Batch optimization

With a defined model and a list of raw materials (possibly with set bounds), the batch composition can be calculated by fitting the raw material contents in the way that the resulting batch composition fits the model curve with a minimum squared deviation summed up over all component sizes.
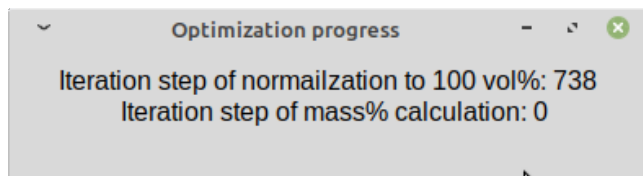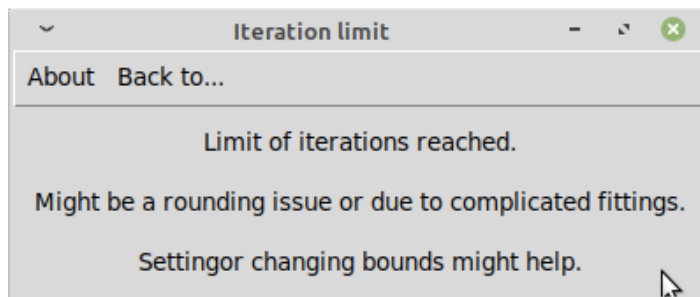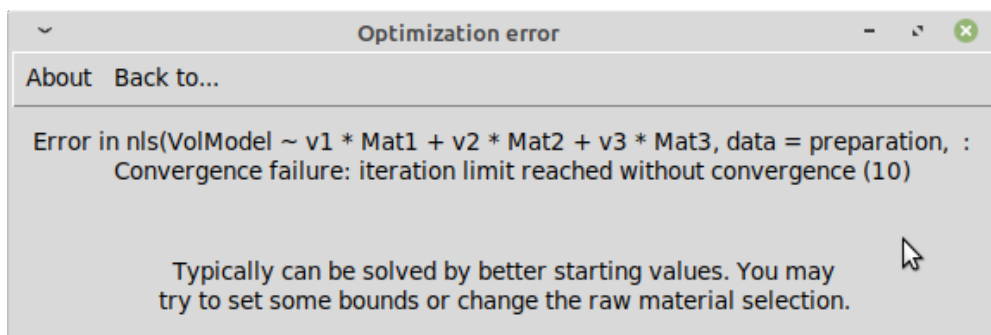

Figure 1: Batch optimization progress

This batch optimization process is parted into two or three steps depending on if it is a volume or weight optimization, respectively. For the volume optimization, it is iterated that the batch adds up to $100\,\mathrm{vol\%}$ and then the optimal content of every raw material is numerically calculated. If bounds in wt% have to be considered, in-between the two steps iterations take place to put the raw materials in question within the set wt%-bounds. The progress of the optimization is displayed (Figure 1) excluding the last step.

(a) Iteration limit reached

(b) Optimization error

Figure 2: Optimization issues

During the optimization, errors can occur. It is possible that due to rounding issues or 'bonded' materials (materials having exactly the same particle size distribution), a 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 (for the vol% and wt% iterations together). 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 setting (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
- Changing the raw material selection might help if e.g. 'bonds' exist

If the last optimization step, the calculation of the optimal contents for all mateials which is done by the nls()-function, fails, another error message is displayed (Figure 2(b)). It shows the returned error of the nls()-function and suggests the latter two points listed above to solve the problem as either the starting values are insufficient or the problem is not solvable by a unique set of raw material contents as is for example the case if 'bonds' exist.