Cyber Physical Systems course project

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Temperature Control of a Continuous Stirred Tank Reactor (CSTR)

1. Goal of the project

The goal of this project is to develop controllers able to regulate the temperature inside a Continuous Stirred Tank Reactor (CSTR). As will be explained in what follows, a CSTR is a highly nonlinear system, with strong dynamic nature. In order to achieve this objective, both a Proportional Integral Derivative (PID) controller and a Model Predictive Control (MPC) strategy have been developed. Some desirable properties of the system are stated in the form of Signal Temporal Logic (STL) formulas, and it has been verified against different reference inputs that both control strategies are able to satisfy these desiderata. Lastly, requirement falsification for the MPC controller has been made minimizing the robustness over N iterations during which parameters of the controller are considered as control inputs and randomly sampled.

2. Plant model

An exothermic CSTR [2] is a tank reactor extensively used in chemical industries in order to convert a chemical A into a mixed product AB, via a first order reaction $A \rightarrow_{k \cdot C_A} B$. The reaction rate per unit volume is modelled as the product $k \cdot C_A$, where C_A is the concentration of A, and the rate constant $k = k(T)$ is computed by the Arrhenius law:

$$k(T) = k_0 e^{-\frac{E_a}{R \cdot T}}$$

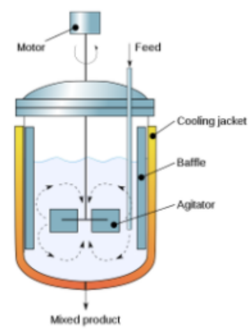
Under the assumptions that: the CSTR is perfectly mixed, the mass densities of the feed and product streams are equal and constant (denoted by ρ) and the liquid volume V in the reactor is kept constant, the model consists of the following mole and energy balances on the content of the reactor:

$$\frac{dC_A}{dt} = \frac{q}{V} \cdot (C_{Af} - C_A) - k(T) \cdot C_A$$

$$\frac{dT}{dt} = \frac{q}{V}(T_f - T) + \frac{-\Delta H_R}{\rho \cdot C_p} k(T) \cdot C_A + \frac{UA}{\rho \cdot C_p \cdot V}(T - T_c)$$

Hence the state of the system consists of $X = [C_A, T]$ (i.e. concentration of the reactant A and reactor temperature, respectively), while T_c (i.e. the temperature of the cooling jacket) is the controlled variable, that can be adjusted within the interval $[250K, 350K]$. The values of the constants are stated and explained in the following table:

Quantity	Value	Unit
Arrhenius pre-exponential	7.2e+10	1/min
Activation Energy	72750	J/mol
Gas constant	8.314	$J/(mol \cdot K)$
Reactor Volume	100	m^3
Density	1000	kg/m^3
Heat capacity	0.239	$J/(kg \cdot K)$
Enthalpy of reaction	-50000	J/mol
Heat transfer coefficient	50000	$J/(min \cdot K)$
Feed flowrate	100	m^3/min
Feed concentration	1	mol/m^3
Feed temperature	350	K
Initial concentration	0.87	mol/m^3
Initial temperature	324	K



Depending on the reactant A and on the product that we want to obtain, it is desirable that the internal temperature of the reactor T sets to a constant reference value (low if we want concentration of A to be high, and viceversa). However, without any form of control, this cannot be easily achieved, due to the dynamics of the system:

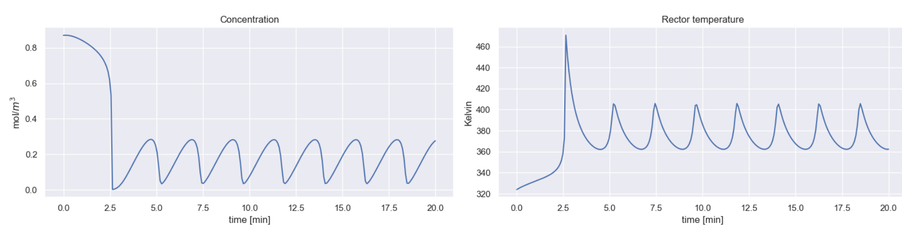


Figure 1: Simulation of the system with constant input $u = 305K$

In what follows, we will also assume that the measurements are noisy, hence along with the controller also a state estimator will be necessary.

