SeborgCSTR_basics

March 13, 2018

1 Use of Modelica + Python in Process Systems Engineering Education

1.1 Basic analysis of "Seborg reactor"

1.1.1 Bernt Lie

1.1.2 University College of Southeast Norway

Basic import and definitions

```
In [1]: from OMPython import ModelicaSystem
        import numpy as np
        import numpy.random as nr
        %matplotlib inline
        import matplotlib.pyplot as plt
        import pandas as pd
        LW1 = 2.5
        LW2 = LW1/2
        Cb1 = (0.3,0.3,1)
        Cb2 = (0.7,0.7,1)
        Cg1 = (0,0.6,0)
        Cg2 = (0.5,0.8,0.5)
        Cr1 = "Red"
        Cr2 = (1,0.5,0.5)
        LS1 = "solid"
        LS2 = "dotted"
        LS3 = "dashed"
        figpath = "../figs/"
```

1.1.3 Nonlinear reactor model from Seborg et al.

Process diagram

Original state space model We consider the original Seborg et al. model, written as:

$$\frac{dc_{\mathrm{A}}}{dt} = \frac{\dot{V}_{\mathrm{i}}}{V}\left(c_{\mathrm{A,i}} - c_{\mathrm{A}}\right) - a \cdot r$$

$$C_p \frac{dT}{dt} = \frac{\dot{V}_\mathrm{i}}{V} C_{p,\mathrm{i}} \left(T_\mathrm{i} - T\right) + \left(-\Delta_\mathrm{r} \tilde{H}\right) rV + \dot{Q}$$

Here:

$$r = k c_\mathrm{A}^a$$

$$k = k_0 \exp\left(-\frac{E}{RT}\right)$$

$$\dot{Q} = \mathcal{U} A \left(T_\mathrm{c} - T\right)$$

In the original Seborg et al. model, $a = 1$, while Δ_r is constant, $\dot{V}_\mathrm{e} = \dot{V}_\mathrm{i}$, and $C_p = C_{p,\mathrm{i}}$ is constant.

Modelica code for original Seborg et al model "ModSeborgCSTRorg" within package "SeborgCSTR"

```
model ModSeborgCSTRorg
   // Model of ORiGinal Seborg CSTR in ode form
   // author:  Bernt Lie
   //          University of Southeast Norway
   //          November 7, 2017
   //
   // Parameters
   parameter Real V = 100 "Reactor volume, L";
   parameter Real rho = 1e3 "Liquid density, g/L";
   parameter Real a = 1 "Stoichiometric constant, -";
   parameter Real EdR = 8750 "Activation temperature, K";
   parameter Real k0 = exp(EdR/350) "Pre-exponential factor, 1/min";
   parameter Real cph = 0.239 "Specific heat capacity of mixture, J.g-1.K-1";
   parameter Real DrHt = -5e4 "Molar enthalpy of reaction, J/mol";
   parameter Real UA = 5e4 "Heat transfer parameter, J/(min.K)";

   // Initial state parameters
   parameter Real cA0 = 0.5 "Initial concentration of A, mol/L";
   parameter Real T0 = 350 "Initial temperature, K";
   // Declaring variables
   // -- states
   Real cA(start = cA0, fixed = true) "Initializing concentration of A in reactor, mol/L";
   Real T(start = T0, fixed = true) "Initializing temperature in reactor, K";
   // -- auxiliary variables
   Real r "Rate of reaction, mol/(L.s)";
   Real k "Reaction 'constant', ...";
   Real Qd "Heat flow rate, J/min";
   // -- input variables
   input Real Vdi "Volumetric flow rate through reactor, L/min";
   input Real cAi "Influent molar concentration of A, mol/L";
```

```
    input Real Ti "Influent temperature, K";
    input Real Tc "Cooling temperature', K";
    // -- output variables
    output Real y_T "Reactor temperature, K";
  // Equations constituting the model
  equation
    // Differential equations
    der(cA) = Vdi*(cAi-cA)/V- a*r;
    der(T) = Vdi*(Ti-T)/V + (-DrHt)*r/(rho*cph) + Qd/(rho*V*cph);
    // Algebraic equations
    r = k*cA^a;
    k = k0*exp(-EdR/T);
    Qd = UA*(Tc-T);
    // Outputs
    y_T = T;
  end ModSeborgCSTRorg;
```

1.1.4 Nominal model study

Instantiating model

```
In [2]: sr_org = ModelicaSystem("SeborgCSTR.mo","SeborgCSTR.ModSeborgCSTRorg")
```

```
2018-03-13 14:45:03,198 - OMPython - INFO - OMC Server is up and running at file:///c:/users/ber
```

Checking quantity names for model

```
In [3]: pd.DataFrame(sr_org.getQuantities())
```

Out[3]:

	Changeable	Description	Name
0	false	Initializing temperature in reactor, K	T
1	false	Initializing concentration of A in reactor, mol/L	cA
2	false	der(Initializing temperature in reactor, K)	der(T)
3	false	der(Initializing concentration of A in reactor...	der(cA)
4	false	None	$cse1
5	false	Heat flow rate, J/min	Qd
6	true	Cooling temperature', K	Tc
7	true	Influent temperature, K	Ti
8	true	Volumetric flow rate through reactor, L/min	Vdi
9	true	Influent molar concentration of A, mol/L	cAi
10	false	Reaction 'constant', ...	k
11	false	Rate of reaction, mol/(L.s)	r
12	false	Reactor temperature, K	y_T
13	true	Molar enthalpy of reaction, J/mol	DrHt
14	true	Activation temperature, K	EdR
15	true	Initial temperature, K	T0
16	true	Heat transfer parameter, J/(min.K)	UA
17	true	Reactor volume, L	V

18	true	Stoichiometric constant, -	a
19	true	Initial concentration of A, mol/L	cA0
20	true	Specific heat capacity of mixture, J.g-1.K-1	cph
21	false	Pre-exponential factor, 1/min	k0
22	true	Liquid density, g/L	rho

	Value	Variability	alias	aliasvariable
0	None	continuous	noAlias	None
1	None	continuous	noAlias	None
2	None	continuous	noAlias	None
3	None	continuous	noAlias	None
4	None	continuous	noAlias	None
5	None	continuous	noAlias	None
6	None	continuous	noAlias	None
7	None	continuous	noAlias	None
8	None	continuous	noAlias	None
9	None	continuous	noAlias	None
10	None	continuous	noAlias	None
11	None	continuous	noAlias	None
12	None	continuous	noAlias	None
13	-50000.0	parameter	noAlias	None
14	8750.0	parameter	noAlias	None
15	350.0	parameter	noAlias	None
16	50000.0	parameter	noAlias	None
17	100.0	parameter	noAlias	None
18	1.0	parameter	noAlias	None
19	0.5	parameter	noAlias	None
20	0.239	parameter	noAlias	None
21	None	parameter	noAlias	None
22	1000.0	parameter	noAlias	None

Observe the artifically named variable "$cse1" this is a variable that the system has created, and is not found in the underlying Modelica code.

Setting simulation length

```
In [4]: sr_org.getSimulationOptions()
```

```
Out[4]: {'solver': 'dassl',
         'startTime': 0.0,
         'stepSize': 0.002,
         'stopTime': 1.0,
         'tolerance': 1e-06}
```

```
In [5]: sr_org.setSimulationOptions(stopTime=15,stepSize=0.05)
```

Checking input

```
In [6]: u = sr_org.getInputs()
```

```
In [7]: u
```

```
Out[7]: {'Tc': None, 'Ti': None, 'Vdi': None, 'cAi': None}
```

```
In [8]: u.keys()
```

```
Out[8]: ['Vdi', 'cAi', 'Tc', 'Ti']
```

```
In [9]: u.values()
```

```
Out[9]: [None, None, None, None]
```

Setting nominal inputs

```
In [10]: sr_org.setInputs(Tc=300)
         sr_org.setInputs(Ti=350)
         sr_org.setInputs(Vdi=100)
         sr_org.setInputs(cAi=1)
```

```
In [11]: u = sr_org.getInputs()
         u.keys()
```

```
Out[11]: ['Vdi', 'cAi', 'Tc', 'Ti']
```

```
In [12]: u["Ti"]
```

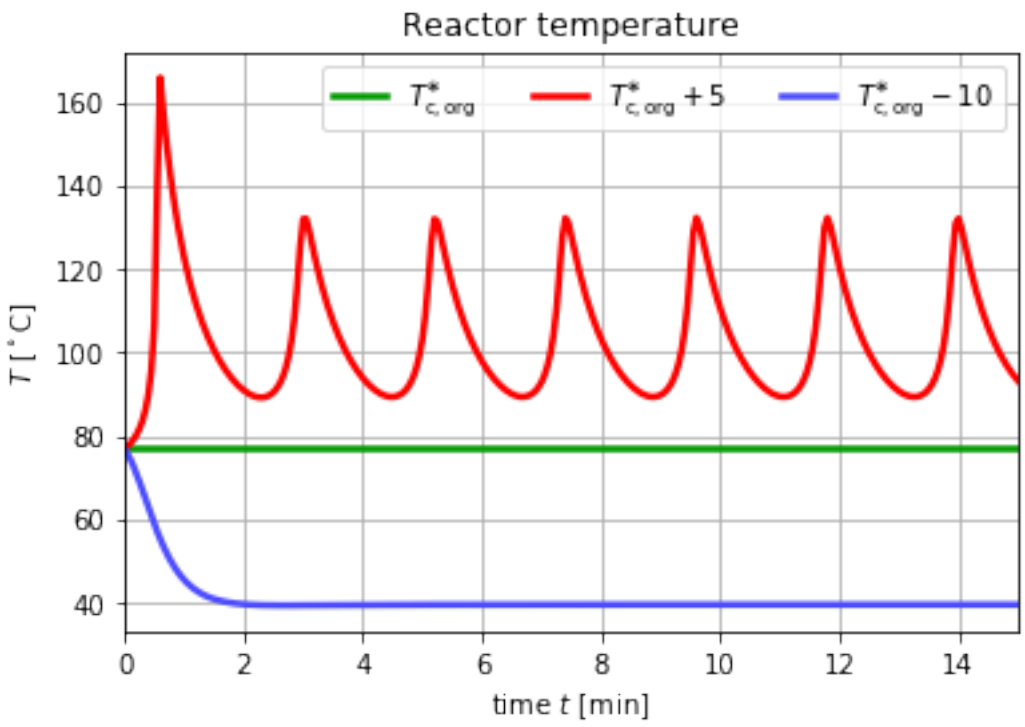
```
Out[12]: [(0.0, 350), (15.0, 350)]
```

Simulating system for three cases of inputs, and extracting results

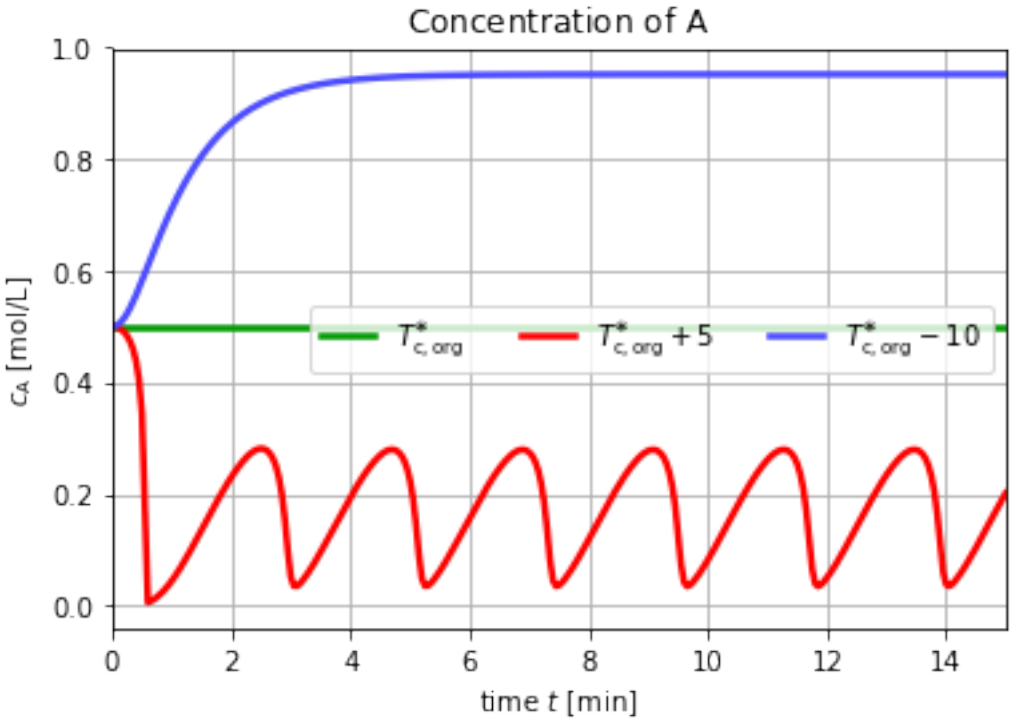
```
In [13]: sr_org.setInputs(Tc=300)
         sr_org.simulate()
         tm_org0, T_org0, Tc_org0, cA_org0 = sr_org.getSolutions("time","T","Tc","cA")
         sr_org.setInputs(Tc=300+5)
         sr_org.simulate()
         tm_org0p, T_org0p, Tc_org0p, cA_org0p = sr_org.getSolutions("time","T","Tc","cA")
         sr_org.setInputs(Tc=300-10)
         sr_org.simulate()
         tm_org0m, T_org0m, Tc_org0m, cA_org0m = sr_org.getSolutions("time","T","Tc","cA")
```

Plotting results

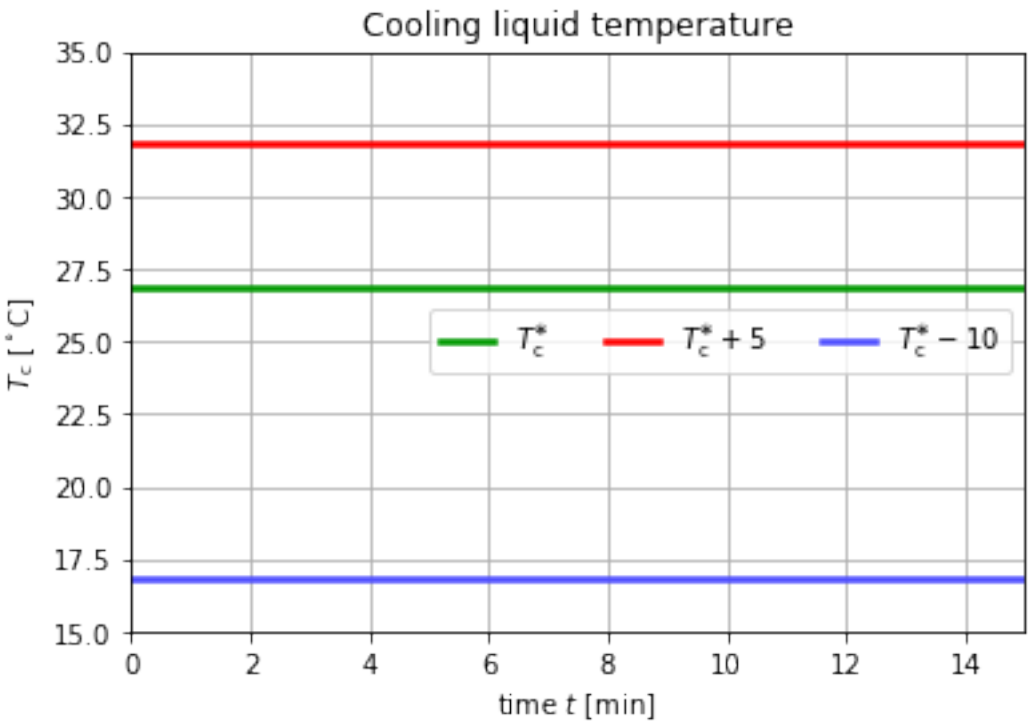
```
In [14]: plt.plot(tm_org0,T_org0-273.15,LW=LW1,color=Cg1,label=r"$T_{\mathrm{c,org}}^{\ast}$")
         plt.plot(tm_org0p,T_org0p-273.15,LW=LW1,color=Cr1,label=r"$T_{\mathrm{c,org}}^{\ast}+5$
         plt.plot(tm_org0m,T_org0m-273.15,LW=LW1,color=Cb1,label=r"$T_{\mathrm{c,org}}^{\ast}-10
         plt.legend(ncol=3)
         plt.title("Reactor temperature")
         plt.xlabel(r"time $t$ [min]")
         plt.ylabel(r"$T$ [${}^\circ \mathrm{C}$]")
         plt.grid()
         plt.xlim(0,15)
         figfile = "tempSeborgCSTRorg.pdf"
         plt.savefig(figpath+figfile)
```



