Information of the folder structure and the present files

The following page should provide an information of the file structure for the ammonia reactor in Brunsbüttel. The initial model was based on the publication: J. Morud and S. Skogestad. *AIChE Journal* 44, **1998**, 888-895. However, several modifications were performed to the model to adjust it for the respective investigations. There are in general several decision variables in each of the files.

If present, the folder "Plot_functions" includes functions for plotting of the results. These files are loading the data automatically. This is computer specific and may lead to problems. If problems arise, it may be possible to load the data also manually and remove the automatic loading.

Prog1. Steady State Analysis

This folder performs a steady state analysis of the system. The files are:

Main_SSAna.m	Steady state optimization and stability simulations.
Main_SSAna_RedFlow.m	Calculation of simple recycles
Main_SSAna_vanHeerden.m	Van Heerden Analysis of the reactor

Prog2. Controller Analysis

This folder allows different control structure evaluations and SOC variable definition. The possible control structures are: Self-optimizing control, extremum-seeking control, economic NMPC, and steady-state gradient control using transient measurements. The files are:

Main_ContEval_SOCdef.m	File in which the SOC variables for the system are defined as well as in which the loss is calculated.
Main_ContEval_SlaTuning.m	File in which the slave temperature loops are tuned.
Main_ContEval_MasTuning_Open.m	Open loop tuning of the master controllers using the SIMC rules.
Main_ContEval_MasTuning_Closed.m	Closed loop tuning of the SOC master controllers using the SIMC rules.
Main_ContEval.m	Evaluation of several different control structures.

Prog3. Recycle loop

This folder defines and evaluates SOC variables with an added, simplified recycle loop. It has to be noted, that there are several similar files with only slight changes. They differ by the used model and the way the SOC variables are calculated. The present files can be sorted according to the following characteristics

Main_SOC_def_Verx.m	Definition and loss calculation of the SOC variables using either a recycle loop or not.
Main_SSAna_RecLoop_Verx.m	Steady-state evaluation of the different SOC variables with and without recycle loop.

The files used for the publication J. Straus and S Skogestad. IFAC-PapersOnLine 51(18), **2018**, 536-541. are saved in Ver6.

Prog4. SOC for surrogate

This folder defines and evaluates SOC variables in the context of surrogate model generation. The files were used for the publication Straus an Skogestad, *Computers & Chemical Engineering* 119, **2018**, 143-151. It requires the installation of Gurobi for solving the MIQP. The files are:

Main_SOCdef_Surr.m	Calculation of the SOC variables using several different approaches
Main_NormEval.m	Calculation and evaluation of different norm types with respect to the calculation of SOC variables.
Main_SurrogateDef.m	Calculation of the surrogate model and evaluation of the fit of the model
Main_SurrogateDef_VaruQ.m	Plot of a case exemplifying that varying u for surrogate model fitting is not a solution
Rosenbrock.m	Definition of the Rosenbrock function and calculation of Figure 3 in the publication

Util1. Casadi3.1.0

The whole framework of CASADI. This folder should not be touched.

Util2. Functions

This folder provides all functions necessary for the model. Due to the nature of the development, several different models are existing resulting in several files. The used files are normally described in the header of the individual functions. Alternatively, it can be deduced from the analysis files in the Prog folders.

Util3. Splinter 3.0

The whole framework of Splinter version 3.0. This folder should not be touched.

Util4. MATLAB2tikz

The whole framework of the program MATLAB2tikz. This folder should not be touched.

Data

Data files for all programs. It can be that there are a lot of redundant files inside this folder.

All functions were written by Julian Straus.