Nonlinear Model Predictive Control of an Adiabatic CSTR

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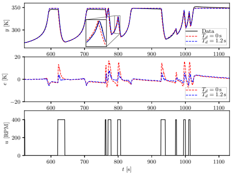
About Eskild

- Chemical engineer from the Technical University of Denmark 2017
- Research assistant at DTU Compute July to September 2017
- Employed at Novo Nordisk in Hillerød

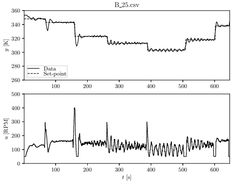
I am not affiliated with any research institution. The presentation is the result of an effort in my spare time.

Key points and learnings

Novel system for experimental evaluation of NMPC.

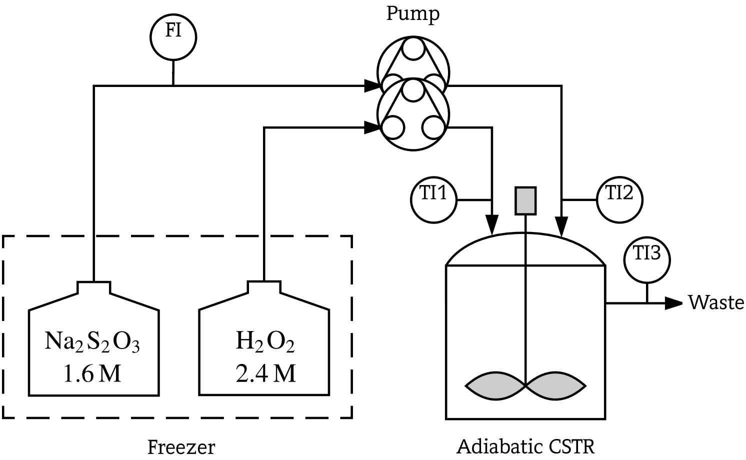


A non-linear model with input time delay.



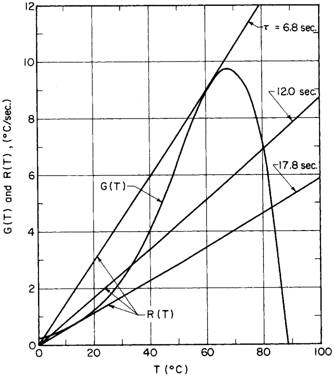
Unstable system stabilized with NMPC.

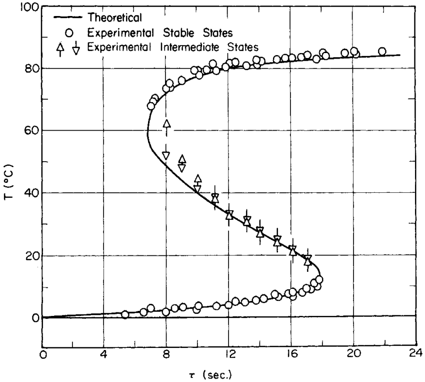
Topic for today



$$Na_2S_2O_3 + 2\,H_2O_2 \longrightarrow \frac{1}{2}\,Na_2SO_4 + \frac{1}{2}\,Na_2S_3O_6 + 2\,H_2O \quad (1)$$

Topic for today





S. A. Vejtasa and R. A. Schmitz, AIChE Journal, 1970

- Relatively easy to perform experiments
- The goal: To control the temperature to any set-point.

How to achieve the goal?

$$\begin{aligned}
\min_{x,\,u} \quad & \frac{1}{2}\sum_{i=0}^{N-1} x_i^T\, Q_c\, x_i + u_i^T\, Q_u\, u_i \,\mathrm{d}t + \frac{1}{2}\, x_N^T\, Q_f\, x_N \\
\text{s.t.} \quad & x_0 = \hat{x}_0 \\
& x_{i+1} = f(x_i, u_i), \quad i = 0, ..., N-1 \\
& u_{\min} \le u_i \le u_{\max}, \quad i = 0, ..., N-1 \\
& \Delta u_{\min} \le u_{i+1} - u_i \le \Delta u_{\max}, \quad i = 0, ..., N-2
\end{aligned}$$

Model

Consider the reaction as

$$\mathrm{A} + 2\,\mathrm{B} \longrightarrow \frac{1}{2}\,\mathrm{C} + \frac{1}{2}\,\mathrm{D} + 2\,\mathrm{E} \tag{3}$$

with 2nd order reaction rate

$$-r_{\mathrm{A}} = c_{\mathrm{A}}\, c_{\mathrm{B}}\, \exp\left(A - \frac{B}{T}\right) \tag{4}$$