In [15]:
```
plt.plot(tm_org0,cA_org0,LW=LW1,color=Cg1,label=r"$T_{\mathrm{c,org}}^{\ast}$")
plt.plot(tm_org0p,cA_org0p,LW=LW1,color=Cr1,label=r"$T_{\mathrm{c,org}}^{\ast}+5$")
plt.plot(tm_org0m,cA_org0m,LW=LW1,color=Cb1,label=r"$T_{\mathrm{c,org}}^{\ast}-10$")
plt.legend(ncol=3,loc=7)
plt.title("Concentration of $\mathrm{A}$")
plt.xlabel(r"time $t$ [min]")
plt.ylabel(r"$c_{\mathrm{A}}$ [mol/L]")
plt.grid()
plt.xlim(0,15)
figfile = "concSeborgCSTRorg.pdf"
plt.savefig(figpath+figfile)
```



In [16]:
```
plt.plot(tm_org0,Tc_org0-273.15,LW=LW1, color=Cg1, label=r"$T_\mathrm{c}^{\ast}$")
plt.plot(tm_org0p,Tc_org0p-273.15,LW=LW1,color=Cr1, label=r"$T_\mathrm{c}^{\ast}+5$")
plt.plot(tm_org0m,Tc_org0m-273.15,LW=LW1,color=Cb1, label=r"$T_\mathrm{c}^{\ast}-10$")
plt.title("Cooling liquid temperature")
plt.xlabel(r"time $t$ [min]")
plt.ylabel(r"$T_\mathrm{c}$ [${}^\circ \mathrm{C}$]")
plt.grid()
plt.axis(ymin=15,ymax=35)
plt.xlim(0,15)
plt.legend(ncol=3,loc=7)
figfile = "coolSeborgCSTRorg.pdf"
plt.savefig(figpath+figfile)
```



1.1.5 Analysis: why oscillations?

Steady state model: steady concentration gives

$$\frac{dc_\mathrm{A}}{dt} = 0 \Rightarrow 0 = \frac{\dot{V}_\mathrm{i}}{V}\left(c_\mathrm{A,i} - c_\mathrm{A}\right) - kc_\mathrm{A} \Rightarrow c_\mathrm{A}(T) = \frac{\dot{V}_\mathrm{i}/V}{k_0 \exp\left(-\frac{E/R}{T}\right) + \dot{V}_\mathrm{i}/V} c_\mathrm{A,i}$$

while steady temperature gives

$$C_p \frac{dT}{dt} = 0 \Rightarrow 0 = \frac{\dot{V}_\mathrm{i}}{V} C_p \left(T_\mathrm{i} - T\right) + \left(-\Delta_\mathrm{r}\tilde{H}\right) rV + \dot{Q} \Rightarrow$$

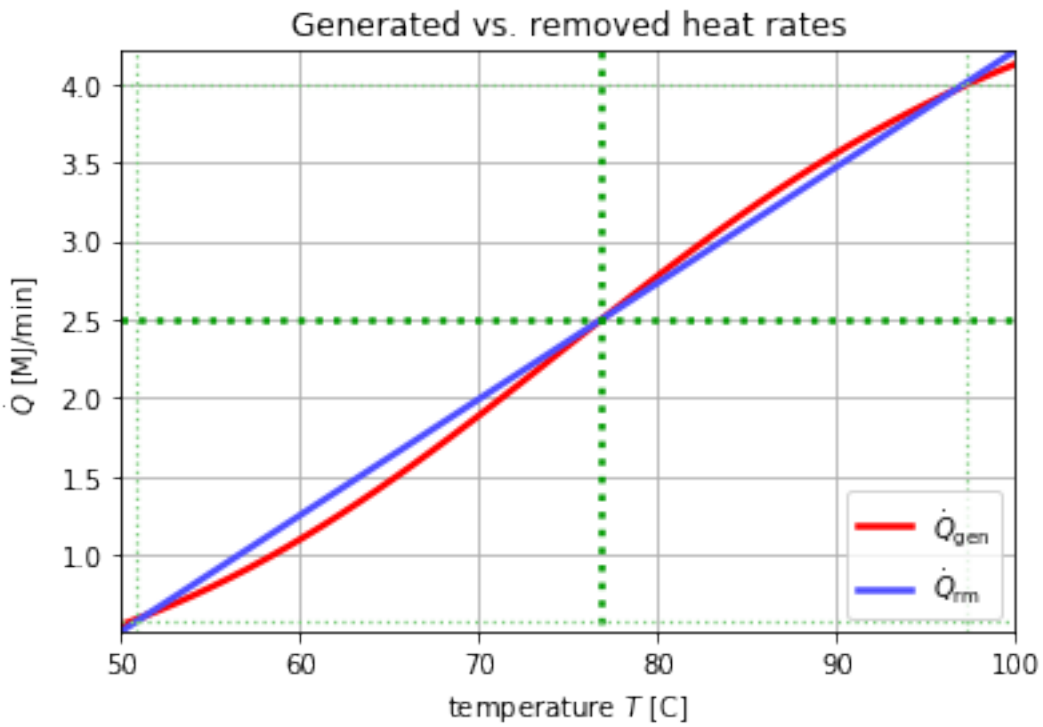
$$0 = \underbrace{\frac{\dot{V}_\mathrm{i}}{V} C_p \left(T_\mathrm{i} - T\right) + \mathcal{U}A\left(T_\mathrm{c} - T\right)}_{=-\dot{Q}_\mathrm{rm}(T)} + \underbrace{\left(-\Delta_\mathrm{r}\tilde{H}\right) k_0 \exp\left(-\frac{E/R}{T}\right) c_\mathrm{A}(T) \cdot V}_{=\dot{Q}_\mathrm{gen}(T)}$$

We now plot "removed heat rate" $\dot{Q}_\mathrm{rm}(T)$ and "generated heat rate" $\dot{Q}_\mathrm{gen}(T)$: at equilibrium, they must be equal.

```
In [17]: EdR = 8750
         k0 = np.exp(EdR/350)
         VdidV = 1
         cAi = 1
         def cA(T):
```

```
        return VdidV/(k0*np.exp(-EdR/T) + VdidV)*cAi
    #
    rho = 1e3
    V = 100
    cph = 0.239
    Cp = rho*V*cph
    DrHt = -5e4
    UA = 5e4
    Ti = 350
    Tc = 300
    def Qdrm(T,Tc):
        return -(VdidV*Cp*(Ti-T) + UA*(Tc-T))

    def Qdgen(T):
        return (-DrHt)*k0*np.exp(-EdR/T)*cA(T)*V
```

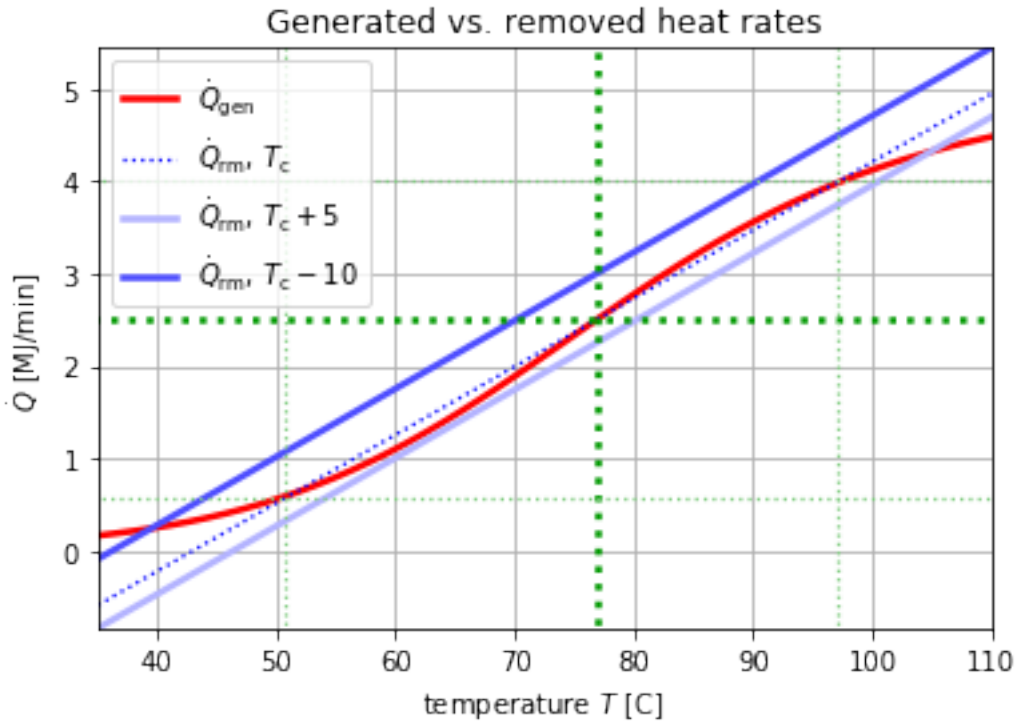
In [18]:
```
TT = np.linspace(50,100)
plt.plot(TT, Qdgen(TT+273.15)/1e6,LW=LW1, color=Cr1, label=r"$\dot{Q}_\mathrm{gen}$")
plt.plot(TT, Qdrm(TT+273.15,Tc)/1e6,LW=LW1, color=Cb1, label=r"$\dot{Q}_\mathrm{rm}$")
plt.plot((350-273.15)*np.array([1,1]), [0,5],LW=LW1,color=Cg1,LS=LS2)
plt.plot([50,100], Qdrm(350,Tc)/1e6*np.array([1,1]),LW=LW1,color=Cg1,LS=LS2)
plt.plot((50.8)*np.array([1,1]), [0,5],LW=LW2,color=Cg2,LS=LS2)
plt.plot([50,100], Qdrm(50.8+273.15,Tc)/1e6*np.array([1,1]),LW=LW2,color=Cg2,LS=LS2)
plt.plot((97.2)*np.array([1,1]), [0,5],LW=LW2,color=Cg2,LS=LS2)
plt.plot([50,100], Qdrm(97.2+273.15,Tc)/1e6*np.array([1,1]),LW=LW2,color=Cg2,LS=LS2)
plt.title("Generated vs. removed heat rates")
plt.xlabel(r"temperature $T$ [C]")
plt.ylabel(r"$\dot{Q}$ [MJ/min]")
plt.grid()
plt.xlim(50,100)
plt.ylim(np.min(Qdrm(TT+273.15,Tc)/1e6), np.max(Qdrm(TT+273.15,Tc)/1e6))
plt.legend()
figfile = "equilSeborgCSTRorg.pdf"
plt.savefig(figpath+figfile)
```



Observe that the system has 3 equilibrium points. For the Seborg reactor, we start the system at $T = 350 - 273.15$ [C], which is at the intersection of the thick green, dotted lines. If the reactor is operated so that the temperature becomes higher than $350 - 273.15$ [C], a higher heat rate is generated than removed, and the temperature increases. If, on the other hand, the temperature is operated so that the temperature becomes lower than $350 - 273.15$ [C], then the removal heat rate is higher than the generated heat rate, and the reactor is cooled. In summary: the equilibrium point given by the green cross is **unstable**. Similar arguments leads to the conclusion that the other two equilibrium points (at ca. $T = 50.8$ [C] and ca. $T = 97.2$ [C]) are **stable**. This analysis does not explain *oscillations*, but it seems reasonable that oscillations may occur: * If the temperature increases, generated heat rate ($\dot{Q}_{\mathrm{gen}}$) will first increase. However, concentration of species A drops and eventually the reaction rate will draw to a halt - and generated heat rate will drop. Thus, the reactor temperature will drop. * As the reactor cools down, species A will increase in concentration due to addition of fresh A in the influent. Then, eventually, the reaction rate will "ignite" again, and the generated heat rate will again increase, leading to increasing temperature. * This will take place cyclically.

```
In [19]: TT = np.linspace(35,110)
         plt.plot(TT, Qdgen(TT+273.15)/1e6,LW=LW1, color=Cr1, label=r"$\dot{Q}_\mathrm{gen}$")
         plt.plot(TT, Qdrm(TT+273.15,Tc)/1e6,LW=LW2, color="blue", LS = LS2, label=r"$\dot{Q}_\m
         plt.plot(TT, Qdrm(TT+273.15,Tc+5)/1e6,LW=LW1, color=Cb2, label=r"$\dot{Q}_\mathrm{rm}$,
         plt.plot(TT, Qdrm(TT+273.15,Tc-10)/1e6,LW=LW1, color=Cb1, label=r"$\dot{Q}_\mathrm{rm}$
         #
         plt.plot((350-273.15)*np.array([1,1]), [-1,6],LW=LW1,color=Cg1,LS=LS2)
         plt.plot([30,110], Qdrm(350,Tc)/1e6*np.array([1,1]),LW=LW1,color=Cg1,LS=LS2)
```

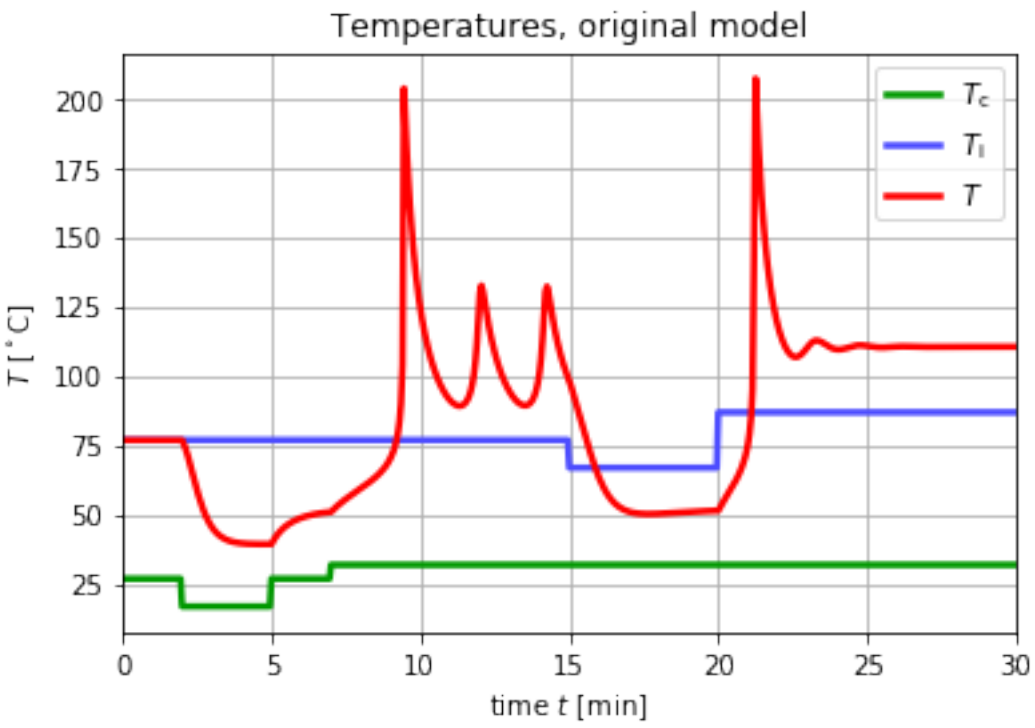
```
plt.plot((50.8)*np.array([1,1]), [-1,6],LW=LW2,color=Cg2,LS=LS2)
plt.plot([30,110], Qdrm(50.8+273.15,Tc)/1e6*np.array([1,1]),LW=LW2,color=Cg2,LS=LS2)
plt.plot((97.2)*np.array([1,1]), [-1,6],LW=LW2,color=Cg2,LS=LS2)
plt.plot([30,110], Qdrm(97.2+273.15,Tc)/1e6*np.array([1,1]),LW=LW2,color=Cg2,LS=LS2)
#
plt.title("Generated vs. removed heat rates")
plt.xlabel(r"temperature $T$ [C]")
plt.ylabel(r"$\dot{Q}$ [MJ/min]")
plt.grid()
plt.xlim(35,110)
plt.ylim(np.min(Qdrm(TT+273.15,Tc+5)/1e6), np.max(Qdrm(TT+273.15,Tc-10)/1e6))
plt.legend()
figfile = "equil_1_SeborgCSTRorg.pdf"
plt.savefig(figpath+figfile)
```



Observe that for cooling temperature $T_c - 10$, the initial temperature leads to reduced temperature until the single equilibrium point at ca. $T_c = 40$ [C] is reached. For the warmer cooling temperature (= less cooling) of $T_c + 5$, the initial temperature leads to increased temperature. While it may seem like there is a single, stable equilibrium at ca. $T_c = 103$ [C] (and possibly a point which is difficult to interpret at ca. $T_c = [60, 65]$ [C], it is important to realize that this analysis is purely based on steady state analysis, and that the dynamics may (and: in fact does!) influence the behavior.

