Results of 'Verify a recipe' main function

The results are presented in a window (Figure 1) with 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.
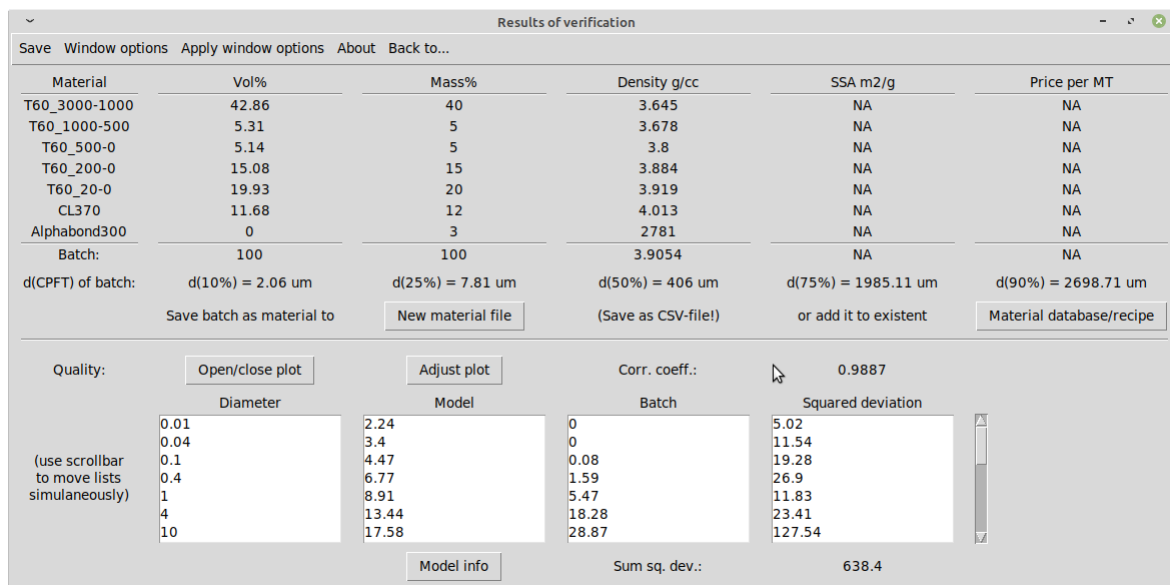

Figure 1: Results window

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

- 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. 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.
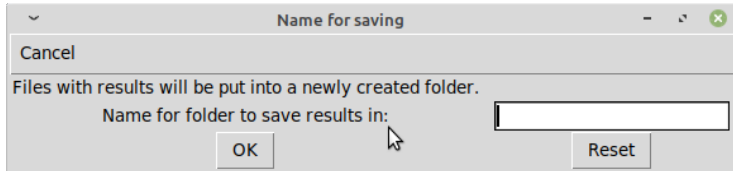
Coming to the results table (cf. Figure 1), there the materials with their contents in vol% and wt% in the batch are listed together with information from the database if saved there. The last
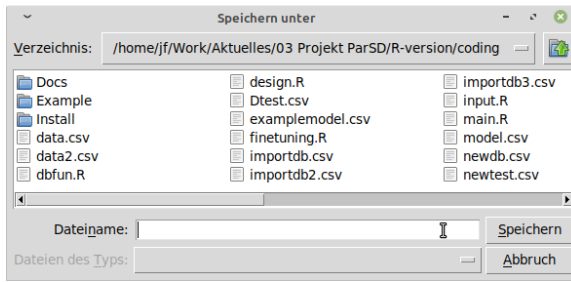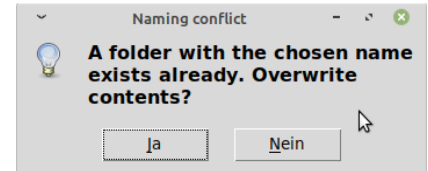
(a) Save-as dialog
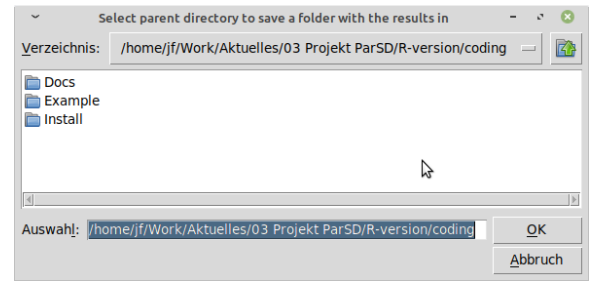
(b) Select parent directory

