Results of 'Calculate model parameters' main function and their fine-tuning

The results and fine-tuning window (Figure 1 has an extended menu bar, followed by the parameter table of the model 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.

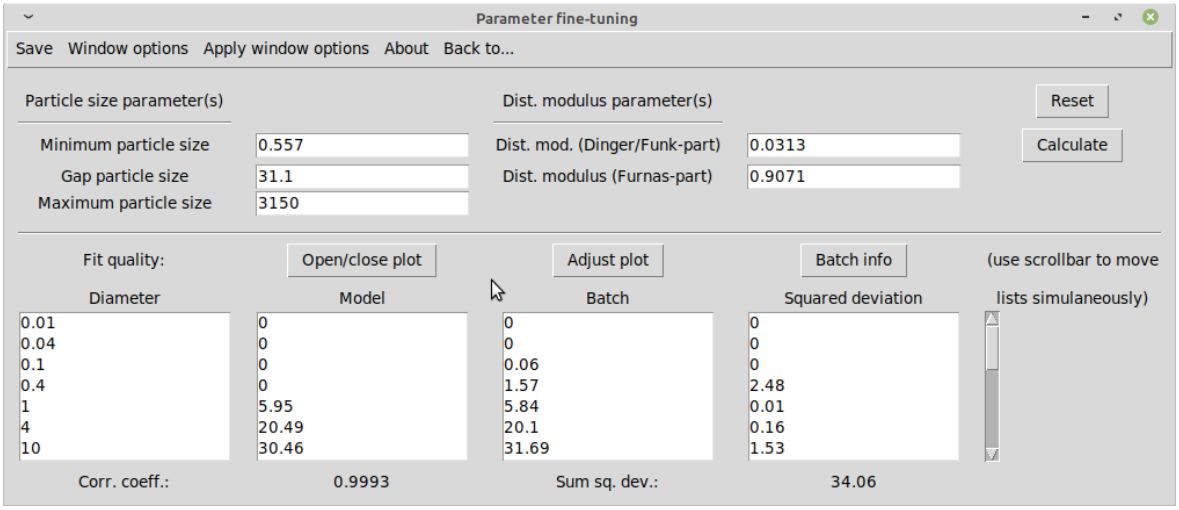


Figure 1: Results and fine-tuning dialog

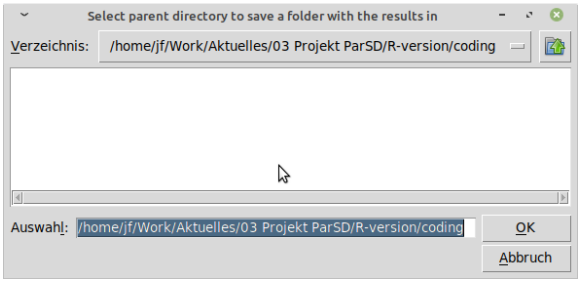
The menu item 'Save' gives the user the possibilities to save the fine-tuned...

- 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 (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 (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 (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 (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, thus, 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)).

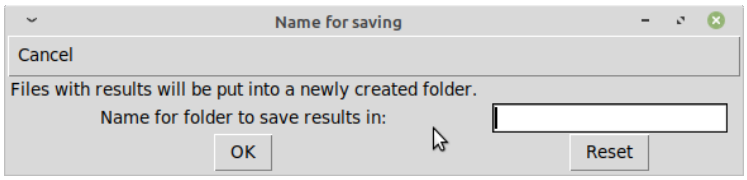
The menu item 'Apply window options' is a button which activates the settings decided for in the menu item 'Window options'. The window options accessible are the listbox height and the distance between the window elements. The listboxes are the boxes in the lower part of the results window showing the comparison of the model and batch particle size distributions. The distance between the window elements also refers to the vertical distance between the lines.

Coming to the editable parameter table in the upper part (cf. Figure 1), there the optimized parameters of the chosen model are presented. They can be edited (fine-tuned) and by 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 parameter results.