1.1.6 Time varying inputs

```
In [20]: uTc = [(0,300),(2,300),(2,300-10),(5,300-10),(5,300),(7,300),(7,300+5),(30,300+5)]
         uTi = [(0,350),(15,350),(15,340),(20,340),(20,360),(30,360)]

In [21]: sr_org.setInputs(Tc=uTc)
         sr_org.setInputs(Ti=uTi)

In [22]: sr_org.setSimulationOptions(stopTime=30)
         sr_org.simulate()

In [23]: tm, T, Tc, Ti = sr_org.getSolutions("time","T","Tc","Ti")
         plt.plot(tm,Tc-273.15,LW=LW1,color=Cg1,label=r"$T_{\mathrm{c}}$")
         plt.plot(tm,Ti-273.15,LW=LW1,color=Cb1,label=r"$T_{\mathrm{i}}$")
         plt.plot(tm,T-273.15,LW=LW1,color=Cr1,label=r"$T$")
         plt.title("Temperatures, original model")
         plt.xlabel(r"time $t$ [min]")
         plt.ylabel(r"$T$ [${}^\circ \mathrm{C}$]")
         plt.grid()
         plt.xlim(0,30)
         plt.legend()
         figfile = "varInputSeborgCSTRorg.pdf"
         plt.savefig(figpath+figfile)
```



SeborgCSTR_control_basic

March 13, 2018

1 Use of Modelica + Python in Process Systems Engineering Education

1.1 Basic control of "Seborg reactor"

1.1.1 Bernt Lie

1.1.2 University College of Southeast Norway

Basic import and definitions

```
In [1]: from OMPython import ModelicaSystem
        import numpy as np
        import numpy.random as nr
        %matplotlib inline
        import matplotlib.pyplot as plt
        import pandas as pd
        LW1 = 2.5
        LW2 = LW1/2
        Cb1 = (0.3,0.3,1)
        Cb2 = (0.7,0.7,1)
        Cg1 = (0,0.6,0)
        Cg2 = (0.5,0.8,0.5)
        Cr1 = "Red"
        Cr2 = (1,0.5,0.5)
        LS1 = "solid"
        LS2 = "dotted"
        LS3 = "dashed"
        figpath = "../figs/"
```

1.1.3 Basic control design

Instantiating models and setting inputs

```
In [2]: sr_org = ModelicaSystem("SeborgCSTR.mo","SeborgCSTR.ModSeborgCSTRorg")
```

```
2018-03-13 16:09:31,720 - OMPython - INFO - OMC Server is up and running at file:///c:/users/ber
```

```
In [3]: sr_org.setSimulationOptions(stopTime=15,stepSize=0.05)
        #
        sr_org.setInputs(Tc=300)
        sr_org.setInputs(Ti=350)
        sr_org.setInputs(Vdi=100)
        sr_org.setInputs(cAi=1)
```

Linearizing model

```
In [4]: sr_org.getLinearizationOptions()

Out[4]: {'numberOfIntervals': 500.0,
         'startTime': 0.0,
         'stepSize': 0.002,
         'stopTime': 1.0,
         'tolerance': 1e-08}

In [5]: A_org, B_org, C_org, D_org = sr_org.linearize()

2018-03-13 16:09:39,717 - OMPython - INFO - OMC Server is up and running at file:///c:/users/ber


In [6]: A_org

Out[6]: array([[  4.37955768e+00,   2.09205021e+02],
               [ -3.57142857e-02,  -2.00000000e+00]])

In [7]: B_org

Out[7]: array([[  2.09205021e+00,   1.00000000e+00,   1.70530257e-15,
                  0.00000000e+00],
               [  0.00000000e+00,   0.00000000e+00,   5.00000000e-03,
                  1.00000000e+00]])

In [8]: C_org

Out[8]: array([[ 1.,  0.]])

In [9]: D_org

Out[9]: array([[ 0.,  0.,  0.,  0.]])

In [10]: sr_org.getLinearInputs()

Out[10]: ['Tc', 'Ti', 'Vdi', 'cAi']

In [11]: sr_org.getLinearStates()

Out[11]: ['T', 'cA']

In [12]: sr_org.getLinearOutputs()

Out[12]: ['y_T']
```

Theoretical results With $x = (T, n_A)$, $u = (T_{c,i}, T_i, \dot{V}, c_{A,i})$ and $y = c_A$, the linearized model is:

$$\frac{dx^\delta}{dt} = Ax^\delta + Bu^\delta$$

$$y^\delta = Cx^\delta + Du^\delta$$

where:

$$A = \begin{pmatrix} 4.3796 & 2.0921 \\ -3.5714 & -2 \end{pmatrix}$$

$$B = \begin{pmatrix} 2.0921 & 1 & 0 & 0 \\ 0 & 0 & 0.5 & 100 \end{pmatrix}$$

$$C = \begin{pmatrix} 0 & 0.01 \end{pmatrix}$$

$$D = \begin{pmatrix} 0 & 0 & 0 & 0 \end{pmatrix}$$

This means that OMPython/the Python API has correctly linearized the model.

```
In [13]: np.linalg.eig(A_org)
```

```
Out[13]: (array([ 2.83388381, -0.45432613]), array([[ 0.99997271, -0.99973316],
                 [-0.00738812,  0.0230998 ]]))
```

Transfer function from T_c to T (from MATLAB due to some lack of support for control toolbox in Python):

Observe... At the initial state, the system is open loop unstable due to the eigenvalue at +2.83388381. Observe also that with T_c as the control input/manipulatable variable and T as the controlled output, the system has a zero at $2.092 \cdot s + 4.184 = 0 \Rightarrow s = -2$; in other words, the zero dynamics is stable!

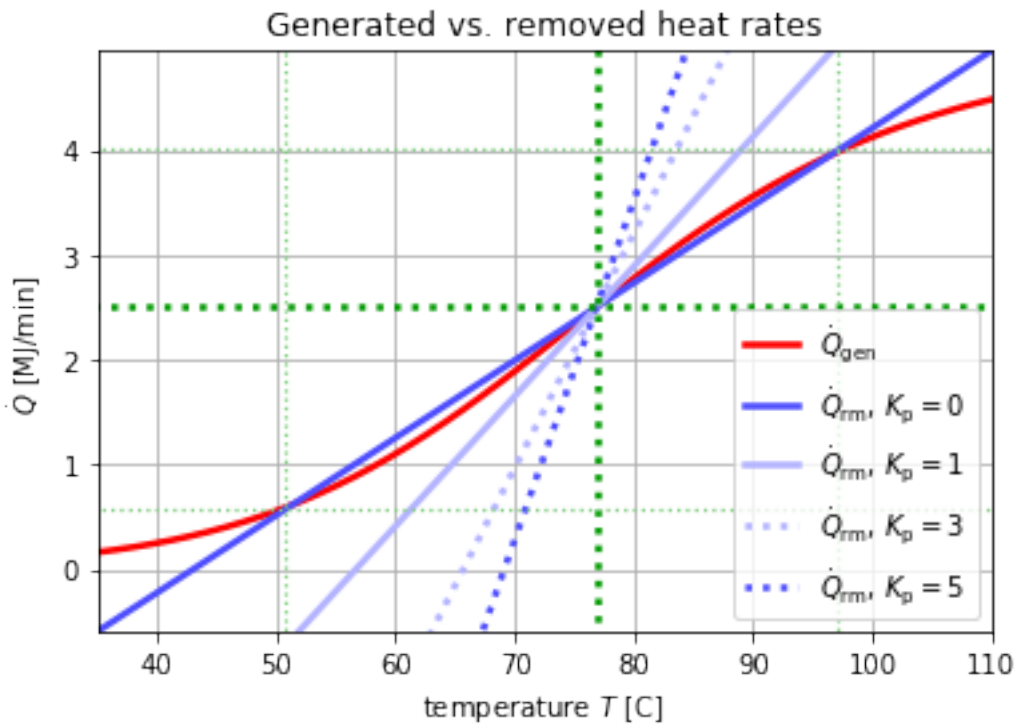
Tuning P-controller A P-controller for controlling output $y = T$ via control input $u = T_c$ will have form $u = T_c^* + K_p(T_{ref} - T)$. This will change the expression for $\dot{Q}_{rm}$ to:

$$-\dot{Q}_{rm} = \frac{\dot{V}_i}{V} C_p (T_i - T) + \mathcal{U}A \left(T_c^* + K_p(T_{ref} - T) - T\right)$$

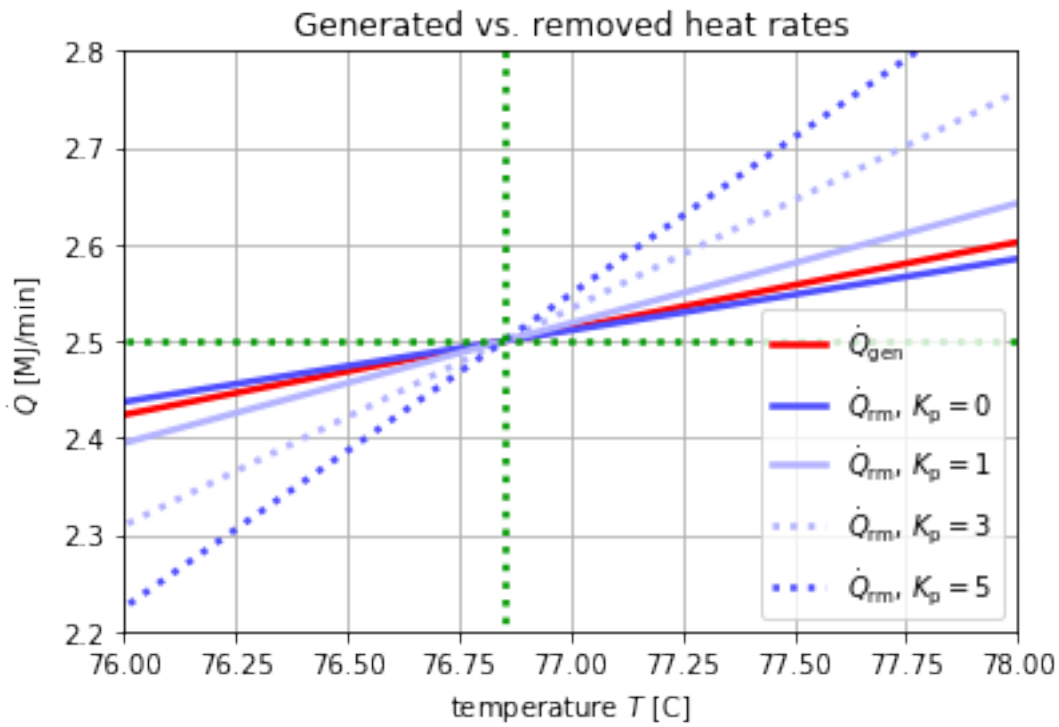
```
In [14]: EdR = 8750
         k0 = np.exp(EdR/350)
         VdidV = 1
         cAi = 1
         def cA(T):
             return VdidV/(k0*np.exp(-EdR/T) + VdidV)*cAi
         #
```

```
rho = 1e3
V = 100
cph = 0.239
Cp = rho*V*cph
DrHt = -5e4
UA = 5e4
Ti = 350
Tcast = 300
Tref = 350
Kp = 0

def Qdrm(T,Kp):
    return -(VdidV*Cp*(Ti-T) + UA*(Tcast+Kp*(Tref-T)-T))

def Qdgen(T):
    return (-DrHt)*k0*np.exp(-EdR/T)*cA(T)*V
```

In [15]:
```
TT = np.linspace(35,110)
plt.plot(TT, Qdgen(TT+273.15)/1e6,LW=LW1, color=Cr1, label=r"$\dot{Q}_\mathrm{gen}$")
plt.plot(TT, Qdrm(TT+273.15,Kp)/1e6,LW=LW1, color=Cb1, label=r"$\dot{Q}_\mathrm{rm}$, $
plt.plot(TT, Qdrm(TT+273.15,1)/1e6,LW=LW1, color=Cb2, label=r"$\dot{Q}_\mathrm{rm}$, $K
plt.plot(TT, Qdrm(TT+273.15,3)/1e6,LW=LW1, color=Cb2, LS = LS2, label=r"$\dot{Q}_\mathr
plt.plot(TT, Qdrm(TT+273.15,5)/1e6,LW=LW1, color=Cb1, LS = LS2, label=r"$\dot{Q}_\mathr
#
plt.plot((350-273.15)*np.array([1,1]), [-1,6],LW=LW1,color=Cg1,LS=LS2)
plt.plot([30,110], Qdrm(350,Kp)/1e6*np.array([1,1]),LW=LW1,color=Cg1,LS=LS2)
plt.plot((50.8)*np.array([1,1]), [-1,6],LW=LW2,color=Cg2,LS=LS2)
plt.plot([30,110], Qdrm(50.8+273.15,Kp)/1e6*np.array([1,1]),LW=LW2,color=Cg2,LS=LS2)
plt.plot((97.2)*np.array([1,1]), [-1,6],LW=LW2,color=Cg2,LS=LS2)
plt.plot([30,110], Qdrm(97.2+273.15,Kp)/1e6*np.array([1,1]),LW=LW2,color=Cg2,LS=LS2)
#
plt.title("Generated vs. removed heat rates")
plt.xlabel(r"temperature $T$ [C]")
plt.ylabel(r"$\dot{Q}$ [MJ/min]")
plt.grid()
plt.xlim(35,110)
plt.ylim(np.min(Qdrm(TT+273.15,Kp)/1e6), np.max(Qdrm(TT+273.15,Kp)/1e6))
plt.legend()
figfile = "equil_controlled_SeborgCSTRorg.pdf"
plt.savefig(figpath+figfile)
```




```
In [16]: plt.plot(TT, Qdgen(TT+273.15)/1e6,LW=LW1, color=Cr1, label=r"$\dot{Q}_\mathrm{gen}$")
         plt.plot(TT, Qdrm(TT+273.15,Kp)/1e6,LW=LW1, color=Cb1, label=r"$\dot{Q}_\mathrm{rm}$, $
         plt.plot(TT, Qdrm(TT+273.15,1)/1e6,LW=LW1, color=Cb2, label=r"$\dot{Q}_\mathrm{rm}$, $K
         plt.plot(TT, Qdrm(TT+273.15,3)/1e6,LW=LW1, color=Cb2, LS = LS2, label=r"$\dot{Q}_\mathr
         plt.plot(TT, Qdrm(TT+273.15,5)/1e6,LW=LW1, color=Cb1, LS = LS2, label=r"$\dot{Q}_\mathr
         #
         plt.plot((350-273.15)*np.array([1,1]), [-1,6],LW=LW1,color=Cg1,LS=LS2)
         plt.plot([30,110], Qdrm(350,Kp)/1e6*np.array([1,1]),LW=LW1,color=Cg1,LS=LS2)
         plt.plot((50.8)*np.array([1,1]), [-1,6],LW=LW2,color=Cg2,LS=LS2)
         plt.plot([30,110], Qdrm(50.8+273.15,Kp)/1e6*np.array([1,1]),LW=LW2,color=Cg2,LS=LS2)
         plt.plot((97.2)*np.array([1,1]), [-1,6],LW=LW2,color=Cg2,LS=LS2)
         plt.plot([30,110], Qdrm(97.2+273.15,Kp)/1e6*np.array([1,1]),LW=LW2,color=Cg2,LS=LS2)
         #
         plt.title("Generated vs. removed heat rates")
         plt.xlabel(r"temperature $T$ [C]")
         plt.ylabel(r"$\dot{Q}$ [MJ/min]")
         plt.grid()
         plt.xlim(76,78)
         plt.ylim(2.2,2.8)
         plt.legend()
         figfile = "equil_detail_controlled_SeborgCSTRorg.pdf"
         plt.savefig(figpath+figfile)
```

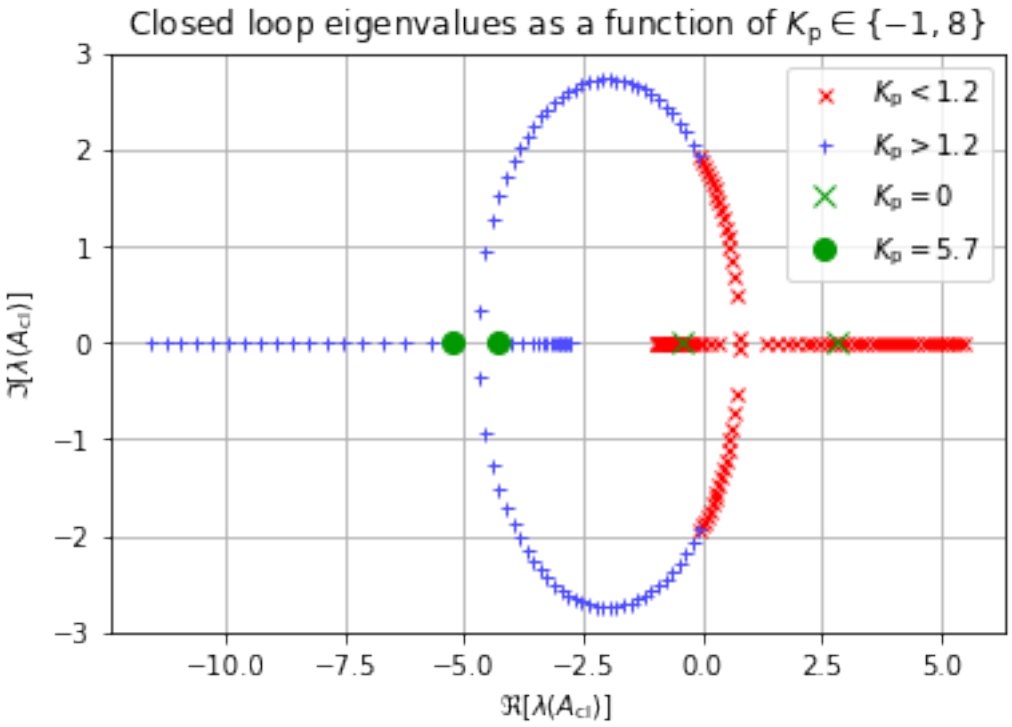


Observe... With $K_p = 0$, we have seen that the system is (open loop) unstable. With $K_p = 1$, the system *appears* to have a stable equilibrium point, and the larger the value for the gain is, the larger the stability margin becomes. (This is contrary to open-loop stable systems.) However, as we will see below: the choice $K_p = 1$ is not sufficient go guarantee stability: we need to consider both the effect in temperature and in concentration!

