Concentration determination

Henceforth only the list of molecules to be checked for their concentration, as assembled according to methods mentioned in the determination of molecules chapter[REF] are used. At this stage the strictness of the list can be adjusted by only allowing molecules present in a certain amount or more of the previously determined regions of low p-values to be processed further. In order to process the molecules further and compare them to the measured data, the information of the molecules are first transcribed to match the format of the measured data. This comes down to scrapping all the information outside of the relevant wavelength region, and matching the wavenumber spacing as used in the measured data through interpolation. Furthermore the measured data and molecules need to be in the same physical quantity, for which in this case absorbance is the most useful. The absorbance of the molecules is determined by:

A(C) = C \* path\_length L \* molar\_absorptivity epsilon

where the absorbance *A* is determined by the concentration C, the optical path length of the laser in the gas L, and the molar absorptivity e. Since the path length is measured from the setup and the molar absorptivity of the molecules is obtained from the databases, the absorbance is left as a function of the concentration. Note that the wavenumber dependency of the molar absorptivity is left out since all calculations are done over the set wavelength region as determined by the measurement. The concentrations are determined through what is essentially a curve fitting problem as the absorbances of the molecules can be laid over the measured absorbance and then best fitted to match by tweaking the concentrations of the molecules. This curve-fitting problem can be expressed as a non-linear least squares problem as:

r(k, C) = absorbance\_spectrum(k) – sum(epsilon\_i(k)\*L\*C\_i)\_over\_molecule\_list

with C = {c\_(first molecule), …., c\_(last molecule)},

and S(C) = sum(r(k,C)^2)\_over\_wavenumber

where r is a residue quantity, and S is the quantity to be minimized. This non-linear least squares problem is solved using the Levenberg–Marquardt algorithm to get the concentrations.

This method is used with the following inputs:

The list of molecules[APPENDIX REF] as found in the last chapter[REF].

Molar absorptivity data per wavenumber of all molecules in the above list.

The regions of low p-values[APPENDIX REF].

The list[APPENDIX REF] denoting the presence of the various molecules in the region of low p-value.

Absorbance data of the breath of 70 healthy and 70 asthmatic children as measured with the setup[REF][appendix chapter: Cannot freely give measurement data (right?), for questions contact X].

The wavenumber vector from 832 to 1250[CHECK] cm-1 with an increment of 0.5 cm-1.

The path length of 54.36 cm of the laser through the gas.

The following parameters are used:

Molecules with presence in one or more of the low p-value regions are further processed.

Initial guesses for the concentrations of the standard molecules are given as 1 part per million (ppm), for CO2 and H2O [OPMAAK] 1000 ppm, and for the other molecules 0.01 ppm.

This results in the concentrations as seen in [APPENDIX REF TO TABLE OF MOLECULES+CONCENTRATIONS] of which the most prominent are plotted below: [FIGURE]