Then mass/energy balances for CSTR conditions are

$$\frac{\mathrm{d}T}{\mathrm{d}t} = \frac{q}{V}(T_{\mathrm{in}} - T) + \frac{(-\Delta H_r)}{\rho\, c_p}\, c_{\mathrm{A}}\, c_{\mathrm{B}}\, \exp\left(A - \frac{B}{T}\right) \tag{5a}$$

$$\frac{\mathrm{d}c_{\mathrm{A}}}{\mathrm{d}t} = \frac{q}{V}(c_{\mathrm{A,\,in}} - c_{\mathrm{A}}) - c_{\mathrm{A}}\, c_{\mathrm{B}}\, \exp\left(A - \frac{B}{T}\right) \tag{5b}$$

$$\frac{\mathrm{d}c_{\mathrm{B}}}{\mathrm{d}t} = \frac{q}{V}(c_{\mathrm{B,\,in}} - c_{\mathrm{B}}) - 2\, c_{\mathrm{A}}\, c_{\mathrm{B}}\, \exp\left(A - \frac{B}{T}\right). \tag{5c}$$

Model

Further assume constant T_{in}, $c_{\text{A, in}}$ and $c_{\text{B, in}}$ yielding:

$$\frac{\mathrm{d}T}{\mathrm{d}t} = \frac{q}{V}\,(T_{\text{in}} - T) + \theta\,R(T) \tag{6a}$$

with reaction rate and parameters

$$R(T) = 2\,c_{\text{B, in}} \left(1 - \frac{T - T_{\text{in}}}{\theta}\right) \left(\phi - \frac{T - T_{\text{in}}}{2\,\theta}\right) \exp\left(A - \frac{B}{T}\right) \tag{6b}$$

$$\phi = \frac{c_{\text{A, in}}}{c_{\text{B, in}}} \tag{6c}$$

$$\theta = \frac{(-\Delta H_r)\,c_{\text{B, in}}}{2\,\rho\,c_p} \tag{6d}$$

This model presents multiple advantages:

- The assumptions are plausible
- Just one temperature measurement is required
- The model is unidimensional

Model assumptions

The model rests on certain equipment specific assumptions:

- State is measurable instantaneously
- Reactor is adiabatic
- Good correlation between pump set-point and throughput

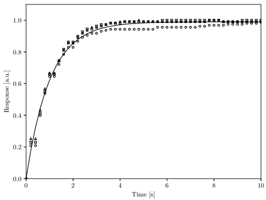


Figure: Thermocouple time constant approximately $1\,\mathrm{s}$.

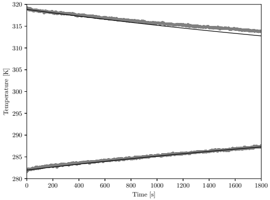


Figure: Reactor is approximately adiabatic.

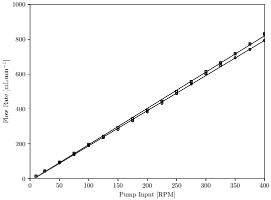


Figure: Pump response is linear and similar for both feeds.

Identification

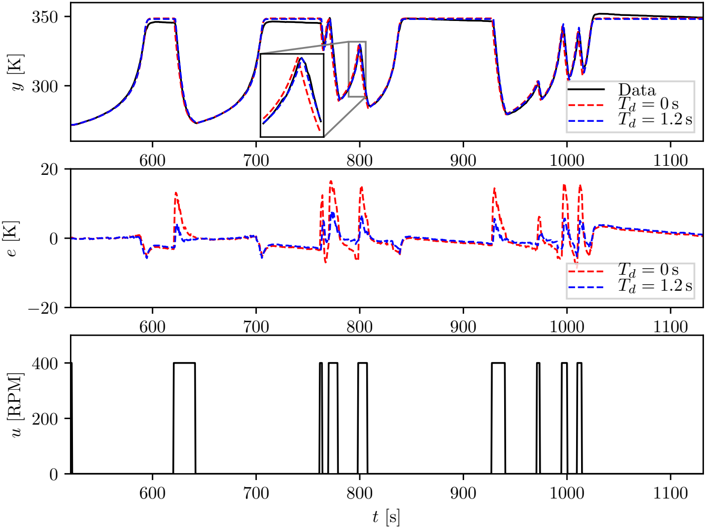
- Step response experiment
- Reasonable parameter estimates are available
- Accuracy of models for similar systems has been shown to be good
- Fit via least squares

Identification experiment is constructed based on a binary input signal subject to a desired output excitation profile.