Root locus diagram for system with P-controller

```
In [17]: A_ol = A_org
         B_ol = np.zeros((A_ol.shape[0],1))
         B_ol[:,0] = B_org[:,0]
         C_ol = C_org
         #
         KKp = np.linspace(-1,1.2)
         Eig = np.zeros((KKp.size,2),np.dtype(complex))
         #
         for (i,Kp) in enumerate(KKp):
             A_cl = A_org - Kp*B_ol*C_ol
             Eig[i,:] = np.linalg.eig(A_cl)[0]
         #
         plt.plot(np.real(Eig)[:,0],np.imag(Eig)[:,0],"x",color=Cr1,markersize=5)
         plt.plot(np.real(Eig)[:,1],np.imag(Eig)[:,1],"x",color=Cr1,markersize=5, label=r"$K_\ma
         #
```

```
KKp = np.linspace(1.2,8)
Eig = np.zeros((KKp.size,2),np.dtype(complex))
#
for (i,Kp) in enumerate(KKp):
    A_cl = A_org - Kp*B_ol*C_ol
    Eig[i,:] = np.linalg.eig(A_cl)[0]
#
plt.plot(np.real(Eig)[:,0],np.imag(Eig)[:,0],"+",color=Cb1,markersize=5)
plt.plot(np.real(Eig)[:,1],np.imag(Eig)[:,1],"+",color=Cb1,markersize=5, label=r"$K_\ma
#
Eig0 = np.linalg.eig(A_ol)[0]
plt.plot(np.real(Eig0)[0],np.imag(Eig0)[0],"x",color=Cg1,markersize=8)
plt.plot(np.real(Eig0)[1],np.imag(Eig0)[1],"x",color=Cg1,markersize=8, label=r"$K_\math
#
Eig1 = np.linalg.eig(A_org - 5.7*B_ol*C_ol)[0]
plt.plot(np.real(Eig1)[0],np.imag(Eig1)[0],"o",color=Cg1,markersize=8)
plt.plot(np.real(Eig1)[1],np.imag(Eig1)[1],"o",color=Cg1,markersize=8, label=r"$K_\math
#
plt.grid()
plt.xlabel(r"$\Re [ \lambda (A_\mathrm{cl}) ]$")
plt.ylabel(r"$\Im [ \lambda (A_\mathrm{cl}) ]$")
plt.title(r"Closed loop eigenvalues as a function of $K_\mathrm{p}\in\{-1,8\}$")
plt.legend()
figfile = "ClosedLoop_Eigenvals_SeborgCSTRorg.pdf"
plt.savefig(figpath+figfile)
```



Observe... The system appears to be stable with a P-controller when $K_p > 1.2$ or so. With $K_p \approx 5.7$, both eigenvalues become real with similar values. Some modification may be needed if we add integral action, but probably not much. We could probably choose $T_i \in \{2, 5\}$ or so (some 10 times closed loop timeconstant of ca. $1/5$).

1.1.4 Simulation of system with P-controller

Modelica model for PI control system

```
model PIconSeborgCSTRorg
  // Simulation of Seborg Reactor
  // author:  Bernt Lie
  //          University of Southeast Norway
  //          January 10, 2018
  //
  // Instantiate model of Seborg Reactor (sr)
  ModSeborgCSTRorg srORG;
  // Declaring parameters
  parameter Real Kp = 0 "Proportional gain in P-controller";
  parameter Real Tc_min = 273.15 "Minimum cooling temperature (freezing point), K";
  // Declaring variables
  // -- inputs
  Real _Vdi "Volumetric flow rate through reactor, L/s";
  Real _cAi "Influent molar concentration of A, mol/s";
  Real _Ti "Influent temperature, K";
  Real _Tc_nom "Nominal cooling temperature, K";
  Real T_ref "Temperature reference, K";
  // -- outputs
  output Real _cA_org "Molar concentration of A, mol/L";
  output Real _T_org "Reactor temperature, K";
  output Real _Tc_org "Controlled cooling temperature, K";
  // Equations
equation
  // -- input values
  _Vdi = 100;
  _cAi = 1;
  _Ti = 350;
  _Tc_nom = 300;
  T_ref = if time < 3 then 350 else 360;
  // -- injecting input functions to model inputs
  srORG.Vdi = _Vdi;
  srORG.cAi = _cAi;
  srORG.Ti = _Ti;
  srORG.Tc = max(Tc_min,_Tc_nom + Kp*(T_ref - _T_org));
  // -- outputs
```

```
    _cA_org = srORG.cA;
    _T_org = srORG.T;
    _Tc_org = srORG.Tc;
  end PIconSeborgCSTRorg;
```

Instantiating controlled system

```
In [18]: c_sr_org = ModelicaSystem("SeborgCSTR.mo","SeborgCSTR.PIconSeborgCSTRorg")

2018-03-13 16:09:44,849 - OMPython - INFO - OMC Server is up and running at file:///c:/users/ber


In [19]: pd.DataFrame(c_sr_org.getQuantities())
```

Out[19]:

	Changeable	Description
0	false	Initializing temperature in reactor, K
1	false	Initializing concentration of A in reactor, mol/L
2	false	der(Initializing temperature in reactor, K)
3	false	der(Initializing concentration of A in reactor...
4	false	None
5	false	Temperature reference, K
6	false	Reactor temperature, K
7	false	Nominal cooling temperature, K
8	false	Controlled cooling temperature, K
9	false	Influent temperature, K
10	false	Volumetric flow rate through reactor, L/s
11	false	Molar concentration of A, mol/L
12	false	Influent molar concentration of A, mol/s
13	false	Heat flow rate, J/min
14	false	Reaction 'constant', ...
15	false	Rate of reaction, mol/(L.s)
16	true	Proportional gain in P-controller
17	true	Minimum cooling temperature (freezing point), K
18	true	Molar enthalpy of reaction, J/mol
19	true	Activation temperature, K
20	true	Initial temperature, K
21	true	Heat transfer parameter, J/(min.K)
22	true	Reactor volume, L
23	true	Stoichiometric constant, -
24	true	Initial concentration of A, mol/L
25	true	Specific heat capacity of mixture, J.g-1.K-1
26	false	Pre-exponential factor, 1/min
27	true	Liquid density, g/L
28	false	Cooling temperature', K
29	false	Influent temperature, K
30	false	Volumetric flow rate through reactor, L/min
31	false	Influent molar concentration of A, mol/L
32	false	Reactor temperature, K

	Name	Value	Variability	alias	aliasvariable
0	srORG.T	None	continuous	noAlias	None
1	srORG.cA	None	continuous	noAlias	None
2	der(srORG.T)	None	continuous	noAlias	None
3	der(srORG.cA)	None	continuous	noAlias	None
4	$cse1	None	continuous	noAlias	None
5	T_ref	350.0	continuous	noAlias	None
6	_T_org	None	continuous	noAlias	None
7	_Tc_nom	None	continuous	noAlias	None
8	_Tc_org	None	continuous	noAlias	None
9	_Ti	None	continuous	noAlias	None
10	_Vdi	None	continuous	noAlias	None
11	_cA_org	None	continuous	noAlias	None
12	_cAi	None	continuous	noAlias	None
13	srORG.Qd	None	continuous	noAlias	None
14	srORG.k	None	continuous	noAlias	None
15	srORG.r	None	continuous	noAlias	None
16	Kp	0.0	parameter	noAlias	None
17	Tc_min	273.15	parameter	noAlias	None
18	srORG.DrHt	-50000.0	parameter	noAlias	None
19	srORG.EdR	8750.0	parameter	noAlias	None
20	srORG.T0	350.0	parameter	noAlias	None
21	srORG.UA	50000.0	parameter	noAlias	None
22	srORG.V	100.0	parameter	noAlias	None
23	srORG.a	1.0	parameter	noAlias	None
24	srORG.cA0	0.5	parameter	noAlias	None
25	srORG.cph	0.239	parameter	noAlias	None
26	srORG.k0	None	parameter	noAlias	None
27	srORG.rho	1000.0	parameter	noAlias	None
28	srORG.Tc	None	continuous	alias	_Tc_org
29	srORG.Ti	None	continuous	alias	_Ti
30	srORG.Vdi	None	continuous	alias	_Vdi
31	srORG.cAi	None	continuous	alias	_cAi
32	srORG.y_T	None	continuous	alias	srORG.T

In [20]:
```
c_sr_org.setSimulationOptions(stopTime=15,stepSize=0.05)
```

Parameters & Simulation

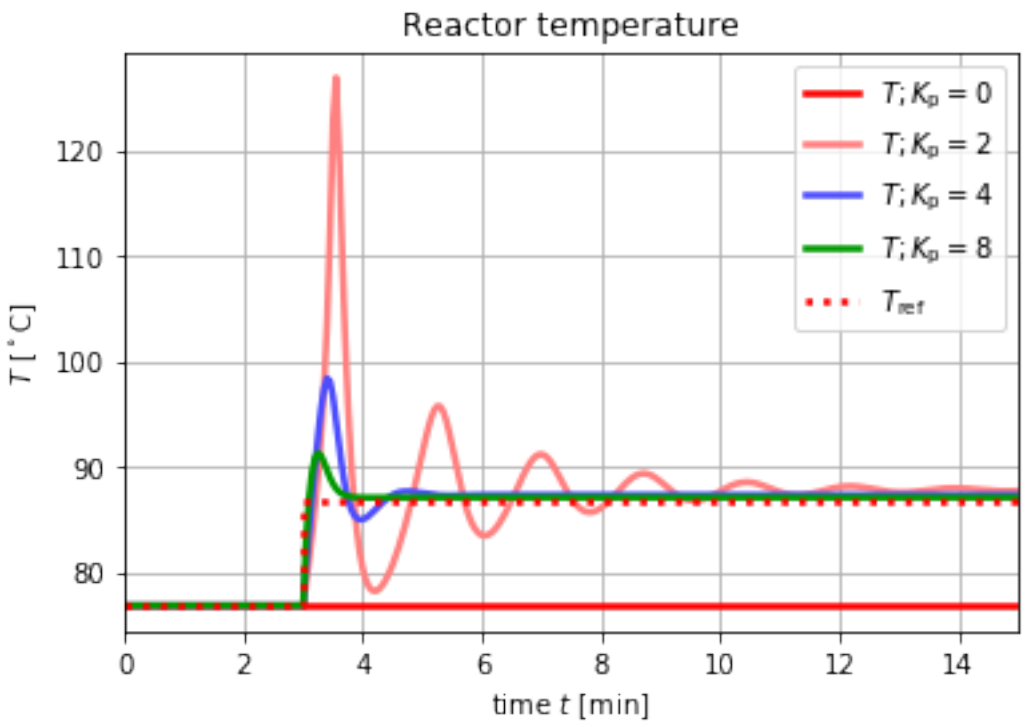
In [21]:
```
c_sr_org.getParameters()
```

Out[21]:
```
{'Kp': 0.0,
 'Tc_min': 273.15,
 'srORG.DrHt': -50000.0,
 'srORG.EdR': 8750.0,
 'srORG.T0': 350.0,
 'srORG.UA': 50000.0,
```

```
 'srORG.V': 100.0,
 'srORG.a': 1.0,
 'srORG.cA0': 0.5,
 'srORG.cph': 0.239,
 'srORG.k0': None,
 'srORG.rho': 1000.0}
```

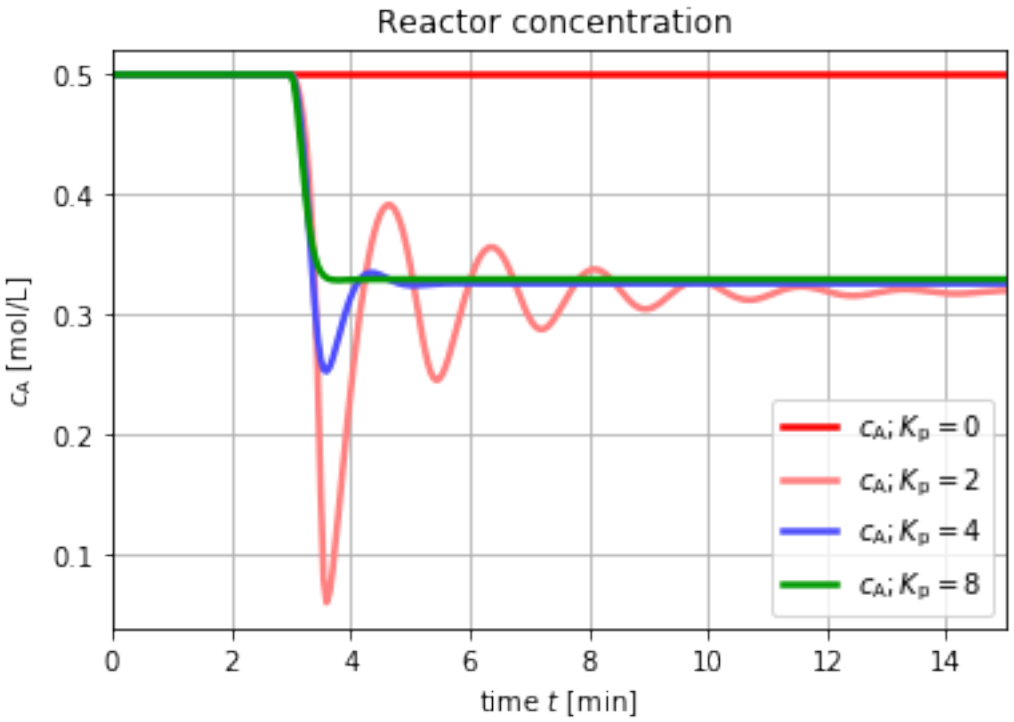
Plotting results

```
In [22]: c_sr_org.setParameters(Tc_min = -1e3)
         c_sr_org.setParameters(Kp=0)
         c_sr_org.simulate()
         tm_corg, T_corg, Tc_corg, cA_corg, T_ref = c_sr_org.getSolutions("time","_T_org","_Tc_o
         plt.plot(tm_corg,T_corg-273.15,LW=LW1,color=Cr1,label=r"$T; K_\mathrm{p} = 0$")
         #
         c_sr_org.setParameters(Kp=2)
         c_sr_org.simulate()
         tm_corg, T_corg, Tc_corg, cA_corg, T_ref = c_sr_org.getSolutions("time","_T_org","_Tc_o
         plt.plot(tm_corg,T_corg-273.15,LW=LW1,color=Cr2,label=r"$T; K_\mathrm{p} = 2$")
         #
         c_sr_org.setParameters(Kp=4)
         c_sr_org.simulate()
         tm_corg, T_corg, Tc_corg, cA_corg, T_ref = c_sr_org.getSolutions("time","_T_org","_Tc_o
         plt.plot(tm_corg,T_corg-273.15,LW=LW1,color=Cb1,label=r"$T; K_\mathrm{p} = 4$")
         #
         c_sr_org.setParameters(Kp=8)
         c_sr_org.simulate()
         tm_corg, T_corg, Tc_corg, cA_corg, T_ref = c_sr_org.getSolutions("time","_T_org","_Tc_o
         plt.plot(tm_corg,T_corg-273.15,LW=LW1,color=Cg1,label=r"$T; K_\mathrm{p} = 8$")
         #
         plt.plot(tm_corg,T_ref-273.15,LW=LW1,color=Cr1,LS=LS2,label=r"$T_{\mathrm{ref}}$")
         #
         plt.title("Reactor temperature")
         plt.xlabel(r"time $t$ [min]")
         plt.ylabel(r"$T$ [${}^\circ \mathrm{C}$]")
         plt.legend()
         plt.grid()
         plt.xlim(0,15)
         figfile = "T_PIconSeborgCSTRorg.pdf"
         plt.savefig(figpath+figfile)
```



