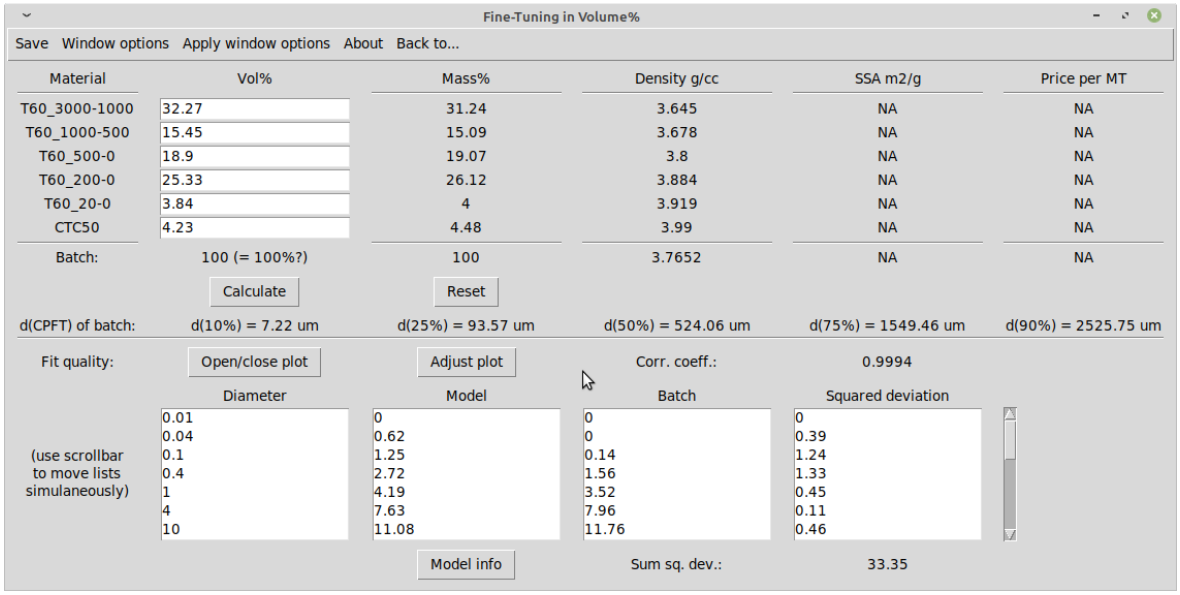
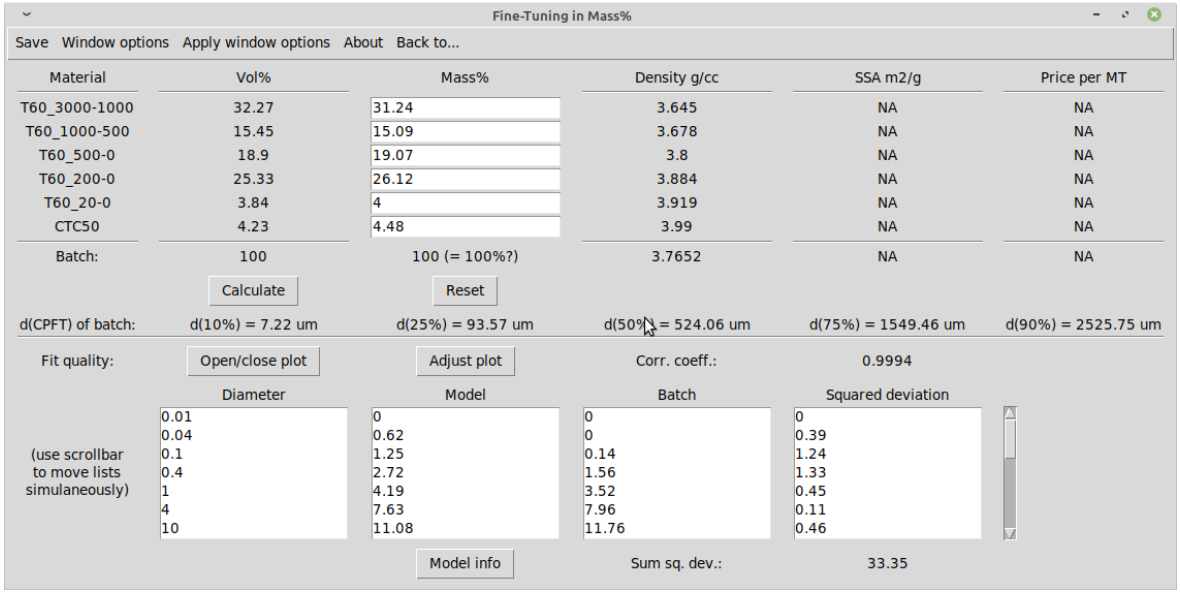
Fine-tuning of results of 'Design a batch' main function