Table: Nominal model parameters.

Parameter	Nominal value
V	$105\,\mathrm{mL}$
$c_{\mathrm{A,\,in}}$	$\frac{1.6}{2}\,\mathrm{mol\,L^{-1}}$
$c_{\mathrm{B,\,in}}$	$\frac{2.4}{2}\,\mathrm{mol\,L^{-1}}$
T_{in}	$0.5°\mathrm{C}$
ρ	$1\,\mathrm{kg\,L^{-1}}$
c_p	$4186\,\mathrm{J\,(kg\,K)^{-1}}$
A	$24.6\,\mathrm{L\,(s\,mol)^{-1}}$
B	$8500\,\mathrm{K}$
ΔH_R	$-560\,\mathrm{kJ\,mol^{-1}}$

Identification experiment



The fit appears to be very good, especially when a time-delay is incorporated into the model.

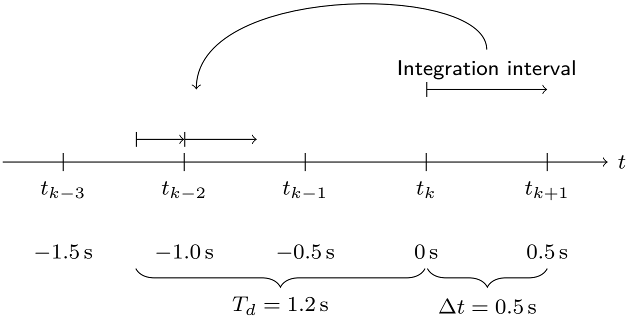
Integration of ODE with constant input time delay

Parameters:

- $\Delta t = 0.5\,\mathrm{s}$
- $T_d = 1.2\,\mathrm{s}$

$n = 2$, $\frac{T_d}{\Delta t} = 2.4$ is non-integer.

1. Integrate over the interval $0.2\,\mathrm{s}$ using $q = u(t_{k-3})$
2. Integrate over the interval $0.3\,\mathrm{s}$ using $q = u(t_{k-2})$



Model for State Estimation (EKF)

Model and disturbance model

$$\frac{\mathrm{d}T}{\mathrm{d}t} = \frac{q}{V}\,(T_{\mathrm{in}} - T) + \theta\,R(T) + x_d \tag{7a}$$

$$\frac{\mathrm{d}x_d}{\mathrm{d}t} = 0 \tag{7b}$$

Reaction rate and parameters

$$R(T) = 2\,c_{\mathrm{B,\,in}}\left(1 - \frac{T - T_{\mathrm{in}}}{\theta}\right)\left(\phi - \frac{T - T_{\mathrm{in}}}{2\,\theta}\right)\exp\left(A - \frac{B}{T}\right) \tag{7c}$$

$$\phi = \frac{c_{\mathrm{A,\,in}}}{c_{\mathrm{B,\,in}}} \tag{7d}$$

$$\theta = \frac{(-\Delta H_r)\,c_{\mathrm{B,\,in}}}{2\,\rho\,c_p} \tag{7e}$$

The way we in reality obtain the disturbance state from the measurement of the temperature, y:

$$x_d = y - T$$

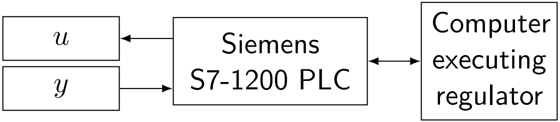
Time delay in the input

$$q(t) = u(t - T_d)$$

$$T_s = 0.5\,\mathrm{s},\;\; T_d = 1.2\,\mathrm{s}$$

NMPC simulator

It's important to connect to the process



Yet, even more important to connect to a simulator beforehand

Switching between process and simulator is a matter of changing an IP address.

Almost ready for NMPC!