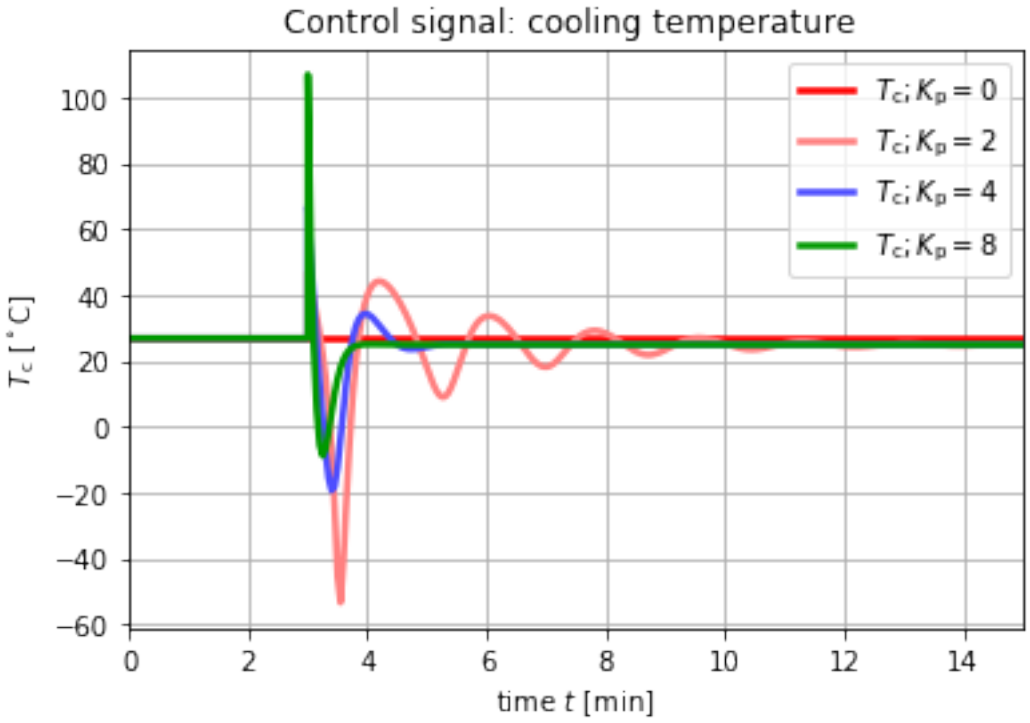
In [23]:
```
c_sr_org.setParameters(Kp=0)
c_sr_org.simulate()
tm_corg, T_corg, Tc_corg, cA_corg, T_ref = c_sr_org.getSolutions("time","_T_org","_Tc_o
plt.plot(tm_corg,cA_corg,LW=LW1,color=Cr1,label=r"$c_\mathrm{A}; K_\mathrm{p} = 0$")
#
c_sr_org.setParameters(Kp=2)
c_sr_org.simulate()
tm_corg, T_corg, Tc_corg, cA_corg, T_ref = c_sr_org.getSolutions("time","_T_org","_Tc_o
plt.plot(tm_corg,cA_corg,LW=LW1,color=Cr2,label=r"$c_\mathrm{A}; K_\mathrm{p} = 2$")
#
c_sr_org.setParameters(Kp=4)
c_sr_org.simulate()
tm_corg, T_corg, Tc_corg, cA_corg, T_ref = c_sr_org.getSolutions("time","_T_org","_Tc_o
plt.plot(tm_corg,cA_corg,LW=LW1,color=Cb1,label=r"$c_\mathrm{A}; K_\mathrm{p} = 4$")
#
c_sr_org.setParameters(Kp=8)
c_sr_org.simulate()
tm_corg, T_corg, Tc_corg, cA_corg, T_ref = c_sr_org.getSolutions("time","_T_org","_Tc_o
plt.plot(tm_corg,cA_corg,LW=LW1,color=Cg1,label=r"$c_\mathrm{A}; K_\mathrm{p} = 8$")
#
plt.title("Reactor concentration ")
plt.xlabel(r"time $t$ [min]")
plt.ylabel(r"$c_\mathrm{A}$ [mol/L]")
```

```
plt.legend()
plt.grid()
plt.xlim(0,15)
figfile = "cA_PIconSeborgCSTRorg.pdf"
plt.savefig(figpath+figfile)
```



In [24]:
```
c_sr_org.setParameters(Kp=0)
c_sr_org.simulate()
tm_corg, T_corg, Tc_corg, cA_corg, T_ref = c_sr_org.getSolutions("time","_T_org","_Tc_o
plt.plot(tm_corg,Tc_corg-273.15,LW=LW1,color=Cr1,label=r"$T_\mathrm{c}; K_\mathrm{p} =
#
c_sr_org.setParameters(Kp=2)
c_sr_org.simulate()
tm_corg, T_corg, Tc_corg, cA_corg, T_ref = c_sr_org.getSolutions("time","_T_org","_Tc_o
plt.plot(tm_corg,Tc_corg-273.15,LW=LW1,color=Cr2,label=r"$T_\mathrm{c}; K_\mathrm{p} =
#
c_sr_org.setParameters(Kp=4)
c_sr_org.simulate()
tm_corg, T_corg, Tc_corg, cA_corg, T_ref = c_sr_org.getSolutions("time","_T_org","_Tc_o
plt.plot(tm_corg,Tc_corg-273.15,LW=LW1,color=Cb1,label=r"$T_\mathrm{c}; K_\mathrm{p} =
#
c_sr_org.setParameters(Kp=8)
c_sr_org.simulate()
```

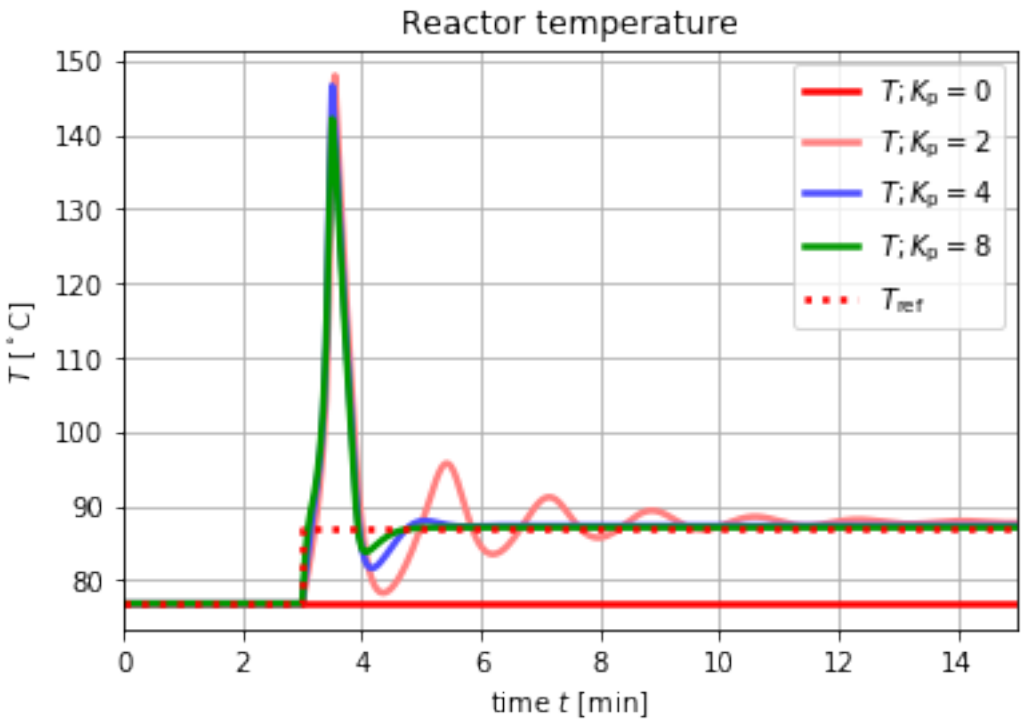
```
tm_corg, T_corg, Tc_corg, cA_corg, T_ref = c_sr_org.getSolutions("time","_T_org","_Tc_o
plt.plot(tm_corg,Tc_corg-273.15,LW=LW1,color=Cg1,label=r"$T_\mathrm{c}; K_\mathrm{p} =
#
plt.title("Control signal: cooling temperature ")
plt.xlabel(r"time $t$ [min]")
plt.ylabel(r"$T_\mathrm{c}$ [${}^\circ \mathrm{C}$]")
plt.legend()
plt.grid()
plt.xlim(0,15)
figfile = "Tc_PIconSeborgCSTRorg.pdf"
plt.savefig(figpath+figfile)
```



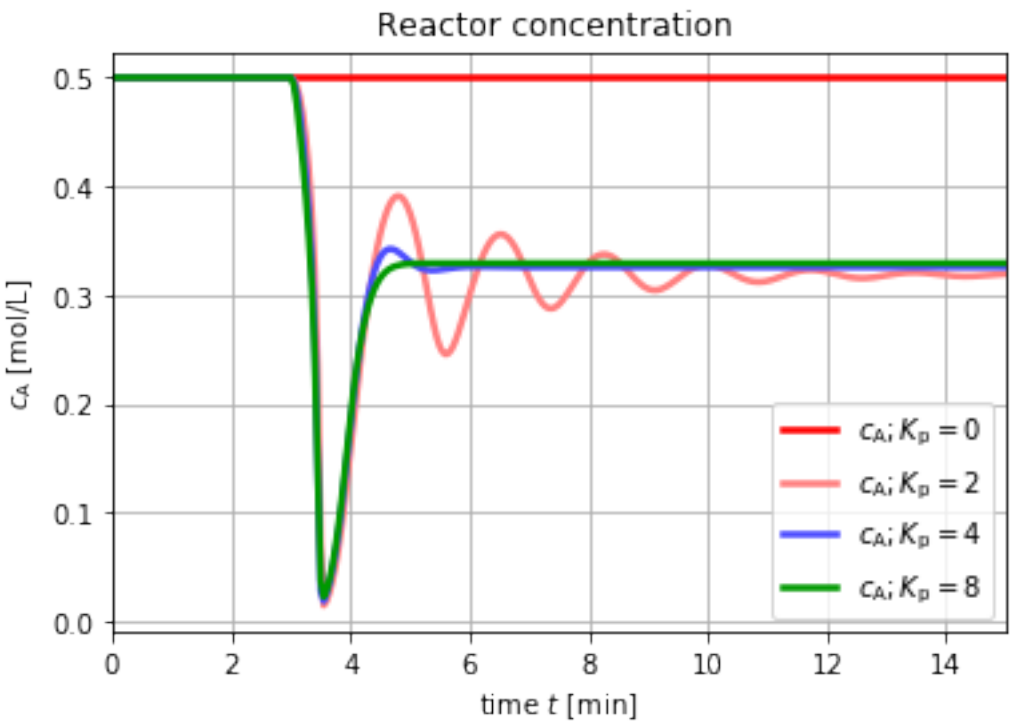
Observe... The design value for K_p based on a linear model does not give good performance; a larger control gain should be chosen to ensure decent performance for the nonlinear system. We also see that the controllers give *negative* cooling temperature, which is not realistic. Let us see what happens if we constrain the cooling temperature (the control input) to $T_c > 4$ [C].

In [25]:
```
c_sr_org.setParameters(Tc_min = 4+273.15)
c_sr_org.setParameters(Kp=0)
c_sr_org.simulate()
tm_corg, T_corg, Tc_corg, cA_corg, T_ref = c_sr_org.getSolutions("time","_T_org","_Tc_o
plt.plot(tm_corg,T_corg-273.15,LW=LW1,color=Cr1,label=r"$T; K_\mathrm{p} = 0$")
#
```

```
c_sr_org.setParameters(Kp=2)
c_sr_org.simulate()
tm_corg, T_corg, Tc_corg, cA_corg, T_ref = c_sr_org.getSolutions("time","_T_org","_Tc_o
plt.plot(tm_corg,T_corg-273.15,LW=LW1,color=Cr2,label=r"$T; K_\mathrm{p} = 2$")
#
c_sr_org.setParameters(Kp=4)
c_sr_org.simulate()
tm_corg, T_corg, Tc_corg, cA_corg, T_ref = c_sr_org.getSolutions("time","_T_org","_Tc_o
plt.plot(tm_corg,T_corg-273.15,LW=LW1,color=Cb1,label=r"$T; K_\mathrm{p} = 4$")
#
c_sr_org.setParameters(Kp=8)
c_sr_org.simulate()
tm_corg, T_corg, Tc_corg, cA_corg, T_ref = c_sr_org.getSolutions("time","_T_org","_Tc_o
plt.plot(tm_corg,T_corg-273.15,LW=LW1,color=Cg1,label=r"$T; K_\mathrm{p} = 8$")
#
plt.plot(tm_corg,T_ref-273.15,LW=LW1,color=Cr1,LS=LS2,label=r"$T_{\mathrm{ref}}$")
#
plt.title("Reactor temperature")
plt.xlabel(r"time $t$ [min]")
plt.ylabel(r"$T$ [${}^\circ \mathrm{C}$]")
plt.legend()
plt.grid()
plt.xlim(0,15)
figfile = "T_constr_PIconSeborgCSTRorg.pdf"
plt.savefig(figpath+figfile)
```

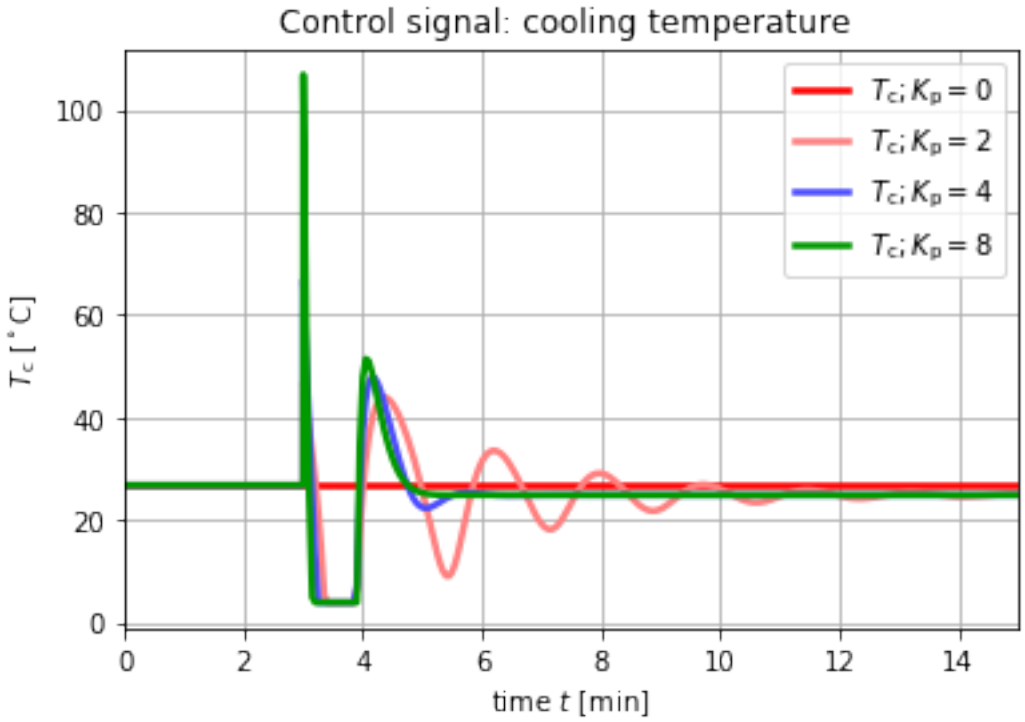


In [26]:
```
c_sr_org.setParameters(Kp=0)
c_sr_org.simulate()
tm_corg, T_corg, Tc_corg, cA_corg, T_ref = c_sr_org.getSolutions("time","_T_org","_Tc_o
plt.plot(tm_corg,cA_corg,LW=LW1,color=Cr1,label=r"$c_\mathrm{A}; K_\mathrm{p} = 0$")
#
c_sr_org.setParameters(Kp=2)
c_sr_org.simulate()
tm_corg, T_corg, Tc_corg, cA_corg, T_ref = c_sr_org.getSolutions("time","_T_org","_Tc_o
plt.plot(tm_corg,cA_corg,LW=LW1,color=Cr2,label=r"$c_\mathrm{A}; K_\mathrm{p} = 2$")
#
c_sr_org.setParameters(Kp=4)
c_sr_org.simulate()
tm_corg, T_corg, Tc_corg, cA_corg, T_ref = c_sr_org.getSolutions("time","_T_org","_Tc_o
plt.plot(tm_corg,cA_corg,LW=LW1,color=Cb1,label=r"$c_\mathrm{A}; K_\mathrm{p} = 4$")
#
c_sr_org.setParameters(Kp=8)
c_sr_org.simulate()
tm_corg, T_corg, Tc_corg, cA_corg, T_ref = c_sr_org.getSolutions("time","_T_org","_Tc_o
plt.plot(tm_corg,cA_corg,LW=LW1,color=Cg1,label=r"$c_\mathrm{A}; K_\mathrm{p} = 8$")
#
plt.title("Reactor concentration ")
plt.xlabel(r"time $t$ [min]")
plt.ylabel(r"$c_\mathrm{A}$ [mol/L]")
plt.legend()
plt.grid()
plt.xlim(0,15)
figfile = "cA_constr_PIconSeborgCSTRorg.pdf"
plt.savefig(figpath+figfile)
```



In [27]:
```
c_sr_org.setParameters(Kp=0)
c_sr_org.simulate()
tm_corg, T_corg, Tc_corg, cA_corg, T_ref = c_sr_org.getSolutions("time","_T_org","_Tc_o
plt.plot(tm_corg,Tc_corg-273.15,LW=LW1,color=Cr1,label=r"$T_\mathrm{c}; K_\mathrm{p} =
#
c_sr_org.setParameters(Kp=2)
c_sr_org.simulate()
tm_corg, T_corg, Tc_corg, cA_corg, T_ref = c_sr_org.getSolutions("time","_T_org","_Tc_o
plt.plot(tm_corg,Tc_corg-273.15,LW=LW1,color=Cr2,label=r"$T_\mathrm{c}; K_\mathrm{p} =
#
c_sr_org.setParameters(Kp=4)
c_sr_org.simulate()
tm_corg, T_corg, Tc_corg, cA_corg, T_ref = c_sr_org.getSolutions("time","_T_org","_Tc_o
plt.plot(tm_corg,Tc_corg-273.15,LW=LW1,color=Cb1,label=r"$T_\mathrm{c}; K_\mathrm{p} =
#
c_sr_org.setParameters(Kp=8)
c_sr_org.simulate()
tm_corg, T_corg, Tc_corg, cA_corg, T_ref = c_sr_org.getSolutions("time","_T_org","_Tc_o
plt.plot(tm_corg,Tc_corg-273.15,LW=LW1,color=Cg1,label=r"$T_\mathrm{c}; K_\mathrm{p} =
#
plt.title("Control signal: cooling temperature ")
plt.xlabel(r"time $t$ [min]")
plt.ylabel(r"$T_\mathrm{c}$ [${}^\circ \mathrm{C}$]")
```

```
plt.legend()
plt.grid()
plt.xlim(0,15)
figfile = "Tc_constr_PIconSeborgCSTRorg.pdf"
plt.savefig(figpath+figfile)
```



Observe... The constraint in the control input dramatically reduces the performance of the controller.

