Information of the folder structure and the present files

The following page should provide an information of the file structure for the simple ammonia loop. The philosophy behind the chosen modelling approach is given by a maximum flexibility in the construction of process flow diagrams. Furthermore, the programs in the folder "Prog 1. Adaptive Sampling" allow an easy adjustment for all types of models, including Aspen HYSYS files.

Prog1. Adaptive Sampling

This folder contains all programs and functions for adaptive sampling of the sections of the simple ammonia loop. The structure of the folder is:

- Calculation Files: Functions used for calculating the sampling domain in other independent variables, extracting the dependent variables from the state matrix, and calculation of dependent variables which are not incorporated in the nonlinear system of equations.
- Constraint Files: Functions calculating the right-hand side of the nonlinear system of equations for the different sections of the simple ammonia loop.
- Definition Files: Functions for giving the boundary conditions of the simple ammonia loop.
- LocalSave: .mat files saved for subsequent analysis.
- Plot Functions. Plot functions used in the creation of my thesis and the paper "J. Straus and S. Skogestad. *Computers & Chemical Engineering* 121, **2019**, 75-85. These files are **not** loading the data automatically. Hence, the user has to load this data manually from the folder "LocalSave". No warranty is given for these plot functions as they are quite specific in their application and the required data.
- Sampling Files: Files used for sampling the points used in surrogate model generation.

There exist several programs within the main folder. The tasks of these programs are written in the header of the respective program.

Furthermore, there exist several functions/files in the main folder which are required for the programs.

Prog2. Optimization of Combined Flowsheet

This folder is used for comparing the results of an optimization on the surrogate model-based process and the original process. The folder structure is similar to the folder "Prog1. Adaptive Sampling". However, the following new folder is added:

- Inequality Files: Functions containing the inequality constraints for the optimization of the simple ammonia loop.

The optimization can be performed using different surrogate models, *e.g.* Latin hypercube sampling or Random sampling based surrogate models.

Util1. Splinter 3.0

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

Util2. Bsplines and Datatables

This folder contains the required datatables and bsplines for running the problem. This folder should not be touched.

Util3. Sampling functions

This folder provides the used sampling functions. If other design of experiments plans should be used, then the functions "GridDef.m" and "GridDef_add.m" shall be correspondingly adjusted.

Util4. Unit operations

This folder contains two subfolders with the unit operations of the system. The first folder, "Optimization", contains the unit operations for the optimization of the simple ammonia loop. The second folder, "Simulation", contains the unit operations for simulation of the simple ammonia loop. Th unit operations differ as certain state variables are in the sampling calculated outside the nonlinear systems of equations whereas the optimization requires them to be calculated internally.

All functions and programs in the "Prog" folders were written by Julian Straus.