The fine-tuning windows for either the vol% or wt% version differ only by the column which is editable, cf. Figure 1. The windows have an extended menu bar, followed by the results table containing the batch properties and in the lower part can be found a detailed comparison of the model and batch particle size distributions characterizing the quality of the fit.



(a) Vol% fine-tuning

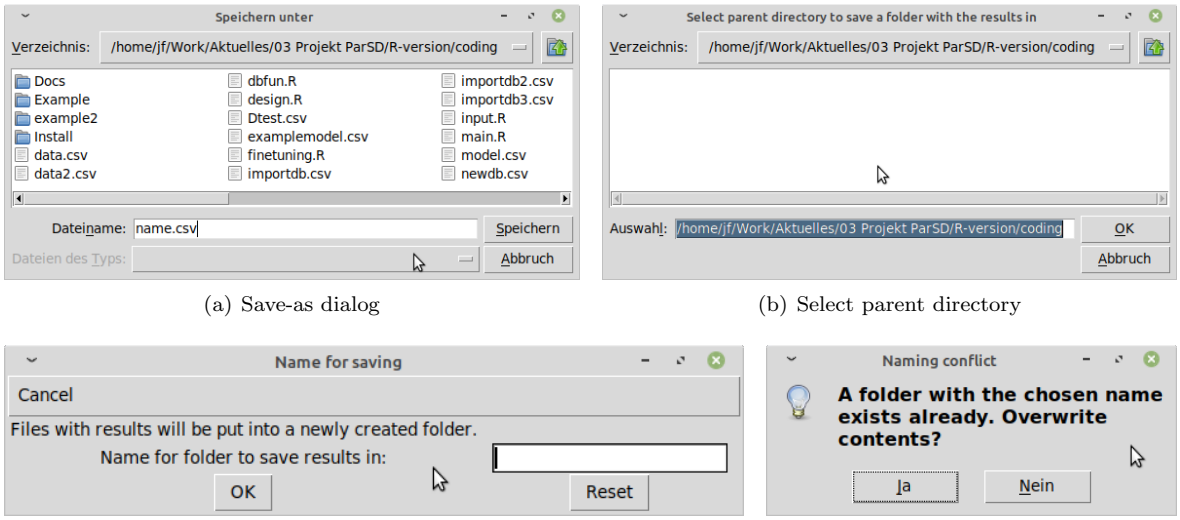


(b) Wt% fine-tuning

Figure 1: Fine-tuning dialogs for fine-tuning in vol% or wt%

The menu item 'Save' gives the user the possibilities to save the fine-tuned...

- recipe, which is a subset database containing the materials used for the present calculation. Has to be saved as CSV file in the Save-As window by adding the file extension to the filename as shown in Figure 2(a).
- batch, which is the table shown in the results window giving the contents of the materials. Has to be saved as CSV file in the Save-As window by adding the file extension to the filename as shown in Figure 2(a).
- model (comparison), which is the lower part of the results-window including information to the model (type and parameters). Has to be saved as CSV file in the Save-As window by adding the file extension to the filename as shown in Figure 2(a).
- graph, as adjusted and displayed by the 'Open/close plot' button. Has to be saved as PNG file in the Save-As window by adding the file extension to the filename (cf. Figure 2(a)).
- complete results (recipe, batch, model (comparison) & plot). In this case, a folder will be created into which the four files will be put. The user is asked to give the parent folder into which the new results folder should be placed (Figure 2(b)) and then to give a name for the results folder (Figure 2(c)). If a folder with this name already exists, the user is informed but can decide to overwrite the contents (Figure 2(d)).