SeborgCSTR_complex_models

March 13, 2018

1 Use of Modelica + Python in Process Systems Engineering Education

1.1 Complex models of "Seborg reactor"

1.1.1 Bernt Lie

1.1.2 University College of Southeast Norway

Basic import and definitions

```
In [1]: from OMPython import ModelicaSystem
        import numpy as np
        import numpy.random as nr
        %matplotlib inline
        import matplotlib.pyplot as plt
        import pandas as pd
        LW1 = 2.5
        LW2 = LW1/2
        Cb1 = (0.3,0.3,1)
        Cb2 = (0.7,0.7,1)
        Cg1 = (0,0.6,0)
        Cg2 = (0.5,0.8,0.5)
        Cr1 = "Red"
        Cr2 = (1,0.5,0.5)
        LS1 = "solid"
        LS2 = "dotted"
        LS3 = "dashed"
        figpath = "../figs/"
```

1.1.3 Nonlinear reactor models based on Seborg et al.

Process diagram

Original state space model The original model is based on several simplifying assumptions: * Reaction species A, B are diluted in a solvent S. * The solvent dominates totally in the mixture, and we can assume constant density in the reaction medium. * Due to constant density (and constant reactor volume), the influent and effluent volumetric flow rates are equal. * Because of dominance of solvent, thermal parameters (heat capacities) are constant and independent of presence of A

and B. * The reaction order is set to unity, $\alpha = 1$. * The heat of reaction is assumed independent of temperature. * We need to include information about the amount of species B in the model.

Complex model 1: rho We maintain that the mixture density is constant, with constant volumetric flow rate through the reactor. However, * The thermal parameters (heat capacities) are allowed to vary with the concentrations of A and B. * We allow for general model order α. * With general model order, the reaction enthalpy may vary with composition and temperature.

Complex model 1 will be given descriptive name related to rho, which indicates constant density (ρ). The following is a DAE implementation in Modelica.

```
model ModSeborgCSTRrho
   // Model of Seborg CSTR when assuming dominant solvent and Constant flow rate Vd
   // author:  Bernt Lie
   //          University of Southeast Norway
   //          November 7, 2017
   //
   // Parameters
   parameter Real V = 100 "Reactor volume, L";
   parameter Real rho = 1e3 "Liquid density, g/L";
   parameter Real m = rho*V "Reactor content mass, g";
   parameter Real mS = m "Reactor solvent mass, g";
   parameter Real a = 1 "Stoichiometric constant, -";
   parameter Real EdR = 8750 "Activation temperature, K";
   parameter Real k0 = exp(EdR/350) "Pre-exponential factor, 1/min";
   parameter Real UA = 5e4 "Heat transfer parameter, J/(min.K)";
   //
   parameter Real HtA_o = 5e4 "Molar enthalpy of A at std state, J/mol";
   parameter Real HtB_o = 0 "Molar enthalpy of B at std state, J/mol";
   parameter Real HhS_o = 0 "Specific enthalpy of solvent at std state, J/g";
   parameter Real cptA = 5 "Molar heat capacity of A, J/(mol.K)";
   parameter Real cptB = cptA "Molar heat capacity of B, J/(mol.K)";
   parameter Real cphS = 0.239 "Specific heat capacity of solvent, J/(g.K)";
   parameter Real cph = cphS "Specific heat capacity of mixture, J/(g.K)";
   parameter Real T_o = 293.15 "Temperature in std state, K";
   parameter Real p_o = 1.01e5 "Pressure in std state, Pa";
   // Initial state parameters
   parameter Real cA0 = 0.5 "Initial concentration of A, mol/L";
   parameter Real nA0 = cA0*V "Initial number of moles of A, mol";
   parameter Real nB0 = 0 "Initial number of moles of B, mol";
   parameter Real T0 = 350 "Initial temperature, K";
   parameter Real HtA0 = HtA_o + cptA*(T0-T_o) "Initial pure molar enthalpy of A, J/mol";
   parameter Real HtB0 = HtB_o + cptB*(T0-T_o) "Initial pure molar enthalpy of B, J/mol";
   parameter Real HhS0 = HhS_o + cphS*(T0-T_o) "Initial pure specific enthalpy of solvent, J/g"
   parameter Real HA0 = nA0*HtA0 "Initial pure enthalpy of A, J";
   parameter Real HB0 = nB0*HtB0 "Initial pure enthalpy of B, J";
   parameter Real HS0 = mS*HhS0 "Initial pure enthalpy of solvent, J";
   parameter Real H0 = HA0 + HB0 + HS0 "Initial total enthalpy of ideal solution, J";
   parameter Real U0 = H0 - p_o*V "Initial internal energy, J";
```

```
  // Declaring variables
  // -- states
  Real nA(start = nA0, fixed = true) "Initializing amount of A in reactor, mol";
  Real nB(start = nB0, fixed = true) "Initializing amount of B in reactor, mol";
  Real U(start = U0, fixed = true) "Initializing internal energy in reactor, J";
  // -- auxiliary variables
  Real ndAi "Influent molar flow rate of A, mol/s";
  Real ndAe "Effluent molar flow rate of A, mol/s";
  Real ndAg "Molar rate of generation of A, mol/s";
  Real ndBi "Influent molar flow rate of B, mol/s";
  Real ndBe "Effluent molar flow rate of B, mol/s";
  Real ndBg "Molar rate of generation of B, mol/s";
  Real mdSi "Influent mass flow rate of solvent, g/min";
  Real mdSe "Effluent mass flow rate of solvent, g/min";
  Real Hdi "Influent enthalpy flow rate, J/min";
  Real Hde "Effluent enthalpy flow rate, J/min";
  Real cA "Molar concentration of A, mol/L";
  Real cB "Molar concentration of B, mol/L";
  Real r "Rate of reaction, mol/(L.s)";
  Real T "Reactor temperature, K";
  Real k "Reaction 'constant', ...";
  Real H "Reactor enthalpy, J";
  Real HA "Enthalpy of pure A, J";
  Real HB "Enthalpy of pure B, J";
  Real HS "Enthalpy of pure solvent, J";
  Real HtA "Molar enthalpy of pure A, J/mol";
  Real HtB "Molar enthalpy of pure B, J/mol";
  Real HhS "Specific enthalpy of pure solvent, J/g";
  Real HdAi "Influent enthalpy flow of pure A,J/min";
  Real HdBi "Influent enthalpy flow of pure B, J/min";
  Real HdSi "Influent enthalpy flow of pure solvent, J/min";
  Real HtAi "Influent molar enthalpy of pure A, J/mol";
  Real HtBi "Influent molar enthalpy of pure B, J/mol";
  Real HhSi "Influent specific enthalpy of solvent, J/g";
  Real HdAe "Effluent enthalpy flow of pure A, J/min";
  Real HdBe "Effluent enthalpy flow of pure B, J/min";
  Real HdSe "Effluent enthalpy flow of pure solvent, J/min";
  Real Qd "Heat flow rate, J/min";
  // -- input variables
  input Real Vdi "Volumetric flow rate through reactor, L/s";
  input Real cAi "Influent molar concentration of A, mol/L";
  input Real Ti "Influent temperature, K";
  input Real Tc "Cooling temperature, K";
  // -- output variables
  output Real y_T "Reactor temperature, K";
  output Real y_cB "Molar concentration of B, mol/L";
// Equations constituting the model
equation
```

```
    // Differential equations
    der(nA) = ndAi - ndAe + ndAg;
    der(nB) = ndBi - ndBe + ndBg;
    der(U) = Hdi - Hde + Qd;
    // Algebraic equations
    nA = cA*V;
    nB = cB*V;
    ndAi = cAi*Vdi;
    ndBi = 0;
    mdSi = rho*Vdi;
    ndAe = cA*Vdi;
    ndBe = cB*Vdi;
    mdSe = mdSi;
    ndAg = -a*r*V;
    ndBg = r*V;
    r = k*cA^a;
    k = k0*exp(-EdR/T);
    U = H-p_o*V;
    H = HA + HB + HS;
    HA = nA*HtA;
    HB = nB*HtB;
    HS = mS*HhS;
    HtA = HtA_o + cptA*(T-T_o);
    HtB = HtB_o + cptB*(T-T_o);
    HhS = HhS_o + cphS*(T-T_o);
    Hdi = HdAi + HdBi + HdSi;
    HdAi = ndAi*HtAi;
    HdBi = ndBi*HtBi;
    HdSi = mdSi*HhSi;
    HtAi = HtA_o + cptA*(Ti-T_o);
    HtBi = 0;
    HhSi = HhS_o + cphS*(Ti-T_o);
    Hde = HdAe + HdBe + HdSe;
    HdAe = ndAe*HtA;
    HdBe = ndBe*HtB;
    HdSe = mdSe*HhS;
    Qd = UA*(Tc-T);
    // Outputs
    y_T = T;
    y_cB = cB;
  end ModSeborgCSTRrho;
```

Complex model 2: is In a more general model, we only assume **ideal solution** in the reaction mixture. The model is given a descriptive name related to is.

For the ideal solution model: * The density of the reaction medium varies with the composition, and influent and effluent volumetric flowrates differ. * The thermal parameters (heat capacities) vary with composition. * We allow for general model order α. * With general model order, the

reaction enthalpy will vary with composition and temperature. * We need to include information about the amount of species B in the model.

It is relatively straightforward to develop a DAE model for this case. It is also possible to develop an ODE model: this time, we need three states (we need to include information about species B). The ODE formulation is simpler than the DAE model, but it is relatively complicated to develop the ODE model. The DAE model is as follows:

```
model ModSeborgCSTRis
   // Model of Seborg CSTR when assuming Ideal Solution, only
   // author:  Bernt Lie
   //          University of Southeast Norway
   //          November 7, 2017
   //
   // Parameters
   parameter Real rhoS_o = 1e3 "Density of pure S, g/L";
   parameter Real rhoA_o = 1.5e3 "Density of pure A, g/L";
   parameter Real rhoB_o = 2.5e3 "Density of pure B, g/L";
   parameter Real MA = 50 "Molar mass of A, g/mol";
   parameter Real MB = MA*a "Molar mass of B, g/mol";
   parameter Real V = 100 "Reactor volume, L";
   parameter Real a = 1 "Stoichiometric constant, -";
   parameter Real k0 = exp(EdR/350) "Pre-exponential factor, 1/min";
   parameter Real EdR = 8750 "Activation temperature, K";
   parameter Real p_o = 1.01e5 "Pressure in std state, Pa";
   //
   parameter Real HhS_o = 0 "Specific enthalpy of solvent at std state, J/g";
   parameter Real HtA_o = 5e4 "Molar enthalpy of A at std state, J/mol";
   parameter Real HtB_o = 0 "Molar enthalpy of B at std state, J/mol";
   //
   parameter Real cphS = 0.239 "Specific heat capacity of solvent, J/(g.K)";
   parameter Real cptA = 5 "Molar heat capacity of A, J/(mol.K)";
   parameter Real cptB = cptA "Molar heat capacity of B, J/(mol.K)";
   //
   parameter Real T_o = 293.15 "Temperature in std state, K";
   //
   parameter Real UA = 5e4 "Heat transfer parameter, J/(min.K)";
   // Initial state parameters
   parameter Real cA0 = 0.5 "Initial concentration of A, mol/L";
   parameter Real nA0 = cA0*V "Initial number of moles of A, mol";
   parameter Real nB0 = 0 "Initial number of moles of B, mol";
   parameter Real mA0 = nA0*MA "Initial mass of A, g";
   parameter Real mB0 = nB0*MB "Initial mass of B, g";
   parameter Real VA0 = mA0/rhoA_o "Initial volume of A, L";
   parameter Real VB0 = mB0/rhoB_o "Initial volume of B, L";
   parameter Real VS0 = V - VA0 - VB0 "Initial volume of S, L";
   parameter Real mS0 = VS0*rhoS_o "Initial mass of S, g";
   parameter Real T0 = 350 "Initial temperature, K";
   parameter Real HhS0 = HhS_o + cphS*(T0-T_o) "Initial pure specific enthalpy of solvent, J/g"
```

```
parameter Real HtA0 = HtA_o + cptA*(T0-T_o) "Initial pure molar enthalpy of A, J/mol";
parameter Real HtB0 = HtB_o + cptB*(T0-T_o) "Initial pure molar enthalpy of B, J/mol";
parameter Real HS0 = mS0*HhS0 "Initial pure enthalpy of solvent, J";
parameter Real HA0 = nA0*HtA0 "Initial pure enthalpy of A, J";
parameter Real HB0 = nB0*HtB0 "Initial pure enthalpy of B, J";
parameter Real H0 = HS0 + HA0 + HB0  "Initial total enthalpy of ideal solution, J";
parameter Real U0 = H0 - p_o*V "Initial internal energy, J";
// Declaring variables
// -- states
Real mS(start = mS0) "Initial amount of S in reactor, kg";
Real nA(start = nA0, fixed = true) "Initializing amount of A in reactor, mol";
Real nB(start = nB0, fixed = true) "Initializing amount of B in reactor, mol";
Real U(start = U0, fixed = true) "Initializing internal energy in reactor, J";
// -- auxiliary variables
// Real mS "Mass of S, g";
Real V_x;
Real mdSi "Influent mass flow rate of S, g/s";
Real mdSe "Effluent mass flow rate of S, g/s";
Real ndAi "Influent molar flow rate of A, mol/s";
Real ndAe "Effluent molar flow rate of A, mol/s";
Real ndAg "Molar rate of generation of A, mol/s";
Real ndBi "Influent molar flow rate of B, mol/s";
Real ndBe "Effluent molar flow rate of B, mol/s";
Real ndBg "Molar rate of generation of B, mol/s";
Real Hdi "Influent enthalpy flow rate, J/min";
Real Hde "Effluent enthalpy flow rate, J/min";
Real Qd "Heat flow rate, J/min";
//
Real VS "Volume of pure S, L";
Real VA "Volume of pure A, L";
Real VB "Volume of pure B, L";
Real mA "Mass of A, g";
Real mB "Mass of B, g";
//
Real Vde "Effluent volumetric flow rate, L/min";
//
Real rhoS "Specific concentration of S, g/L";
Real cA "Molar concentration of A, mol/L";
Real cB "Molar concentration of B, mol/L";
Real r "Rate of reaction, mol/(L.s)";
Real k "Reaction 'constant', ...";
Real T "Absolute temperature, K";
//
Real H "Reactor enthalpy, J";
Real HS "Enthalpy of pure solvent, J";
Real HA "Enthalpy of pure A, J";
Real HB "Enthalpy of pure B, J";
Real HhS "Specific enthalpy of pure solvent, J/g";
```

```
  Real HtA "Molar enthalpy of pure A, J/mol";
  Real HtB "Molar enthalpy of pure B, J/mol";
  Real HdSi "Influent enthalpy flow of pure solvent, J/min";
  Real HdAi "Influent enthalpy flow of pure A,J/min";
  Real HdBi "Influent enthalpy flow of pure B, J/min";
  Real HhSi "Influent specific enthalpy of solvent, J/g";
  Real HtAi "Influent molar enthalpy of pure A, J/mol";
  Real HtBi "Influent molar enthalpy of pure B, J/mol";
  Real HdSe "Effluent enthalpy flow of pure solvent, J/min";
  Real HdAe "Effluent enthalpy flow of pure A, J/min";
  Real HdBe "Effluent enthalpy flow of pure B, J/min";
  //
  Real mdSi_x;
  // -- input variables
  input Real Vdi "Volumetric flow rate through reactor, L/s";
  input Real cAi "Influent molar concentration of A, mol/L";
  input Real Ti "Influent temperature, K";
  input Real Tc "Cooling temperature, K";
  // -- output variables
  output Real y_T "Reactor temperature, K";
  output Real y_cB "Molar concentration of B, mol/L";
// Equations constituting the model
equation
  // Differential equations
  mdSi_x = mdSe + der(mS);
  der(mS) = mdSi - mdSe;
  der(nA) = ndAi - ndAe + ndAg;
  der(nB) = ndBi - ndBe + ndBg;
  der(U) = Hdi - Hde + Qd;
  // Algebraic equations
  V = VS + VA + VB;
  VS = mS/rhoS_o;
  VA = mA/rhoA_o;
  VB = mB/rhoB_o;
  mS = rhoS*V;
  V_x = mS/rhoS_o + nA*MA/rhoA_o + nB*MB/rhoB_o;

  mA = nA*MA;
  mB = nB*MB;
  nA = cA*V;
  nB = cB*V;
  //
  mdSi = rhoS_o*(1-cAi*MA/rhoA_o)*Vdi;
  ndAi = cAi*Vdi;
  ndBi = 0;
  mdSe = rhoS*Vde;
  ndAe = cA*Vde;
  ndBe = cB*Vde;
```

```
    ndAg = -a*r*V;
    ndBg = r*V;
    r = k*cA^a;
    k = k0*exp(-EdR/T);
    //
    U = H-p_o*V;
    H = HS + HA + HB;
    HS = mS*HhS;
    HA = nA*HtA;
    HB = nB*HtB;
    //
    HhS = HhS_o + cphS*(T-T_o);
    HtA = HtA_o + cptA*(T-T_o);
    HtB = HtB_o + cptB*(T-T_o);
    //
    Hdi = HdSi + HdAi + HdBi;
    HdSi = mdSi*HhSi;
    HdAi = ndAi*HtAi;
    HdBi = ndBi*HtBi;
    //
    HhSi = HhS_o + cphS*(Ti-T_o);
    HtAi = HtA_o + cptA*(Ti-T_o);
    HtBi = 0;
    //
    Hde = HdAe + HdBe + HdSe;
    HdSe = mdSe*HhS;
    HdAe = ndAe*HtA;
    HdBe = ndBe*HtB;
    //
    Qd = UA*(Tc-T);
    // Outputs
    y_T = T;
    y_cB = cB;
  end ModSeborgCSTRis;
```

