Matlab®/Simulink® Phenomenological Modelling Approach for Generation of Dynamic WWTP Influent Disturbance Scenarios including pharmaceuticals

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Note that this short document does not by any means provide a complete description of how to use the influent generator, however it may give some useful hints on the topic and avoid some unnecessary frustration. The document assumes that you are familiar with Matlab®/Simulink® and wastewater treatment process modelling and simulation. Please, also read the provided Agreement BSM-X.pdf.

### Unpacking the files

The files have been archived using .zip. Just unzip the files with the software you normally use for this purpose.

### Folders

When the files are unpacked, you will find in the main directory two different folders that include the models, one named BSM-ASMX and the other Influent generator ASM-X. The folder BSM-ASMX contains also two different folders, one containing the ASMX with co-metabolism and one containing the ASMX with inhibition. With both folders the BSM1 can be run with the inclusion of the fate of pharmaceuticals.

The folder Influent generator ASM-X has also two different folders, one containing the influent generator with the occurrence of DCF and the other containing the influent generator with the occurrence of SMX. The folder of DCF contains the stochastic approach of generating the pharmaceutical occurrence profile, while the folder of SMX contains the phenomenological approach.

### File description

#### BSM-ASMX

The files in the folder Co-metabolism and in the folder Inhibition are almost identical. The differences are in the ASMX models that are used during the simulation of the BSM1. There are two Simulink models in the folder, *benchmarkss* for steady state simulation (200 days) and *benchmark* for dynamic simulation (14 days).

There are also 5 different C-files in the folder:

* asm1 *Contains the ASM1 with fate of pharmaceuticals according to co-metabolism or inhibition*
* carboncombiner\_asm1 *Combines streams if carbon is added to the system*
* combiner\_asm1 *Combines two streams of different units into one stream*
* hyddelay\_asm1 *Adds a hydraulic delay to the stream*
* settler1d\_asm1 *Contains the settler model based on the principles of Takács.*

In order to use these C-files in the Simulink models, you have to compile them using the Matlab command *mex*. All C-files can be compiled at once by running the script *mexall\_asm1*.

In principle all the parameters and variables are defined in the different m-files and the actual Simulink blocks and models therein never need to be adjusted (unless you want to rebuild the modelling approach to simulate different pharmaceuticals processes). Within Simulink you only define parameters that are related to the numerical solver, the storing of data and selecting which input data files should be used. The initialization m-files are associated with the different blocks in Simulink (*asm1init, reginit\_asm1, sensorinit\_asm1, settler1dinit\_asm1*) The initialization file *benchmarkinit* calls the other init files in order to initialize a simulation of the *benchmark*(*ss*) model. If you want to use another pharmaceutical, but keep the same processes, you only have to update the parameters in the *asm1init.m* file.It is also valuable to study the init m-files to see how the models are set-up.

There are two input files provided *constinfluent* and *BSM1LT\_Influent\_CMZ*. The first input file is the influent used for the steady state simulation and the second is used for dynamic simulation. This second input file is generated by the influent generator.

The output variables are stored during simulations in the Matlab workspace. The output time information is stored as a general individual variable in Matlab workspace called t (unit days). In principle, all the different inputs are stored during simulation. By default, data are stored as a grab sample every 15 minutes. Note that there is one or two unused dummy states, depending on the use of inert soluble concentration. The file *perf\_plant* can be used to evaluate the performance of the WWTP according to the BSM1 criteria and displays the additional removal indexes of the pharmaceutical. *Smoothing\_data* contains an exponential filter that facilitates the visualization of the results by removing noise variations.

Naturally you can create any other helpful scripts for your specific purposes on your own.

#### Influent generator ASM-X

The files in the folder Phenomenological and in the folder Stochastic are also almost identical. The differences are in the additional files need in the Stochastic folder to use the Markov Chain for the generation of the random profile of the pharmaceutical. Also the Simulink *ASM1\_Influentmodel1\_ff* is different in the two folders.

There are two Simulink models in each folder, *ASM1\_Influentmodel1\_ff* to generate the influent data files and *ASM1\_Influentmodelprimary* to pass the influent data file through a primary clarifier in order to use it in the BSM1 models.

There are 7 different C-files in the folder:

* asm1\_combiner *Combines two streams of different units into one stream*
* asm1\_fractionation.c *Transfers the inputs of COD, TSS and SNH into state variables that are used in ASM1*
* asmX\_fractionation.c *Transfers the inputs of the pharmaceuticals into the state variables that are used in ASM-X*
* firstflush\_ASM1.c *Accounts for the “first flush” effect of the sewer network and re-suspension of the accumulated particulate material*
* primclar\_bsm2.c *Describes the primary clarifier model according to Otterpohl/Freund model*
* unisoilmodel.c *Describes the storage of water in soil*
* sewer\_asm1.c *The sewer system model describing transport of flow rate, components and temperature.*

In order to use these C-files in the Simulink models, you have to compile them using the Matlab command *mex*. All C-files can be compiled at once by running the script *mexall\_asm1*.

In principle all the parameters and variables are defined in the different m files and the actual Simulink blocks and models therein never need to be adjusted (unless you want to rebuild the modelling approach to generate the different WWTP influent scenarios or activate reactions in the sewer). Within Simulink you only define parameters that are related to the numerical solver, the storing of data and selecting which input data files should be used. The initialization file *ASM1\_Influent\_init\_dry* is used to initialize the simulation of the Simulink model *ASM1\_Influentmodel1\_ff*. If you want to use another pharmaceutical, but keep the same processes, you update the parameters in this initialization file.It is also valuable to study the init m-file to see how the model is set-up.