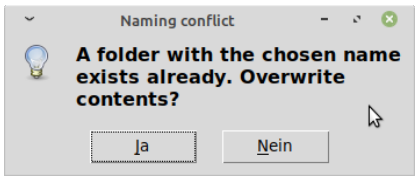
(a) Save-as dialog



(b) Select parent directory



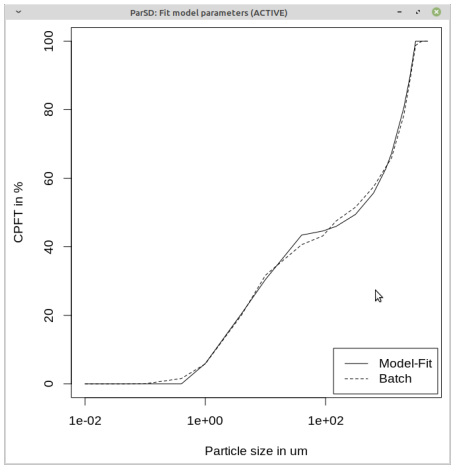
(c) Name results-folder



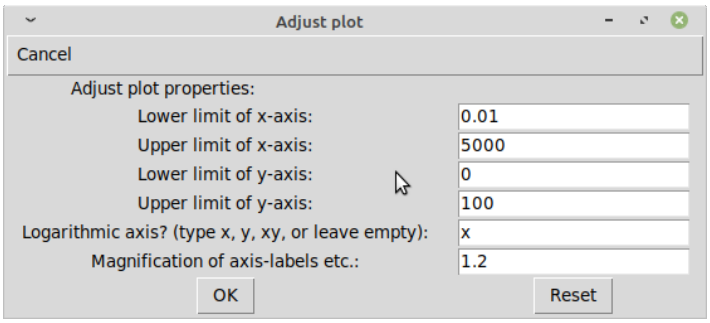
(d) Select parent directory

Figure 2: Save results

In the lower part of the fine-tuning window (Figure 1), the quality of the fit is evaluated. The user can evaluate it visually by plotting the fine-tuned 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 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 showing 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. Furthermore, the batch information can be displayed (Figure 4) by clicking on the button 'Batch info'. It shows a table where the materials with their contents in the batch are listed together with information from the database if saved there. The last line of the table shows the batch properties containing also the calculable (true) batch density, its specific surface area and the costs. Below, for the batch the describing d(CPFT) values are given to summarize the properties of the batch particle size distribution.

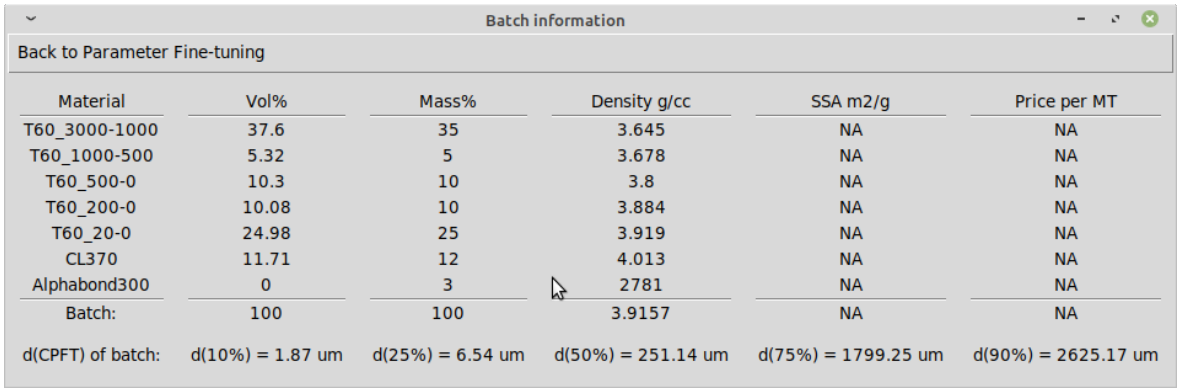


Figure 4: Batch info