3. PID Control

As a first control strategy, a PID controller has been implemented, whose well-known standard form of the control function is the following:

$$u(t) = K_p \left(e(t) + \frac{1}{\tau_i} \int_0^t e(\tau) d\tau + \tau_d \frac{de(t)}{dt} \right)$$

with $e(t) = ref(t) - T(t)$, being $ref(t)$ the reference temperature we aim to follow.

The actual implementation leverages the following discrete formula:

$$u(t) = K_p \left(e(t) + \frac{1}{\tau_i} \sum_{i=0}^{t} e(i)dt + \tau_d \frac{e(t) - e(t-1)}{dt} \right)$$

being dt the time step.

For what concerns the tuning of the parameters $[K_p, \tau_i, \tau_d]$, mainly trial-and-error has been used, however, in order to get an initial guess of such parameters Internal Model Control (IMC) tuning [1] has been used. It works as follows:

- input and output data are obtained by simulation (manually providing $u(t)$, e.g. multiple step input);
- IMC tuning parameters are obtained via model identification, fitting the simulation data (i.e. minimizing the sum of squared errors) to the following *first-order plus dead-time (FOPDT) model*:

$$\tau \frac{dy(t)}{dt} = -y(t) + K \cdot u(t - \theta)$$

- PID parameters are obtained as (with $\tau_c = \max(0.1\tau, 0.8\theta)$):

$$K_p = \frac{1}{K} \cdot \frac{\tau + 0.5\theta}{\tau_c + 0.5\theta}, \ \tau_i = \tau + 0.5\theta, \ \tau_d = \frac{\tau \cdot \theta}{2 \cdot \tau + \theta}$$

In the end, the PID parameter used are $K_p = 1.7, \tau_i = 0.8, \tau_d = 0.2$.

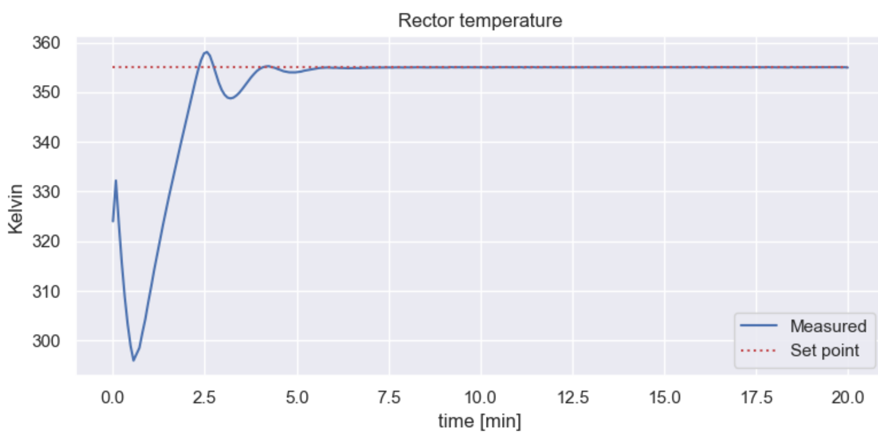


Figure 2: PID control for reference temperature of $355K$

4. MPC Control

As a second control strategy, Model Predictive Control has been tried. The objective of this controller is to find $u^\star$, at each time t, such that:

$$\min_{u^\star} \sum_{i=0}^{H} Q \cdot ||ref(t) - y_{t+i}||^2 + R \cdot ||u^\star_{t+1}||^2$$

$$\text{s.t. } x_{t+k+1} = f(x_{t+k}, y_{t+k}),\ y_{t+k} = g(x_{t+k}),\ 250 \le u_{t+k} \le 350$$

where f, g are the equations describing the system's dynamics, H is the length of the receding horizon.

Parameters of this controller have been set by trial and error to: $Q = 2.0, R = 0.01, H = 10.0$.