1.1.4 Comparing models

Instantiating models

```
In [2]: sr_is = ModelicaSystem("SeborgCSTR.mo","SeborgCSTR.ModSeborgCSTRis")
        sr_rho = ModelicaSystem("SeborgCSTR.mo","SeborgCSTR.ModSeborgCSTRrho")
        sr_org = ModelicaSystem("SeborgCSTR.mo","SeborgCSTR.ModSeborgCSTRorg")

2018-03-13 14:58:39,841 - OMPython - INFO - OMC Server is up and running at file:///c:/users/ber
2018-03-13 14:58:43,240 - OMPython - INFO - OMC Server is up and running at file:///c:/users/ber
2018-03-13 14:58:46,236 - OMPython - INFO - OMC Server is up and running at file:///c:/users/ber
```

Setting up simulations

In [3]:
```
sr_is.setSimulationOptions(stopTime=15,stepSize=0.05)
sr_rho.setSimulationOptions(stopTime=15,stepSize=0.05)
sr_org.setSimulationOptions(stopTime=15,stepSize=0.05)
#
sr_is.setInputs(Tc=300)
sr_is.setInputs(Ti=350)
sr_is.setInputs(Vdi=100)
sr_is.setInputs(cAi=1)
sr_rho.setInputs(Tc=300)
sr_rho.setInputs(Ti=350)
sr_rho.setInputs(Vdi=100)
sr_rho.setInputs(cAi=1)
sr_org.setInputs(Tc=300)
sr_org.setInputs(Ti=350)
sr_org.setInputs(Vdi=100)
sr_org.setInputs(cAi=1)
```

Simulating system for three cases of inputs, and extracting results

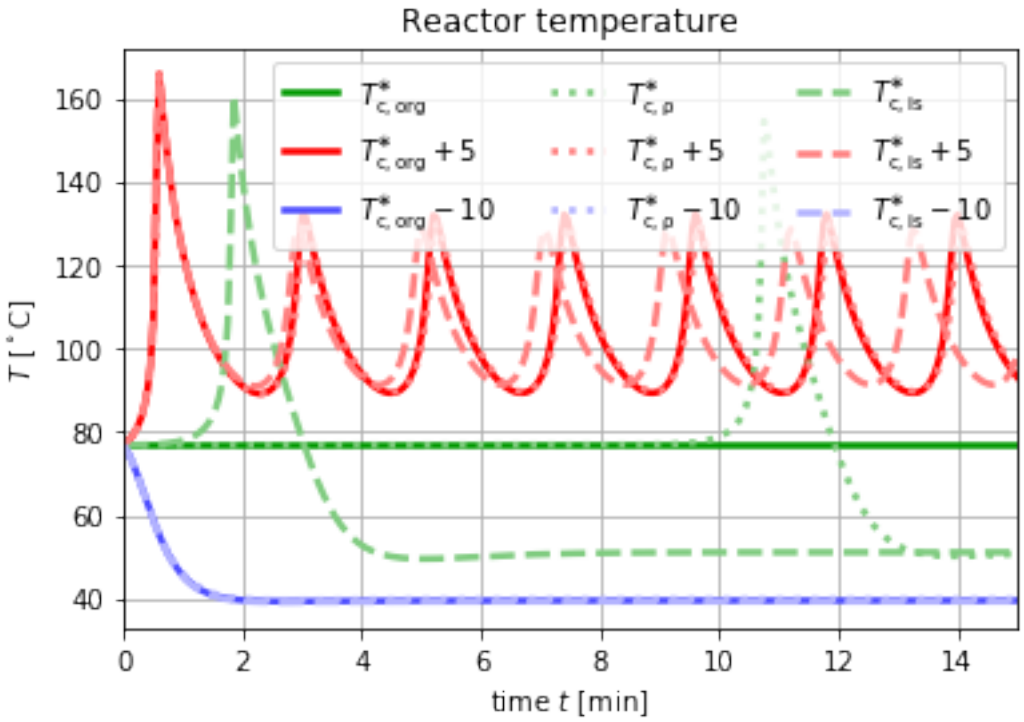
In [4]:
```
sr_is.setInputs(Tc=300)
sr_is.simulate()
tm_is0, T_is0, Tc_is0, cA_is0 = sr_is.getSolutions("time","T","Tc","cA")
sr_is.setInputs(Tc=300+5)
sr_is.simulate()
tm_is0p, T_is0p, Tc_is0p, cA_is0p = sr_is.getSolutions("time","T","Tc","cA")
sr_is.setInputs(Tc=300-10)
sr_is.simulate()
tm_is0m, T_is0m, Tc_is0m, cA_is0m = sr_is.getSolutions("time","T","Tc","cA")
```

In [5]:
```
sr_rho.setInputs(Tc=300)
sr_rho.simulate()
tm_rho0, T_rho0, Tc_rho0, cA_rho0 = sr_rho.getSolutions("time","T","Tc","cA")
sr_rho.setInputs(Tc=300+5)
sr_rho.simulate()
tm_rho0p, T_rho0p, Tc_rho0p, cA_rho0p = sr_rho.getSolutions("time","T","Tc","cA")
sr_rho.setInputs(Tc=300-10)
sr_rho.simulate()
tm_rho0m, T_rho0m, Tc_rho0m, cA_rho0m = sr_rho.getSolutions("time","T","Tc","cA")
```

In [6]:
```
sr_org.setInputs(Tc=300)
sr_org.simulate()
tm_org0, T_org0, Tc_org0, cA_org0 = sr_org.getSolutions("time","T","Tc","cA")
sr_org.setInputs(Tc=300+5)
sr_org.simulate()
tm_org0p, T_org0p, Tc_org0p, cA_org0p = sr_org.getSolutions("time","T","Tc","cA")
sr_org.setInputs(Tc=300-10)
sr_org.simulate()
tm_org0m, T_org0m, Tc_org0m, cA_org0m = sr_org.getSolutions("time","T","Tc","cA")
```

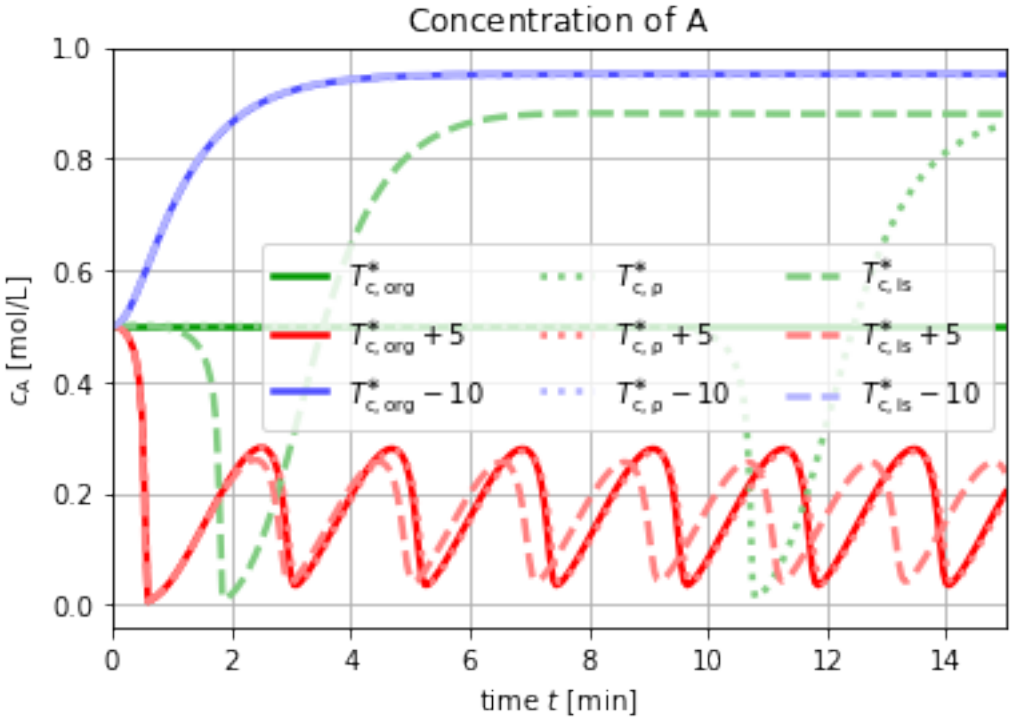
Plotting results

In [7]:
```
plt.plot(tm_org0,T_org0-273.15,LW=LW1,color=Cg1,label=r"$T_{\mathrm{c,org}}^{\ast}$")
plt.plot(tm_org0p,T_org0p-273.15,LW=LW1,color=Cr1,label=r"$T_{\mathrm{c,org}}^{\ast}+5$"
plt.plot(tm_org0m,T_org0m-273.15,LW=LW1,color=Cb1,label=r"$T_{\mathrm{c,org}}^{\ast}-10$
plt.plot(tm_rho0,T_rho0-273.15,LW=LW1,LS=LS2,color=Cg2,label=r"$T_{\mathrm{c,\rho}}^{\as
plt.plot(tm_rho0p,T_rho0p-273.15,LW=LW1,LS=LS2,color=Cr2,label=r"$T_{\mathrm{c,\rho}}^{\
plt.plot(tm_rho0m,T_rho0m-273.15,LW=LW1,LS=LS2,color=Cb2,label=r"$T_{\mathrm{c,\rho}}^{\
plt.plot(tm_is0,T_is0-273.15,LW=LW1,LS=LS3,color=Cg2,label=r"$T_{\mathrm{c,is}}^{\ast}$"
plt.plot(tm_is0p,T_is0p-273.15,LW=LW1,LS=LS3,color=Cr2,label=r"$T_{\mathrm{c,is}}^{\ast}
plt.plot(tm_is0m,T_is0m-273.15,LW=LW1,LS=LS3,color=Cb2,label=r"$T_{\mathrm{c,is}}^{\ast}
plt.legend(ncol=3)
plt.title("Reactor temperature")
plt.xlabel(r"time $t$ [min]")
plt.ylabel(r"$T$ [${}^\circ \mathrm{C}$]")
plt.grid()
plt.xlim(0,15)
figfile = "tempSeborgCSTR.pdf"
plt.savefig(figpath+figfile)
```



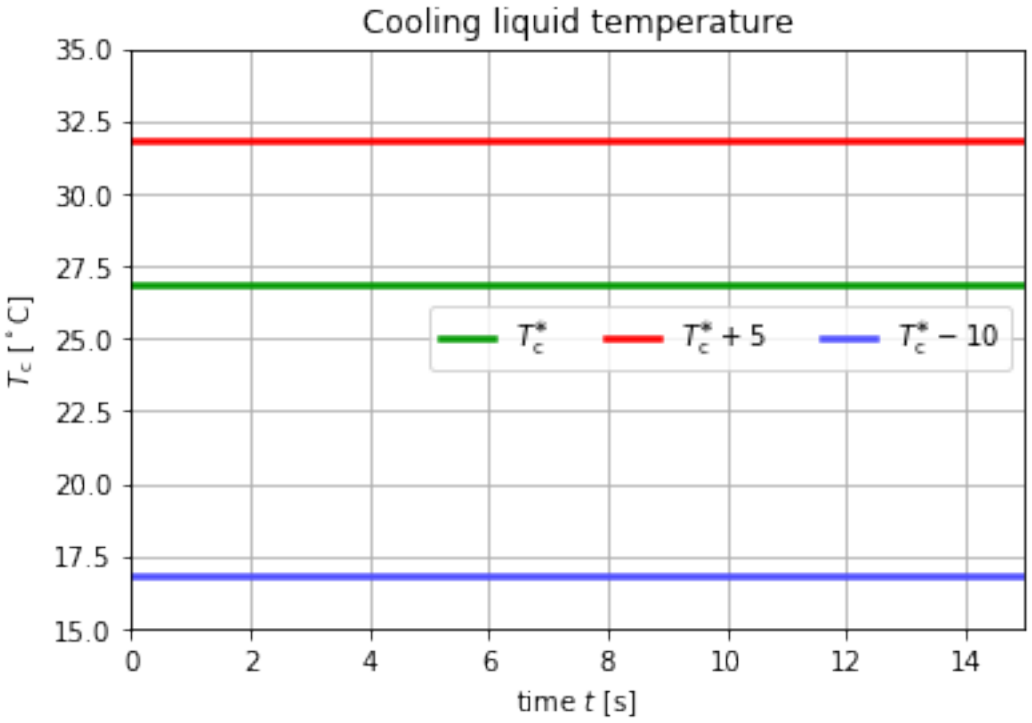
In [8]:
```
plt.plot(tm_org0,cA_org0,LW=LW1,color=Cg1,label=r"$T_{\mathrm{c,org}}^{\ast}$")
plt.plot(tm_org0p,cA_org0p,LW=LW1,color=Cr1,label=r"$T_{\mathrm{c,org}}^{\ast}+5$")
plt.plot(tm_org0m,cA_org0m,LW=LW1,color=Cb1,label=r"$T_{\mathrm{c,org}}^{\ast}-10$")
plt.plot(tm_rho0,cA_rho0,LW=LW1,LS=LS2,color=Cg2,label=r"$T_{\mathrm{c,\rho}}^{\ast}$")
```

```
plt.plot(tm_rho0p,cA_rho0p,LW=LW1,LS=LS2,color=Cr2,label=r"$T_{\mathrm{c,\rho}}^{\ast}+5
plt.plot(tm_rho0m,cA_rho0m,LW=LW1,LS=LS2,color=Cb2,label=r"$T_{\mathrm{c,\rho}}^{\ast}-1
plt.plot(tm_is0,cA_is0,LW=LW1,LS=LS3,color=Cg2,label=r"$T_{\mathrm{c,is}}^{\ast}$")
plt.plot(tm_is0p,cA_is0p,LW=LW1,LS=LS3,color=Cr2,label=r"$T_{\mathrm{c,is}}^{\ast}+5$")
plt.plot(tm_is0m,cA_is0m,LW=LW1,LS=LS3,color=Cb2,label=r"$T_{\mathrm{c,is}}^{\ast}-10$")
plt.legend(ncol=3,loc=7)
plt.title("Concentration of $\mathrm{A}$")
plt.xlabel(r"time $t$ [min]")
plt.ylabel(r"$c_{\mathrm{A}}$ [mol/L]")
plt.grid()
plt.xlim(0,15)
figfile = "concSeborgCSTR.pdf"
plt.savefig(figpath+figfile)
```



In [9]:
```
plt.plot(tm_org0,Tc_org0-273.15,LW=LW1, color=Cg1, label=r"$T_\mathrm{c}^{\ast}$")
plt.plot(tm_org0p,Tc_org0p-273.15,LW=LW1,color=Cr1, label=r"$T_\mathrm{c}^{\ast}+5$")
plt.plot(tm_org0m,Tc_org0m-273.15,LW=LW1,color=Cb1, label=r"$T_\mathrm{c}^{\ast}-10$")
plt.title("Cooling liquid temperature")
plt.xlabel(r"time $t$ [s]")
plt.ylabel(r"$T_\mathrm{c}$ [${}^\circ \mathrm{C}$]")
plt.grid()
plt.axis(ymin=15,ymax=35)
plt.xlim(0,15)
```

```
plt.legend(ncol=3,loc=7)
figfile = "coolSeborgCSTR.pdf"
plt.savefig(figpath+figfile)
```