Prerequisites are coming together

- Model is established, assumptions are acceptable
- Model augmented with a time-delay to improve fit
- Satisfactory fit between model and data obtained

NMPC problem

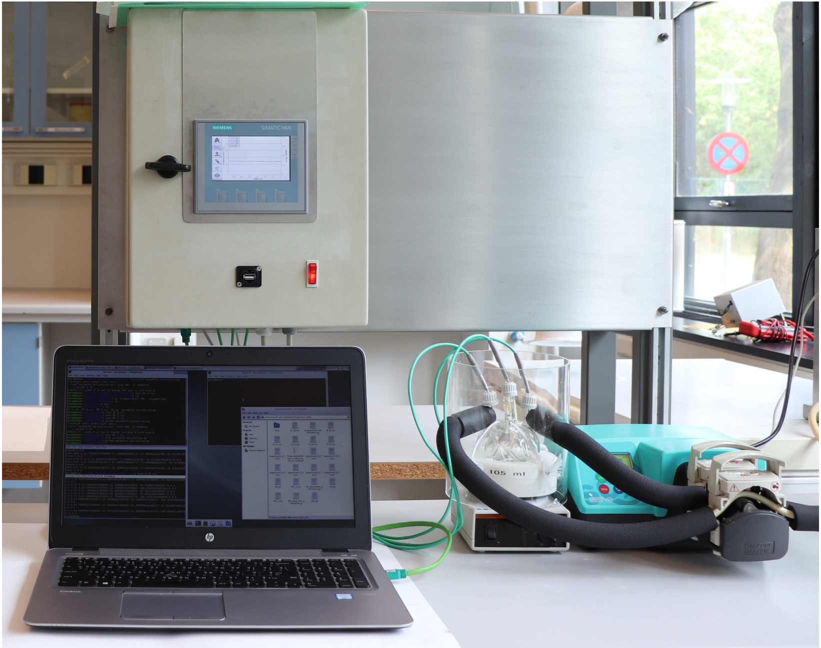
- Problem solved via. direct multiple shooting
- Objective function comprises quadratic term and rate of movement input regularization
- Minimized s.t. constraints: ODE model, input and rate of input change

Algorithm

CasADi

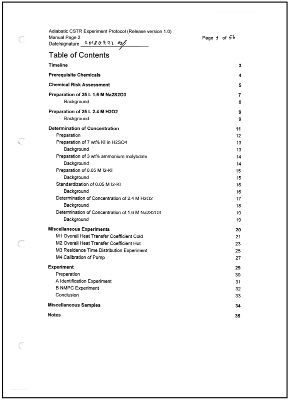
The problem is solved with CasADi in Python.
See `direct_multiple_shooting.py` on their Github for sample code.

Experimental setup



Experimental Procedure

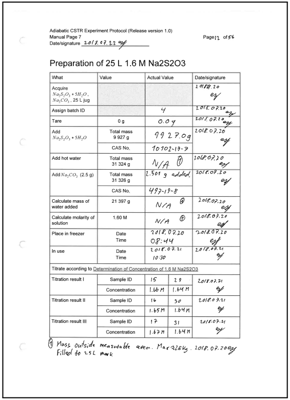
Experiments are performed according to a detailed procedure promoting repeatability and data integrity.



Adiabatic CSTR Experiment Protocol (Release version 1.0)
Manual Page 2
Date/signature 2018.07.22

Page 1 of 56

Table of Contents



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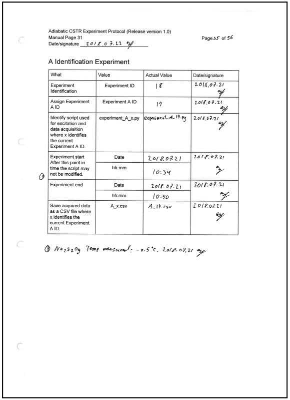
Manual Page 7
Date/signature 2018.07.22

Page 12 of 56

Preparation of 25 L 1.6 M Na2S2O3

What	Value	Actual Value		Date/signature
Acquire $Na_2S_2O_3 * 5H_2O$, Na_2CO_3, 25 L jug				2018.07.20
Assign batch ID		4		2018.07.20
Tare	0 g	0.0 g		2018.07.20
Add $Na_2S_2O_3 * 5H_2O$	Total mass 9 927 g	9927.0 g		2018.07.20
	CAS No.	10102-17-7		
Add hot water	Total mass 31 324 g	N/A ①		2018.07.20
Add Na_2CO_3 (2.5 g)	Total mass 31 326 g	2.501 g added.		2018.07.20
	CAS No.	497-19-8		
Calculate mass of water added	21 397 g	N/A ①		2018.07.20
Calculate molarity of solution	1.60 M	N/A ①		2018.07.20
Place in freezer	Date Time	2018.07.20 08:44		2018.07.20
In use	Date Time	2018.07.21 10:30		2018.07.21
Titrate according to Determination of Concentration of 1.6 M Na2S2O3				
Titration result I	Sample ID	15	29	2018.07.21
	Concentration	1.66 M	1.64 M	
Titration result II	Sample ID	16	30	2018.07.21
	Concentration	1.65 M	1.64 M	
Titration result III	Sample ID	17	31	2018.07.21
	Concentration	1.67 M	1.64 M	