There are 15 input files provided:

* day\_HS.mat *Represents the flow-rate daily profile from households*.
* CODsol\_day\_HS.mat, CODpart\_day\_HS.mat, SNH\_day\_HS.mat, TKN\_day\_HS.mat *Represent the daily profiles for the different pollutants from households.*
* week\_HS.mat *Represents the flow rate weekly profile from households.*
* week\_polHS.mat *Represents the weekly pattern in the different pollutants from households.*
* year\_HS.mat *Represents the yearly pattern in the flow rate and different pollutants from households.*
* week\_IndS.mat *Represents the flow rate weekly profile from industry*.
* CODsol\_week\_IndS.mat, CODpart\_week\_IndS.mat, SNH\_week\_IndS.mat, and TKN\_week\_IndS.mat *Represents the weekly pattern in the different pollutants from industry.*
* year\_IndS.mat *Represents the yearly profile variation for industry. This pattern is applied to both flow-rate and pollutants*.
* XXX\_day\_HS.mat *Represents the daily profile of the pharmaceutical coming from households. This is only used in the phenomenological approach.*

or

* day\_MP.mat *Represents the night time minima of the pharmaceutical. This is only used in the stochastic approach.*

The output variables are stored during simulations in the Matlab workspace. The output time information is stored as a general individual variable in Matlab workspace called t (unit days). In principle, all the different input and stored during simulation. By default, data are stored as a grab sample every 15 minutes. Note that there is one or two unused dummy states, depending on the pharmaceutical used. The file *Figure\_ASM1influent* can be used to evaluate the generation of the influent data; it prints to the screen the different pollutant concentration and loads and plots the dynamic profiles of composite variables (COD, BOD5, TSS, TN, and pharmaceuticals). It also gives values or dispersion such as quartiles. *Smoothing\_data* contains an exponential filter that facilitates the visualization of the results by removing noise variations.

Naturally you can create any other helpful scripts for your specific purposes on your own.

### RUNNING THE BSM1 WITH ASM-X

When the archive has been unzipped, you are ready to run the different models. A few simple instructions are given below to help you through the first time and to test the system on your computer. The idea is to put the path to the benchmark directory into the Matlab path and then change directory (Matlab command cd) into the subdirectory you want to work from.

1. Start Matlab and move to the folder containing the model you want to use (*ASMX\_BSM – CMZ*, *ASMX\_BSM – SMX*).
2. Command mexall\_asm1.m (if you have problems with your C-compiler you must solve this). If you change the C-files (which should normally not be done), you need to re-mex all the C-files that you have modified in order for Simulink to use the modified file.
3. Run the initialization file *benchmarkinit* (initiates all variables and parameters, loads the data files etc. The file *asm1init* contains all variables and parameters with regard to the ASM1 model, *settlerinit* everything for the settlermodel, *reginit* everything for the controllers and soon). In the Simulink window parameters select simulation time, how often data should be stored etc. (if you are running *benchmarkss* with constant input use the ode15s solver but use ode45 if you use dynamic input data or active noise).
4. Command *benchmarks,* the Simulink model will appear in a new window. Run this model.
5. After simulation all data are stored in the Matlab workspace and not to files. Use the *who* command to see what variables you have available.
6. Initialize the steady state values as initial values for the dynamic simulation by running the script *stateset*.
7. Open the *benchmark* Simulink model (again a new window will appear) and run it for 14 days.
8. Evaluate the performance by using m-file *perf\_plant*).

Some useful commands for analysis are also available:

* *stateset* – this command saves all the variables obtained by the steady state simulationinto new variables and also sets them in the workspace so the benchmark is ready for a new simulation.
* perf\_plant – prints to the screen the values of all performance criteria related to the overall plant according to the definitions on the web site;

There is also an m-file included that goes through all these steps (*run\_bsm1*).

### RUNNING THE INFLUENT GENERATOR

When the archive has been unzipped, you are ready to run the different models. A few simple instructions are given below to help you through the first time and to test the system on your computer. The idea is to put the path to the benchmark directory into the Matlab path and then change directory (Matlab command cd) into the subdirectory you want to work from.

1. Start Matlab and move to the folder containing the model you want to use (*ASMX\_Influent generation (SMX), ASMX\_influent generation\_DCF*)
2. Command mexall\_asm1.m (if you have problems with your C-compiler you must solve this). If you change the C-files (which should normally not be done), you need to re-mex all the C-files that you have modified in order for Simulink to use the modified file.
3. **Only applicable for the stochastic approach:** Run the script *realize\_DCF* in order to run the Markov Chain for the random occurrence.
4. Run the initialization file *ASM1\_Influent\_init*. This file will initiate all the variables, parameters, inputs and so on needed to run the simulation.
5. Command the Simulink file you want to use (*benchmarks, benchmark or ASM1\_Influentmodel1\_ff*). The Simulink model will appear in a new window. Run this model.
6. Evaluate the performance by using the m-file *Figure\_ASM1\_Influent*.
7. Open the Simulink model *ASM1\_Influentmodelprimary* (again a new window will appear) and run this model.
8. Evaluate this performance by using the m-file *Figure\_BSM1LT\_Influent*. This should also generate the influent file that can be used in the BSM1-ASM-X models. Save the variable *BSM1LT\_Influent* from the workspace and copy it to the BSM1-ASM-X folder where you want to use it.

There is also an m-file included that goes through all these steps (*run\_influent*). Only the saving of the generated influent file is not done by this script.

### Final remarks

Try to understand the structure of the different m-files and c-files to grasp how they relate to each other. You should compare your results with the results provided in the Excel document. If your results are different, then you are doing something wrong. When you feel confident that you understand this implementation you may start to create your own influent files and control strategies for subsequent simulation studies. Remember, that this implementation is simply a starting point and a fully verified platform tor you to start working on you own and testing different scenarios that you’re interested in.

Enjoy!

Best regards,

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