

Getting started

1. Down-loading the toolbox

The EMSCtoolbox zip-file is down-loaded by clicking on 'Download the EMSC...'. This down-loads the file 'EMSCtoolbox.zip' to your hard-disk.

2. Setting up directories

1.1 Software and demos:

Copy the file 'EMSCtoolbox.zip' into your c:\Matlab\toolbox directory, and unzip the file. This generates directories

C:\Matlab\toolbox \EMSC

with sub-directories

C:\Matlab\toolbox\EMSC\Documentation

and

C:\Matlab\toolbox\EMSC\DemoDirectory

Directory ...Matlab\toolbox\EMSC contains the central EMSC software as well as some Matlab data files used for the demos.

Directory ...Matlab\toolbox\EMSC\DemoDirectory contains some local EMSC software and demo data sets. Keep DemoDirectory unchanged, to see how the standard setup should be.

Once you have become familiar with using the toolbox on the default data that follows the toolbox, you should copy the directory DemoDirectory to your normal Matlab works space, rename it to a more informative project name, and your place input data (and, optionally, your own new method definitions) in this directory.

3. Setting up the Matlab path

Under the menu entry 'File\SetPath' in the Matlab browser you can permanently add the toolbox directory 'EMSC'. This means that all the functions and data in the toolbox can be called from any working directory.

4. Running the software with the default data files

- a. Go to the directory where you want to run the toolbox from.

In Matlab Command window; type e.g.

```
cd c:\Matlab\toolbox \EMSC\ DemoDirectory <return>
```

- b. You can set the path by typing (skip this step if you added the path to your Matlab browser, in step 3.)

```
EMSC_SetPath <return>
```

- c. Start the EMSC program by typing

```
EMSC_Main<return>
```

- d. Follow the dialogue: Repeatedly, give one integer index (here called DataCase) followed by <return>, to control the function of the program. Details are given in the enclosed Program Manual and illustrated in the Powerpoint documentation.

Examples of different values of DataCase:

- 1000 = a list of pre-defined input-and method combinations,
- 2000 = more plots
- 101 = conventional MSC on the demo data set (diffuse NIR transmission OD of powder mixtures, published by Martens et al. 2003).
- 102 = default EMSC with only physical parameters
- 151 = default EMSC with automatically optimized reference spectrum
- 99 = all the calibration pre-processing methods already defined in file
EMSC\ DemoDirectory \EMSC_GetUserDefinedDataCases.m
- 199 = all calibration pre-processing methods already defined in file
EMSC\EMSCGetInternalDataCases.m
- 399 = the MSC, EMSC and EISC cases published in Martens et al. (2003)
- 0 = interactive input for calibration pre-processing
- 1 = interactive input for prediction pre-processing
- 3 = default EMSC/EISC with whatever was the last model defined
- 99 = all the default prediction pre-processing methods already defined
in files EMSC\EMSCGetDefaultInputDataForPred.m and
EMSC\ DemoDirectory\EMSC_GetUserDefPredDataCases.m
- 1000 = stop

5. Running the software with your own data files

- a. Go to your project directory, here assumed to be a copy of DemoDirectory, renamed to MyDirectory
- b. You can set the path by typing (skip this step if you added the path to your Matlab browser, in step 3.) EMSC_SetPath <return>
- c. Calibration: Make your own input files (e.g.
EMSC_Z.mat (spectra of a set of samples)
EMSC_Y.mat (main-analyte concentration in this sample set.)
- d. If you intend to run the pre-defined calibration methods (e.g. by responding DataCase=199), you first have to run the program EMSCMakeDefaults to make (more or less) dummy versions of the following files, based on your own input files:
EMSC_Ref.mat (a reference spectrum),
EMSC_Wgts.mat, (Channel weights),
EMSC_GoodSpectra.mat (spectra of one or more “analytes”),
EMSC_BadSpectra.mat (spectra of one or more “interferants”).
- e. Start the EMSC program by typing
EMSC_Main <return>
- f. Follow the dialogue: Repeatedly, give one integer index (here called DataCase) followed by <return>, to control the function of the program. Details are given in the enclosed Program Manual and illustrated in the Powerpoint documentation.
- g. Prediction: Once you have run the program at least once to “calibrate” an EMSC model based on your own calibration sample set, you may pre-process another sample set with the same kind of data, based on the obtained EMSC calibration model.
- h. If you want to set up your own calibration or prediction pre-processing methods - combinations of data input files and pre-processing method definitions - you can modify file EMSC_GetUserDefinedDataCases.m

(calibration or EMSC_GetUserDefPredDataCases (prediction) in MyDirectory, as explained in the program manual.