Problem Set #3: Numerical Optimal Control (cont'd)

Exercise 1: Formulation of OCPs and Solution via CasADi

The aim of this exercise is formulate several optimal control problems. We will use the `Optistack Toolbox`, which is an extension of CasADi used in the first exercise sheet. Information about this toolbox can be found on `https://github.com/casadi/optistack`. It is advisable to install CasADi and optistack prior to the exercise.

Consider a chemical continuous stirred tank reactor (CSTR) in which the exothermic irreversible reaction

$$A \to B$$

takes place. The dynamics of the CSTR are as follows, see [1] for details.

$$\dot{c}_A = \frac{q}{V}(c_{Af} - c_A) - k_0 e^{\frac{-E}{RT}} c_A \tag{1a}$$

$$\dot{T} = \frac{q}{V}(T_f - T) + \frac{-\triangle H}{\rho C_p} k_0 e^{\frac{-E}{RT}} c_A + \frac{UA}{V\rho C_p}(u_1 - T). \tag{1b}$$

The states c_A and T describe the concentration of subtance A and the reactor temperature in K. The coolant stream temperature u is the considered input variable. The objective is to compute an input signal such that the system reaches the set-point $c_{As} = 0.159[mol/l], T_s = 374.985[K]$. The coolant stream temperature u is subject to the input constraint $u \in [270, 330]$. The system parameters are listed in the following table.

Table 1: Parameters for CSTR.

q	100	$[L/min]$	c_{Af}	1	$[mol/L]$
T_f	350	$[K]$	V	100	$[L]$
ρ	1000	$[g/L]$	C_p	0.239	$[J/(g \cdot K)]$
$-\triangle H$	$5 \cdot 10^4$	$[J/mol]$	$\frac{E}{R}$	8750	$[K]$
k_0	$7.2 \cdot 10^{10}$	$[min^{-1}]$	UA	$5 \cdot 10^4$	$[J/(minK)]$

a) We want to calculate optimal open-loop inputs which steer the system (1) to the considered set-point. Formulate three different optimal control problem, such that the solution of each of these problems yields the considered open-loop inputs. Justify and explain your choices.
Hint: We already discussed this part in Problem Set # 2, Ex. 1a).

b) Calculate (i.e. compute numerically) the stationary value for the coolant stream temperature u_s corresponding to the set-point $c_{As} = 0.159[mol/l], T_s = 374.9854[K]$.

c) Solve of one your formulated optimal control problems for $(c_A(0), T(0)) = (0.25, 370)$ using `Optistack` and CasADi.
Hint: Use the templates `RK4.m, parameters.m, P3Ex1_template.m, CSTR_ODE.m` provided on the course moodle page.

References

[1] M. Henson and D. Seborg. *Nonlinear Process Control*. Prentice Hall, Upper Saddle River, NJ, 1997.