(c) Name results-folder

(d) Select parent directory

Figure 2: Save results

line shows the batch properties which contains obviously 100 vol% and wt%, but the line contains also the calculable (true) batch density, its specific surface area and the costs. Subsequently, for the batch the describing d(CPFT) values are given to summarize the properties of the batch particle size distribution. The batch can furthermore be saved as a new material file (database with one material only) or it can be added to an existing recipe or database. In the first case, the user is shown the save-as dialog (Figure 2(a)) where the user decides for a path and name for the new CSV (database) file. In the second case, the user selects a database from the filesystem. In both cases, afterwards, the user is asked to give the batch-material information (Figure 3). The fields are pre-filled, but can be edited—especially the unique identifier might be given a reasonable name.


Figure 3: Give batch-material information to save batch as material

The reason, the Save batch as material-function was included, is that by this also connections between raw materials can be accounted for. An example: Two raw materials should react completely

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with each other, so their ratio is fixed. If also their together amount is fixed, it can just be defined in the batch (by equal lower and upper bounds for both raw materials), but if their together share of the batch is to be optimized, the user can firstly define their relationship in a batch of two materials, save this batch as 'reaction-phase-material' and work in the further steps with this batch material.

In the lower part of the results window (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 4). The axis ranges and the magnification of the axis-labels can be adjusted and it can be decided if there should be logarithmic axes.
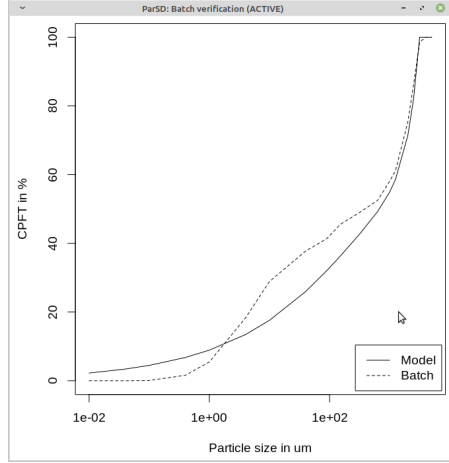
(a) Graph
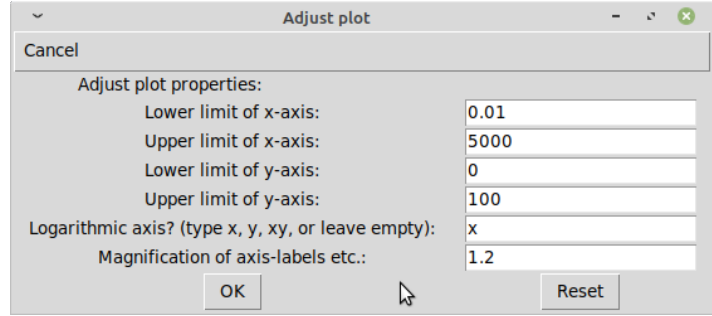
(b) Adjust plot

Figure 4: 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 model information (type and parameters) can be presented (Figure 5) by clicking on the button 'Model info'.
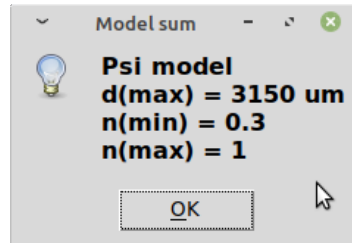

Figure 5: Model info

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