dat`).
  - Low-temperature entropy correction (by means of Debye function) was added.
- 21 December 2016 — CpFit 0.3
  - Automatic search of model terms number was added.
  - t-test for model coefficients (for statistical significance) was added.
  - Negative values of the model cannot be obtained during an optimization now.
  - Confidence intervals for parameters and tabulated values (using two-sided 95 % quantile of t-distribution).
  - Improved export of tabulated values.
  - Zooming for 2D plots.
  - Loading of model parameters from `.csv` files.
  - Estimation of confidence intervals for user-supplied parameters.
- 31 October 2016 — CpFit 0.2 — First public version

Bibliography

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Chapter 6

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