(a) Save-as dialog

(b) Select parent directory

(c) Name results-folder

(d) Select parent directory

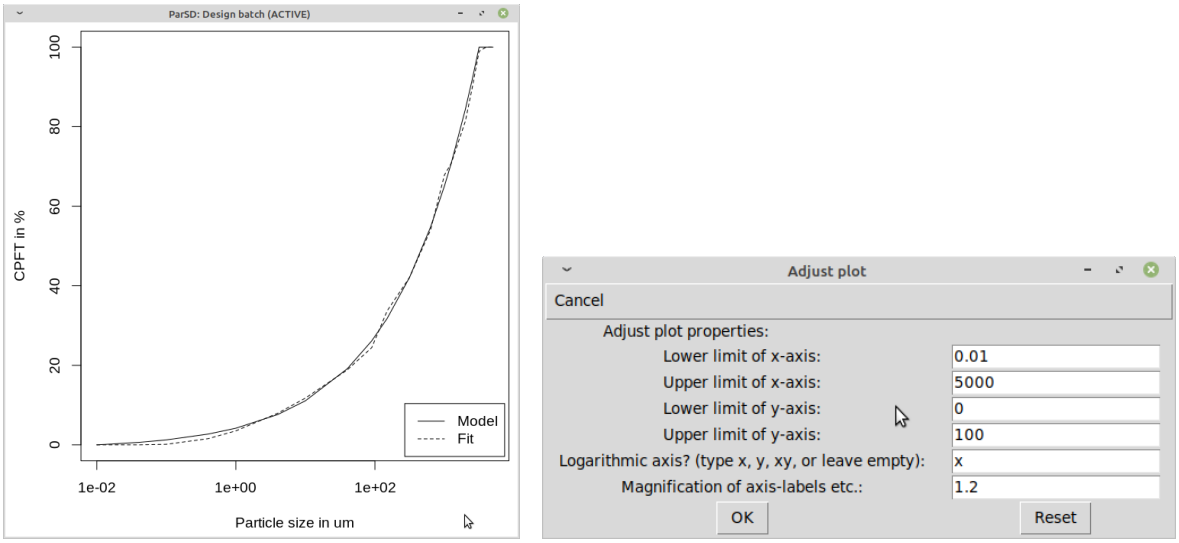
Figure 2: Save fine-tuned results

The menu item 'Apply window options' is a button which activates the settings decided for in the menu item 'Window options'. The window options accessible are the listbox height and the distance between the window elements. The listboxes are the boxes in the lower part of the results window showing the comparison of the model and batch particle size distributions. The distance between the window elements also refers to the vertical distance between the lines. Reason is that for batches containing a lot of materials (up to 20), it is possible that the results window could not fit on the screen for a large distance between the window elements.

Coming to the table in the upper part (cf. Figure 1), there the materials with their contents in the batch are listed together with information from the database if saved there. For vol% fine-tuning, the vol%-column is editable and for wt% fine-tuning the wt%-column. The last line of the table shows the batch properties containing also the calculable (true) batch density, its specific surface area and the costs. By editing (fine-tuning) the contents and then clicking 'Calculate', the complete set-up (batch and fit) is re-calculated for the new values. By the button 'Reset' it is always possible to get again the original non-fine-tuned results. It can be noted that by resetting, the unrounded values are shown. Caution: It is not checked if the edited values sum up to 100 %. In the line below the buttons, for the batch the describing d(CPFT) values are given to summarize the properties of the batch particle size distribution.

In the lower part of the fine-tuning windows (Figure 1), the quality of the fit is evaluated. The user can evaluate it visually by plotting the results (the CPFT curves) and by adjusting the plot to make details visible (Figure 3). The axis ranges and the magnification of the axis-labels can be adjusted

and it can be decided if there should be logarithmic axes.



(a) Graph

(b) Adjust plot

Figure 3: Plot fine-tuned results

The quality of the fit is described by the two numbers correlation coefficient and sum of squared deviations. Firstly, a correlation coefficient (≤ 1) for the correlation between the batch-CPFT(d) values and model-CPFT(d) values of '1' would describe a perfect fit. The second value is the sum of the squared deviations of the batch-CPFT(d) from the model-CPFT(d) for all component sizes d. The single values are shown in the listboxes by row. In the first listbox the component size d, in the second the model-CPFT(d), in the third the batch-CPFT(d) and in the fourth listbox the squared deviation is shown. Furthermore, the model information (type and parameters) can be presented (Figure 4) by clicking on the button 'Model info'.

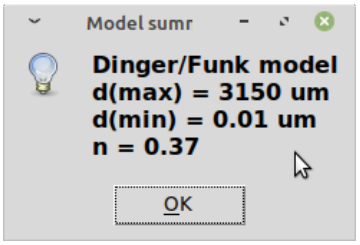


Figure 4: Model info