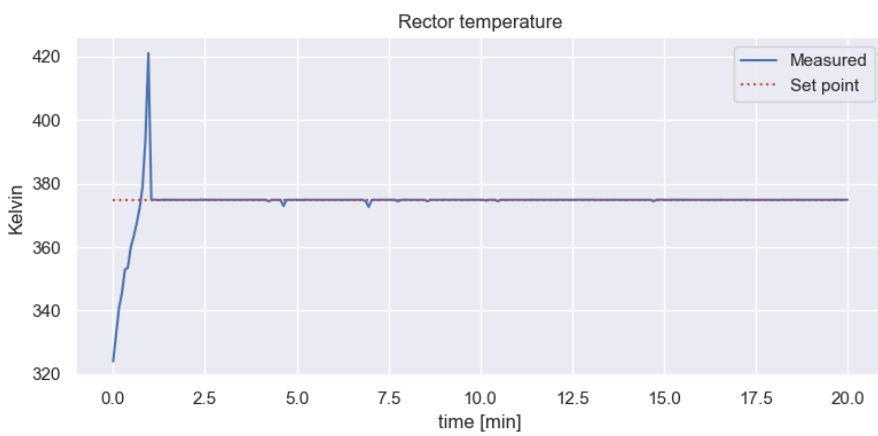


Figure 3: MPC control for reference temperature $ref = 375$

5. Extended Kalman Filter

In order to emulate a real sensor, in both control strategies a random normal noise has been added to the state of the system, and this led to the necessity of including a state observer. The Extended Kalman Filter (EKF) has been used, given the non-linear dynamics of the CSTR system. In order to implement it, at each step of the simulation it was necessary to linearize the dynamics of the system, that is, evaluate the Jacobian of the ODEs describing the CSTR at the predicted state, which is:

$$F_k := \frac{\partial f}{\partial x}\bigg|_{\hat{x}_{k|k+1}, u_k} = \begin{bmatrix} -\frac{q}{V} - k(T) & -k0 \cdot \frac{E_a}{R} \cdot \frac{1}{T^2} \cdot e^{\frac{E_a}{R \cdot T}} \cdot C_A \\ -\frac{\Delta H_R}{\rho \cdot C_p} \cdot k(T) & -\frac{q}{V} - \frac{\Delta H_R}{\rho \cdot C_p} \cdot C_A \cdot (\frac{E_a}{R} \cdot \frac{1}{T^2} \cdot e^{\frac{E_a}{R \cdot T}}) + \frac{UA}{\rho \cdot C_p \cdot V} \end{bmatrix}\Bigg|_{\hat{x}_{k|k+1}, u_k}$$

For brevity I will not report all the equations for the prediction and update steps of the EKF, however the parameters has been set to: $Q_k = \begin{bmatrix} 10^{-2} & 0 \\ 0 & 10^{-4} \end{bmatrix}$, $R_k = \begin{bmatrix} 10^{-4} & 0 \\ 0 & 10^{-2} \end{bmatrix}$

Performance measures of both controllers (equipped with EKF) against fourteen different reference inputs can be found in Appendix A.

6. Requirements of the system

As already stated before, it is important that, at least from a certain point on, the system strictly follows the constant reference temperature it is fed with. For this reason, the following requirements are asked:

- oscillations in the reactor temperature ($o(t) = |T(t) - T(t-1)| \ \forall t$) are admitted in the first time steps, however within the first half of the simulation time they should be contained within $5K$, formally:

$$\phi_1 = \mathbf{FG}_{[0.0, \frac{N}{2}]}(o(t) < 5.0)$$

- in the second half of the simulation, oscillations in the reactor temperature should be contained within $3K$ (i.e. only small oscillations are admitted in the second part of the simulation), formally:

$$\phi_2 = \mathbf{G}_{[\frac{N}{2}, N]}(o(t) < 3.0)$$

- in the last part of the simulation, the temperature should closely follow the reference temperature, i.e. the difference $d(t) = |T(t) - ref(t)|$ should not exceed $3K$, formally:

$$\phi_3 = \mathbf{G}_{[\frac{2}{3}N, N]}(d(t) < 3.0)$$

where N is the final time step.

In order to verify these properties, fourteen different constant references have been provided to the system, and the robustness has been computed both for the PID and the MPC control, resulting always positive, hence witnessing that the requirements are satisfied. Detailed result can be found in the Appendix B.

7. Falsification

As last step, falsification of the property ϕ_3 in the case of MPC control has been performed. In order to do so, the parameters Q and R of the controller were considered as control inputs of the system, so that the falsification procedure was as follows:

```
minSTL = 'inf'
params = [2.0, 0.001]
for i = 1,...,N:
  Q ~ N(2.0, 1)
  R ~ N(0.001, 0.01)
  T = simulate_mpc(Q, R, ref)
  stl = compute_robustness(T, phi_3)
  if stl < minSTL:
    minSTL = stl
    params = [Q, R]
  if minSTL < 0:
    break
```

That is, for $N = 100$ iterations the system is simulated, randomly sampling at every iteration parameters Q, R. If parameters falsifying the requirement are found, they are stored and the procedure stops.