① Mass outside measurable area. Max 32 kg. 2018.07.20
Filled to 25L mark



Adiabatic CSTR Experiment Protocol (Release version 1.0)
Manual Page 31
Date/signature 2018.07.22

Page 35 of 56

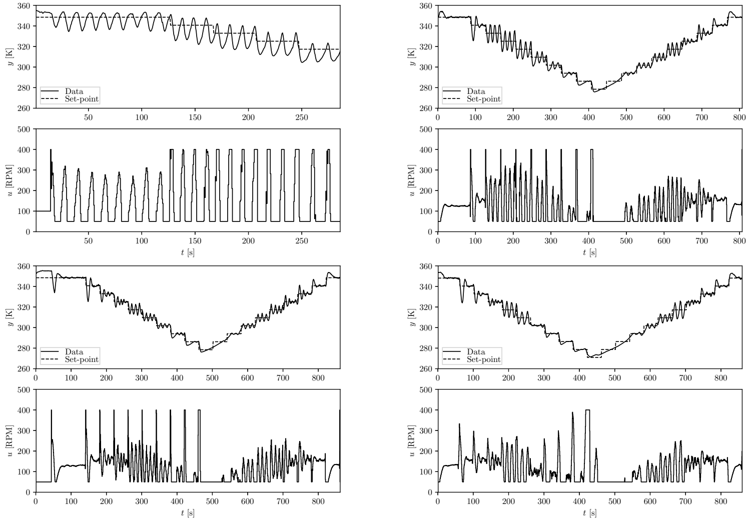
A Identification Experiment

What	Value	Actual Value	Date/signature
Experiment Identification	Experiment ID	18	2018.07.21
Assign Experiment A ID	Experiment A ID	19	2018.07.21
Identify script used for excitation and data acquisition where x identifies the current Experiment A ID.	experiment_A_x.py	experiment_A_19.py	2018.07.21
① Experiment start After this point in time the script may not be modified.	Date	2018.07.21	2018.07.21
	hh:mm	10:34	
Experiment end	Date	2018.07.21	2018.07.21
	hh:mm	10:50	
Save acquired data as a CSV file where x identifies the current Experiment A ID.	A_x.csv	A_19.csv	2018.07.21

① $Na_2S_2O_3$ Temp measured: -0.5 °C. 2018.07.21

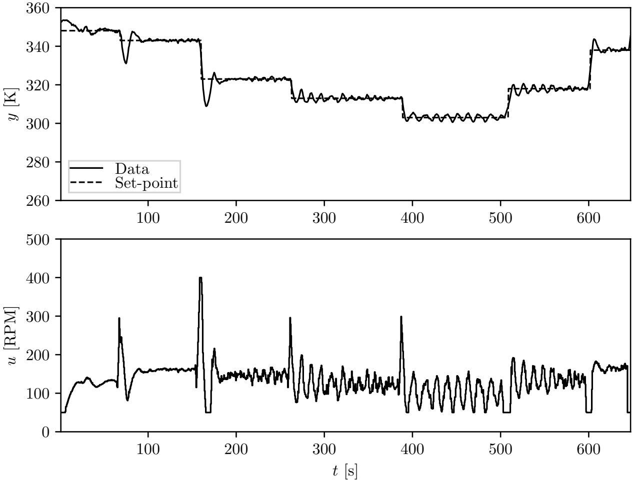
NMPC Results 1-4

Trial 1 to 4



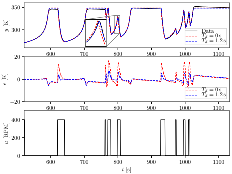
NMPC Results 5

Trial 5 – $T_d = 1.2$, $\alpha = 0.1$, $|\Delta u| \leq 30$



Key points and learnings

Novel system for experimental evaluation of NMPC.



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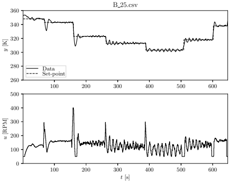

Unstable system stabilized with NMPC.