Technische Universitï¿½t Dortmund
Department of Biochemical and Chemical Engineering
Chair of Process Dynamics and Operations
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Data-Based Dynamic Modeling Assignment SS 21

Submission requirements

- The assignment (written part and MATLAB® files) must be delivered **before 17:00pm on 23.07.2021**.
- The assignment constitutes 15% of your final grade.
- The assignment must be solved **individually**.
- It is required to provide the procedure followed to obtain your results (i.e. only writing the result is not sufficient). Furthermore, justification of your conclusions must be provided.
- Your submission must be a **single PDF file**. You can use the MATLAB® `publish` function to do this, e.g. `publish('task1.m','pdf')`. Make sure text/code is not cut at the page borders!
- Provide your name and matriculation number[1] on every page!
- All MATLAB® code, output, and plots (with appropriate labels) must be included in the PDF file.
  The first line of each MATLAB® file should contain your name and matriculation number[1].
- Upload your PDF file to Moodle.
- If you want to do calculations on paper, they must be easily readable, scanned/photographed with a decent quality, and part of the PDF file.
- Please use the assignment consultation hours published on Moodle.

[1] Not required for Students in the Summer School program

Data-based Dynamic Modeling Assignment Task

In Figure 1, the heating system of a reactor is shown. It consists of a jacketed reactor and a thermostat, which are connected via tubes. The system is an actual lab system used for a

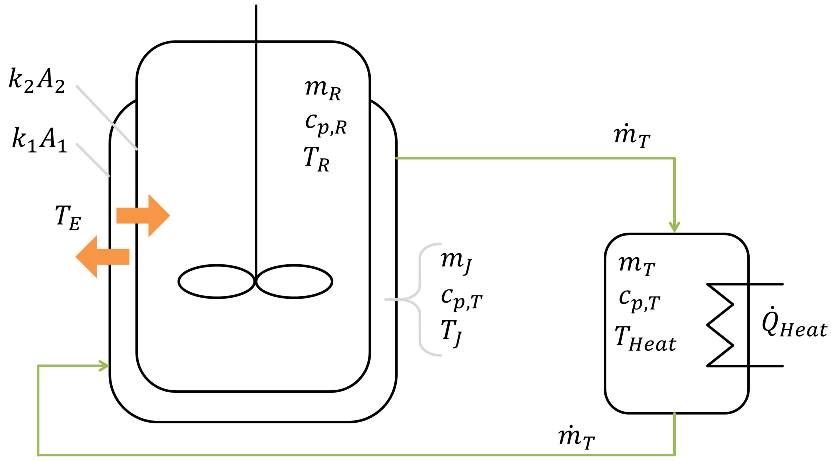

Figure 1: Heating system for a reactor

semi-batch co-polymerization process. The system has to be modeled in order to be able to design appropriate controllers. Your assignment is to use different modeling techniques and to compare and evaluate the resulting models. This system consists of 3 compartments, which can be assumed to be homogeneous: The heater, the jacket and the reactor. The input of the system is the heat source ($\dot{Q}_{Heat}$), the output of the system is the reactor temperature. From the adiabatic heating bath, the liquid is pumped to the jacket of the reactor, the same amount of liquid is pumped back from the jacket to the heater. In the jacket, heat is transferred to the reactor with a heat transfer coefficient k_2. Additionally heat is lost from the jacket to the environment with a heat transfer coefficient k_1. There is no heat created or lost inside the reactor. In a first experiment, a step response to the heat input was given to the system and the reactor temperature was measured. In the file `step_response.mat` several measurements of the heat input and the reactor temperature as well as the timestamps are given.

Tasks

Unfortunately the measurement system of the reactor temperature fails occasionally and assigns an implausible temperature at these sampling instances. Additionally the measurements of the input and the output are affected by noise. Thus your first task is to clean up the data.

a) Remove the outliers caused by the failure of the measurement system. Describe and justify your procedure. **(1 Point)**

b) Choose and apply an appropriate method for smoothing the data after the outlier removal from a). Why did you choose this specific method? **(1 Point)**

c) Use MATLAB® to create a plot of the raw data. In the same plot, add the data without outliers, and the smoothed data. **(0.5 Points)**

d) Use the method of Schwarze with the smoothed data to identify a transfer function $G_{Schwarze}(s)$. Write down the necessary steps. **(1.5 Point)**

e) Choose one of the prepared data sets for numerical transfer function estimation. Justify your choice. Identify a transfer function $G_{tfest}(s)$ using the MATLAB® commands `iddata` and `tfest` based on the chosen data set. Hint: The MATLAB® documentation can be used for reference. **(1 Point)**

f) Plot the data and the responses from the transfer functions $G_{Schwarze}(s)$ and $G_{tfest}(s)$. Comment on the results. **(1 Point)**

The system can be mathematically modeled using the following assumptions:

- Reactor, jacket, and thermostat are perfectly mixed
- Heat is only exchanged between the jacket and the environment and between the reactor and the jacket
- The flow going to and from the thermostat $\dot{m}_T$ is constant
- When $\dot{Q}_{Heat} = 0$, the reactor and the jacket are in thermal equilibrium with the environment.