SeborgCSTR_sensitivity

March 13, 2018

1 Use of Modelica + Python in Process Systems Engineering Education

1.1 Sensitivity analysis of "Seborg reactor"

1.1.1 Bernt Lie

1.1.2 University College of Southeast Norway

Basic import and definitions

```
In [1]: from OMPython import ModelicaSystem
        import numpy as np
        import numpy.random as nr
        %matplotlib inline
        import matplotlib.pyplot as plt
        import pandas as pd
        LW1 = 2.5
        LW2 = LW1/2
        Cb1 = (0.3,0.3,1)
        Cb2 = (0.7,0.7,1)
        Cg1 = (0,0.6,0)
        Cg2 = (0.5,0.8,0.5)
        Cr1 = "Red"
        Cr2 = (1,0.5,0.5)
        LS1 = "solid"
        LS2 = "dotted"
        LS3 = "dashed"
        figpath = "../figs/"
```

1.1.3 Reactor temperature sensitivity to UA from Monte Carlo simulations

Instantiating models and setting inputs

```
In [2]: srp = ModelicaSystem("SeborgCSTR.mo","SeborgCSTR.ModSeborgCSTRorg")
        srm = ModelicaSystem("SeborgCSTR.mo","SeborgCSTR.ModSeborgCSTRorg")
```

```
2018-03-13 14:56:13,187 - OMPython - INFO - OMC Server is up and running at file:///c:/users/ber
2018-03-13 14:56:16,158 - OMPython - INFO - OMC Server is up and running at file:///c:/users/ber
```

```
In [3]: srp.setSimulationOptions(stopTime=10,stepSize=0.05)
        srm.setSimulationOptions(stopTime=10,stepSize=0.05)
        #
        srp.setInputs(Tc=300+5)
        srm.setInputs(Tc=300-10)
        srp.setInputs(Ti=350,Vdi=100,cAi=1)
        srm.setInputs(Ti=350,Vdi=100,cAi=1)
```

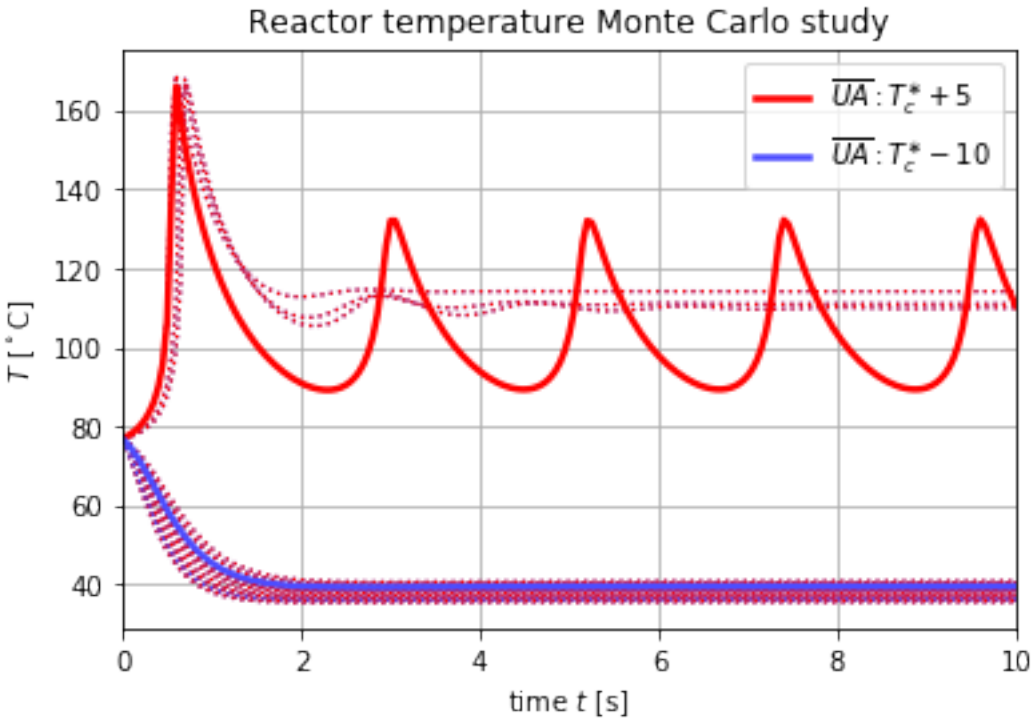
Finding parameter names, and generating random variations of UA with uniform distribution and 5% variation

```
In [4]: p = srp.getParameters()
        p.keys()

Out[4]: ['a', 'cph', 'DrHt', 'cA0', 'T0', 'EdR', 'k0', 'rho', 'V', 'UA']

In [5]: p.values()

Out[5]: [1.0, 0.239, -50000.0, 0.5, 350.0, 8750.0, None, 1000.0, 100.0, 50000.0]

In [6]: UA = p["UA"]
        UA

Out[6]: 50000.0

In [7]: nr.seed(0)
        UUAA = UA*(1 + (nr.rand(20)-0.5)/2)
```

Simulating for nominal values $\overline{UA}$ of UA, as well as for random variations in UA

```
In [8]: srp.simulate()
        tm0p,T0p = srp.getSolutions("time","T")
        srm.simulate()
        tm0m,T0m = srm.getSolutions("time","T")
        #
        for ua in UUAA:
            srp.setParameters(UA=ua);
            srp.simulate()
            tm0p1,T0p1 = srp.getSolutions("time","T")
            srm.setParameters(UA=ua);
            srm.simulate()
            tm0m1,T0m1 = srm.getSolutions("time","T")
            plt.plot(tm0p1,T0p1-273.15,LW=LW2,color=Cr1,LS=LS2,label="_nolabel_")
            plt.plot(tm0m1,T0m1-273.15,LW=LW2,color=Cb1,LS=LS2,label="_nolabel_")
        #
        plt.plot(tm0p,T0p-273.15,LW=LW1,color=Cr1,label=r"$\overline{UA} : T_c^{\ast}+5$")
        plt.plot(tm0m,T0m-273.15,LW=LW1,color=Cb1,label=r"$\overline{UA} : T_c^{\ast}-10$")
        plt.title("Reactor temperature Monte Carlo study")
        plt.xlabel(r"time $t$ [s]")
```

```
plt.ylabel(r"$T$ [${}^\circ \mathrm{C}$]")
plt.grid()
plt.xlim(0,10)
plt.legend()
figfile = "sensitivitySeborgCSTRorg.pdf"
plt.savefig(figpath+figfile)
```



1.1.4 Sensitivity of quantities wrt. parameters

```
In [9]: sr_org = ModelicaSystem("SeborgCSTR.mo","SeborgCSTR.ModSeborgCSTRorg")

2018-03-13 14:56:28,186 - OMPython - INFO - OMC Server is up and running at file:///c:/users/ber


In [10]: sr_org.setSimulationOptions(stopTime=20)

In [11]: sr_org.setInputs(Tc=300)
         sr_org.setInputs(Ti=350)
         sr_org.setInputs(Vdi=100)
         sr_org.setInputs(cAi=1)

In [12]: sr_org.simulate()
         tm = sr_org.getSolutions("time")
```

Function for numerical sensitivity computation

```
In [13]: def sensitivity(obj,Lv,Lp,Le=[1e-2]):
             """
             Method for computing numeric sensitivity of OpenModelica object

             Arguments:
             ----------
             1st arg: obj # OMPython API model object -- should be removed in method?
             2nd arg: Lv  # List of strings of Modelica Variable names
             3rd arg: Lp  # List of strings of Modelica Parameter names
             4th arg: Le  # List of float Excitations of parameters; defaults to single 1e-2

             Returns:
             --------
             1st return: LSname # List of Sensitivity names
             2nd return: Sarray # 2D array of sensitivities, one row per sensitivity name
             """
             # Production quality code should check type and form of input arguments
             #
             nLp = len(Lp) # number of parameter names
             nLe = len(Le) # number of excitations in parameters
             # Adjusting size of Le to that of Lp
             if nLe < nLp:
                 for i in range(nLe,nLp):
                     Le.append(Le[nLe-1]) # expands Le with the last element of Le
             elif nLe > nLp:
                 Le = Le[0:nLp] # truncates Le to same length as Lp
             # Nominal parameters p0
             par0 = obj.getParameters(*Lp)
             # eXcitation parameters parX
             parX = []
             for i,p in enumerate(par0):
                 parX.append(p*(1.+Le[i]))
             # Zip parameter names and parameter values into list of tuples
             # --- preparation for setting excitated parameters via keyword assignment
             Lpar0 = zip(Lp,par0) # List of parameter name/value pairs for resetting to nominal
             LparX = zip(Lp,parX) # List of eXcited parameter name/value pairs
             # Simulate nominal system
             obj.simulate()
             # Get nominal SOLutions of variables of interest (Lv), converted to 2D array
             sol0 = np.asarray(obj.getSolutions(*Lv))
             # Get list of eXcited SOLutions (2D arrays), one for each parameter (Lp)
             solX = []
             for i,d in enumerate(LparX):
                 # change to excited parameter
                 obj.setParameters(**dict([d]))
                 # simulate perturbed system
```

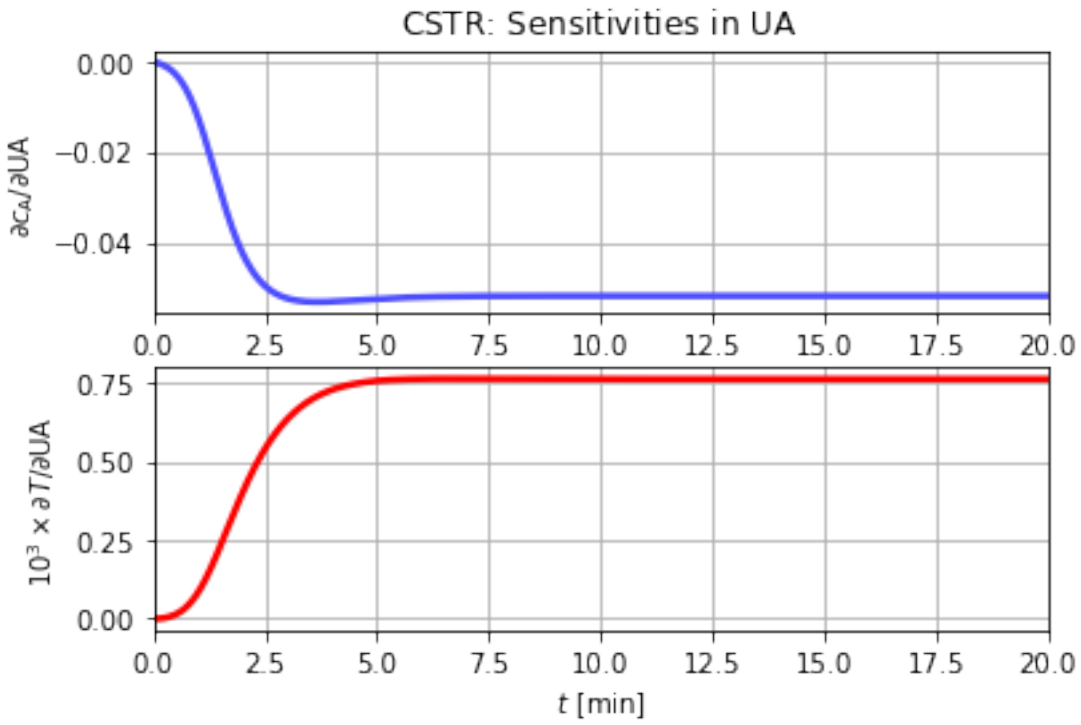
```
            obj.simulate()
            # get eXcited SOLutions (Lv) as 2D array, and append to list
            solX.append(np.asarray(obj.getSolutions(*Lv)))
            # reset parameters to nominal values
            obj.setParameters(**dict(Lpar0))
        # Compute sensitivities and add to list, one 2D array per parameter (Lp)
        LSname = [] # Preparing list of names of sensitivities
        LSarray = [] # Preparing list of 2d sensitivity arrays, 1 per parameter
        for i,sol in enumerate(solX):
            LSarray.append((sol-sol0)/(par0[i]*Le[i]))
            for var in Lv:
                # NOTE: In analytic sensitivities, "var" and "LP[i]" are reversed
                # ... I find the order below more natural
                LSname.append("$Sensitivities." + var + "." + Lp[i])
        # Converting list of 2D arrays to a 2D array by stacking elements in list
        Sarray = np.vstack(LSarray)
        return LSname, Sarray
```

In [14]:
```
Sn, Sa = sensitivity(sr_org,["T","cA"],["UA","EdR"])
```

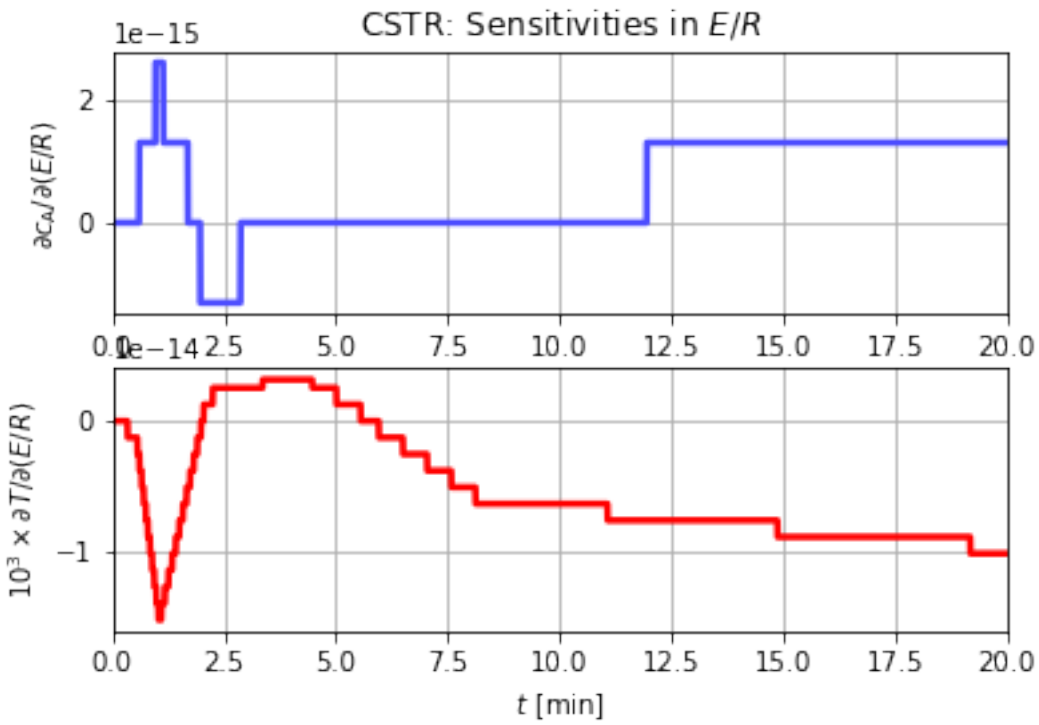
In [15]:
```
Sn
```

Out[15]:
```
['$Sensitivities.T.UA',
 '$Sensitivities.cA.UA',
 '$Sensitivities.T.EdR',
 '$Sensitivities.cA.EdR']
```

In [16]:
```
plt.subplot(2,1,1)
plt.plot(tm,Sa[0],linewidth=LW1,color=Cb1)
plt.ylabel(r'${\partial c_\mathrm{A}}/{\partial \mathrm{UA}}$')
plt.title(r'CSTR: Sensitivities in $\mathrm{UA}$')
plt.grid()
plt.xlim(0,20)
plt.subplot(2,1,2)
plt.plot(tm,Sa[1]*1e3,linewidth=LW1,color=Cr1)
plt.ylabel(r'$10^3 \times{\partial T}/{\partial \mathrm{UA}}$')
plt.xlabel(r'$t $ [min]')
plt.grid()
plt.xlim(0,20)
figfile = "TcA_UA_NumSensitivityReactororg.pdf"
plt.savefig(figpath+figfile)
```




```
In [17]: plt.subplot(2,1,1)
         plt.plot(tm,Sa[2],linewidth=LW1,color=Cb1)
         plt.ylabel(r'${\partial c_\mathrm{A}}/{\partial (E/R)}$')
         plt.title(r'CSTR: Sensitivities in $E/R$')
         plt.grid()
         plt.xlim(0,20)
         plt.subplot(2,1,2)
         plt.plot(tm,Sa[3]*1e3,linewidth=LW1,color=Cr1)
         plt.ylabel(r'$10^3 \times{\partial T}/{\partial (E/R)}$')
         plt.xlabel(r'$t $ [min]')
         plt.grid()
         plt.xlim(0,20)
         figfile = "TcA_EdR_NumSensitivitySeborgCSTRorg.pdf"
         plt.savefig(figpath+figfile)
```



Here, numerical sensitivity has been computed. OpenModelica has support for computing analytic sensitivities, but that has not been properly interfaced to the Python API at the moment.