Results of the falsification can be found in Appendix C.

References

[1] Rice, R. (2010). PID Tuning Guide, online: https://bit.ly/3xjrMeX

[2] Seborg, D. E. (2011). Process dynamics and control. Hoboken, N.J: John Wiley & Sons.

Appendix

A. Controllers' performance

Reference	Overshoot	Rise time	Steady state error	Settling time	Type
320	12.196	7.04	0.004	7.04	PID
320	4	0.08	0.105	0.08	MPC
325	7.205	6.4	0	6.4	PID
325	0.049	0.08	0.086	0	MPC
330	2.196	5.84	0.007	5.76	PID
330	0.004	0.08	0.014	0.08	MPC
335	0.024	5.12	0.021	5.12	PID
335	0.074	0.16	0.034	0.16	MPC
340	0.8	4.48	0.002	4.48	PID
340	0.158	0.16	0.074	0.16	MPC
345	4.221	4	0.013	4.88	PID
345	2.264	0.24	1.653	1.44	MPC
350	76.001	3.52	0	8.56	PID
350	77.905	1.76	1.795	7.68	MPC
355	3.082	2.32	0.051	3.92	PID
355	62.116	0.56	0.128	2.8	MPC
360	109.974	2.24	0.017	7.44	PID
360	59.586	0.8	0.124	0.8	MPC
365	96.388	2.56	0.011	6.8	PID
365	16.285	1.76	2.43	2.32	MPC
370	103.475	2.32	0.024	6.16	PID
370	74.75	3.2	0.598	3.2	MPC
375	94.705	4.8	0.005	5.6	PID
375	46.114	1.04	0.07	1.04	MPC
380	94.503	4.24	0.025	6	PID
380	6.064	1.2	1.514	1.28	MPC
385	83.707	3.44	0.012	6.56	PID
385	59.394	1.2	1.917	1.44	MPC

B. Verification Results

Reference (K)	ϕ_1	ϕ_2	ϕ_3	Type
320	4.93253	2.93253	2.96594	PID
320	4.97122	2.96718	2.86723	MPC
325	4.93568	2.9275	2.95727	PID
325	4.95816	2.95816	2.89236	MPC
330	4.92094	2.92094	2.97335	PID
330	4.97148	2.95784	2.94943	MPC
335	4.94701	2.94701	2.96744	PID
335	4.96729	2.95451	2.9541	MPC
340	4.95634	2.95634	2.97319	PID
340	4.9623	2.95648	2.90227	MPC
345	4.94068	2.94068	2.97096	PID
345	2.75737	0.428719	0.473074	MPC
350	4.30281	2.30281	2.23374	PID
350	2.36445	0.364447	0.64978	MPC
355	4.92214	2.9215	2.94765	PID
355	4.34312	2.34284	2.19566	MPC
360	4.91115	2.91115	2.95645	PID
360	2.60967	0.60967	2.10229	MPC
365	4.91519	2.91519	2.96059	PID
365	4.98001	2.98001	0.559726	MPC
370	4.9444	2.9444	2.95934	PID
370	4.9893	2.92456	2.33	MPC
375	4.91701	2.91701	2.95095	PID
375	4.54535	2.54535	2.86681	MPC
380	4.91814	2.91814	2.95187	PID
380	4.31203	2.31108	1.0324	MPC
385	4.94638	2.91565	2.95505	PID
385	4.00767	0.912368	0.548313	MPC

C. Falsification Results

Reference	Q	R	Robustness
320	1.33663	0.020416	-1.28741
325	0.376885	0.024445	-20.7467
330	0.210134	0.0191757	-31.3692
335	1.60591	0.0040131	-0.423672
340	1.63118	0.00144311	-0.0405561
345	2.45878	0.0092065	-0.10704
350	2.67307	0.0045229	-2.28309
355	1.57202	0.00161315	-3.23189
360	1.67468	0.0150942	-8.42903
365	2.70502	0.00979266	-58.8853
370	2.59014	0.00121103	-5.30934
375	1.73716	0.0150608	-0.0113018
380	1.48972	0.018182	-2.94381
385	0.226472	0.0107259	-8.14433