Your colleague spent several hours doing experiments and evaluating data sheets to provide you with the following parameters of the system:

Table 1: Model variables and parameters

Symbol	Description	Value	Unit
m_R	Mass of the content in the reactor	2	kg
m_J	Mass of the heating medium in the jacket	0.5	kg
m_T	Mass of the heating medium in the thermostat	4	kg
$c_{p,T}$	Heat capacity of the content of the jacket and thermostat	2	$kJ/kg \cdot K$
$c_{p,R}$	Heat capacity of the content of the reactor	4	$kJ/kg \cdot K$
$\dot{m}_T$	In/outlet mass flow of the thermostat	0.02	kg/s
A_1	Heat transfer area between the jacket and environment	0.4	m^2
A_2	Heat transfer area between the jacket and reactor	0.2	m^2
k_1	Heat transfer coefficient of jacket-environment	-	$kW/m^2 \cdot K$
k_2	Heat transfer coefficient of jacket-reactor	-	$kW/m^2 \cdot K$

g) Set up the 3 differential balance equations for the system using the variables listed in Table 1. **(3 Points)**

h) Apply the parameter estimation method from the lecture to estimate the values of k_1 and k_2. Plot the simulation results of the fitted model and the real measurements without outliers in one graph. **(2.5 Points)**

- *Hint: Use the MATLAB® command* `ode45` *for the integration of the derived ODE system.*

i) Apply the Laplace transform to each individual equation to determine the white box model transfer function $G_{WB}(s)$, using the heat transfer coefficients estimated in Task (h). Explain your steps. **(2 Points)**

Assume that the resulting transfer function is of the following form:

$$G(s) = \frac{a_0}{b_0 + b_1 s + b_2 s^2 + b_3 s^3}$$

Use this formulation and the coefficients $a_0 = 25, b_0 = 1, b_1 = 825, b_2 = 13 \cdot 10^4$, and $b_3 = 1 \cdot 10^6$ to proceed with your calculations (**even if you found a different transfer function or other coefficients!**).

j) Calculate the z-domain transfer function $G_{WB}(z)$ manually. Write down your steps. **(4 Points)**

From now on you will use the new data sets `experiment_1.mat` and `experiment_2.mat` to fit ARX models and to test all your model approaches.

k) Plot the inputs and outputs of the data set used in the previous tasks and of the new data sets for parameter estimation (`experiment_1.mat`) and validation (`experiment_2.mat`) in one figure. **Qualitatively** discuss the features of the input signals. **(1.5 Point)**

l) Using frequency response techniques, sketch a method to **quantitatively** compare different input sequences with the goal of choosing the most suitable for model identification. Assume that the noise is white and additive on the output. **(2.0 Points)**

Now use `experiment_1.mat` for the parameter estimation.

m) Identify 4 ARX models on the `experiment_1.mat` dataset and plot the prediction results together with the fitting data. **(1 Point)**

Now use `experiment_2.mat` for validation. Choose a suitable error metric for what follows (e.g.: mean square error, root mean square error, etc.).

n) Compare the prediction performance of the identified models $G_{ARX,i}(z)$ on the validation dataset using the error metric. Plot the results. Is the performance of the ARX model satisfactory? **(1.5 Points)**

o) Identify 4 ARMAX models on the `experiment_1.mat` dataset and repeat the comparison of the previous point on the validation dataset `experiment_2.mat` using the error metric. Plot the validation results. Which model structure is more suitable for the supplied data between ARX and ARMAX? Provide suggestions as to why is this the case. **(2.0 Points)**

Now compare the identified models are compared using the validation data set `experiment_2.mat` and the error metric.

p) Plot the validation data `experiment_2.mat` along with the responses of $G_{Schwarze}(s)$, $G_{tfest}(s)$, $G_{WB}(z)$, and the best model identified among ARX and ARMAX $G_{\mathrm{AR(MA)X}}(z)$. Compare the different simulations using the error metric. How can you explain the differences? Tip: consider the whole model identification procedure.**(3.0 Points)**

q) Rank the different modelling techniques (Graphical, first principles and automatic model identification) from most favourable to least favourable based on the ease of implementation, accuracy and ease of use for the subsequent controller design process. **(1.5 Points)**