Model optimization

With a defined batch composition and a list of model parameters (possibly with set bounds), the parameter values can be calculated by fitting the particle size distributions of the batch and the calculable model to each other minimizing the squared deviation summed up over all component sizes.

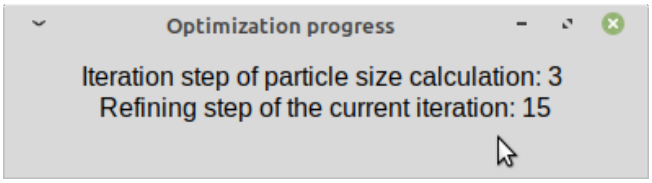


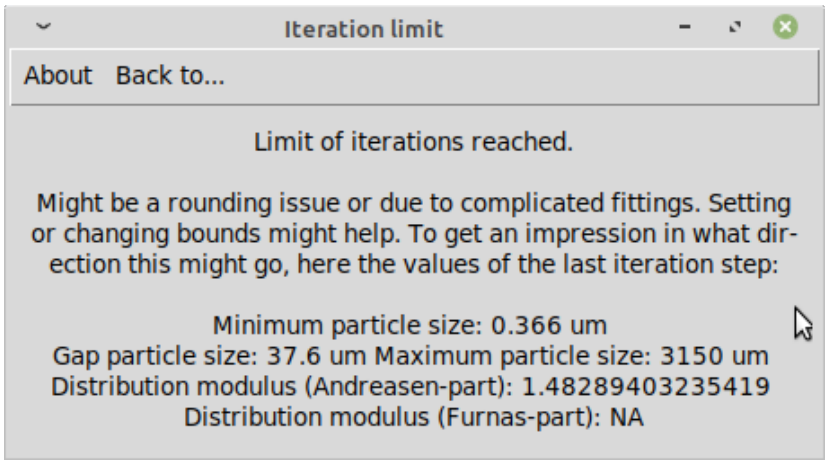
Figure 1: Model optimization progress

This batch optimization process is parted into two steps. The first step is that for the particle sizes—which are not given as constant—a simultaneous optimization of all particle sizes in question is done (referred to as refining steps). For all combinations, the second step, the calculation of the optimal parameters is done. Followingly, the combination of particle sizes returning the lowest of the minimum squared deviations is taken as the result of the first run. Around the particle size values returning this hopefully global minimum now, the ranges for the particle size are slightly narrowed and the whole process starts again. It is proceeded till the lower and upper borders of these ranges for the particle sizes to return minimum values are constant within the set accuracy for the grain sizes (in the Main Window Menu Settings). The progress of the optimization is displayed (Figure 1) showing the overall run in the first line and the refining step in the second line.

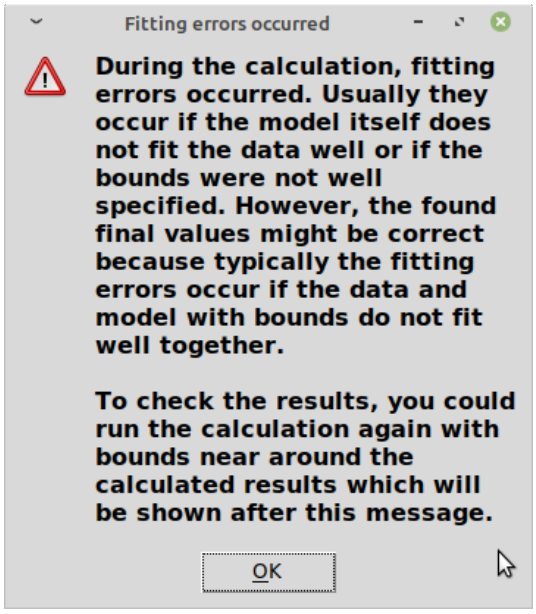
During the optimization, errors can occur. It is possible that due to rounding issues, 'bonded' materials (materials having exactly the same particle size distribution), due to existing local minima besides the global one or due to the possibility that more than one solution exists (especially for the more complex models with a higher number of parameters), a reasonable single solution cannot be calculated. To ensure that the program doesn't run infinitely, on the one hand in the Settings the user specifies a maximum number of iterations of the main runs. If this limit is reached, the user is informed (Figure 2(a)). Possible solutions are:

- Setting the iteration limit to a higher value (in Main Window Menu → Settings)
- Changing the accuracy and grain size accuracy settings (in Main Window Menu → Settings) might help if it is a rounding issue
- Changing bounds might help because this alters the starting values of the optimization process and can influence the result. Moreover, running into a local minimum instead of a global one is less probable with reasonable bounds for e.g. the particle sizes. As this is probably the best solution to the issue, for the last iteration run, the parameter values which returned the minimum sum of squared deviations for the fit are also shown in the error message so that the user has a hint in what direction it might go.
- Changing the raw material selection might help if e.g. 'bonds' exist.

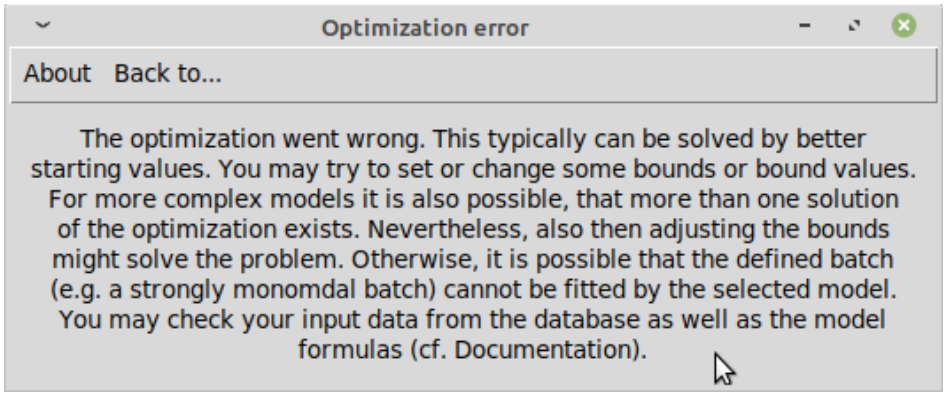
It is probable that not for all refining steps the nls()-function finds a solution because some combinations of particle sizes will be just not reasonable. The user will be informed if this happened (Figure 2(b)). Nevertheless, for the reasonable combinations a minimum might be reached and even if this error or caution message appears, the final result should be fine. However, it is also possible—especially for complex models—that the optimizations (nls()-function calls) for all refining steps fail. For this iteration run, then, no minimum exists and the optimization is aborted showing the message in Figure 2(c). To solve this issue, it is recommended to change the bounds or the selected raw materials.



(a) Iteration limit reached (Main run steps)



(b) Fitting errors (Refining steps)



(c) Optimization error (nls()-functions)

Figure 2: Optimization issues