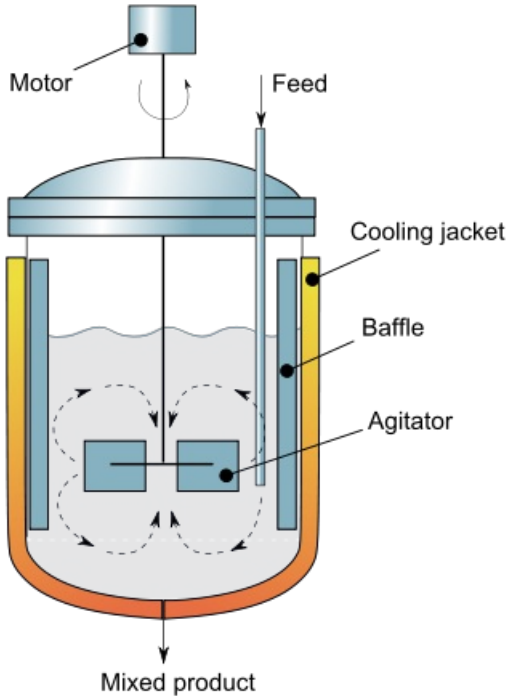
5.2 Exothermic CSTR

In [ ]:

```
!pip install -q pyomo
```

Description

This example is intended as an introduction to the nonlinear dynamics of an exothermic continuous stirred-tank reactor. The example has been studied by countless researchers and students since the pioneering work of Amundson and Aris in the 1950's. The particular formulation and parameter values described below are taken from example 2.5 from Seborg, Edgar, Mellichamp and Doyle (SEMD).



(Diagram By Daniele Pugliesi - Own work, CC BY-SA 3.0, Link)

Arrehenius Law Kinetics for a First-Order Reaction

We assume the kinetics are dominated by a single first order reaction

$$A \xrightarrow{kc_A} \text{Products}$$

The reaction rate per unit volume is modeled as the product kc_A where c_A is the concentration of A. The rate constant $k(T)$ is a increases with temperature following the Arrehenius law

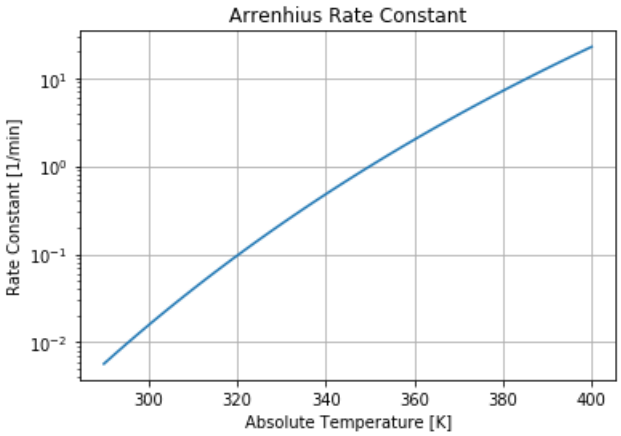
$$k(t) = k_0 e^{-\frac{E_a}{RT}}$$

E_a is the activation energy, R is the gas constant, T is absolute temperature, and k_0 is the pre-exponential factor.

We can see the strong temperature dependence by plotting $k(T)$ versus temperature over typical operating conditions.

In [2]:

```
%matplotlib inline
import matplotlib.pyplot as plt
import numpy as np

Ea  = 72750     # activation energy J/gmol
R   = 8.314     # gas constant J/gmol/K
k0  = 7.2e10    # Arrhenius rate constant 1/min

T = np.linspace(290,400)

# Arrhenius rate expression
def k(T):
    return k0*np.exp(-Ea/R/T)

plt.semilogy(T,k(T))
plt.xlabel('Absolute Temperature [K]')
plt.ylabel('Rate Constant [1/min]')
plt.title('Arrenhius Rate Constant')
plt.grid(True)
```



This graph shows the reaction rate changes by three orders of magnitude over the range of possible operating temperatures. Because an exothermic reaction releases heat faster at higher temperatures, there is a positive feedback that can potentially result in unstable process behavior.

Modeling and Parameter Values

Mathematical Model

The model consists of mole and energy balances on the contents of the well-mixed reactor.

$$V\frac{dc_A}{dt} = q(c_{Ai} - c_A) - Vkc_A$$
$$V\rho C_p\frac{dT}{dt} = wC_p(T_i - T) + (-\Delta H_R)Vkc_A + UA(T_c - T)$$

which are the equations that will be integrated below.

Quantity	Symbol	Value	Units	Comments
Activation Energy	E_a	72,750	J/gmol	
Arrehnius pre-exponential	k_0	7.2 x 10^{10}	1/min	
Gas Constant	R	8.314	J/gmol/K	
Reactor Volume	V	100	liters	
Density	ρ	1000	g/liter	
Heat Capacity	C_p	0.239	J/g/K	
Enthalpy of Reaction	ΔH_r	-50,000	J/gmol	
Heat Transfer Coefficient	UA	50,000	J/min/K	
Feed flowrate	q	100	liters/min	
Feed concentration	$c_{A,f}$	1.0	gmol/liter	
Feed temperature	T_f	350	K	
Initial concentration	$c_{A,0}$	0.5	gmol/liter	
Initial temperature	T_0	350	K	
Coolant temperature	T_c	300	K	Primary Manipulated Variable

Pyomo Model

In [ ]:

```
from pyomo.environ import *
from pyomo.dae import *
from pyomo.dae.simulator import Simulator

Ea  = 72750     # activation energy J/gmol
R   = 8.314     # gas constant J/gmol/K
k0  = 7.2e10    # Arrhenius rate constant 1/min
V   = 100.0     # Volume [L]
rho = 1000.0    # Density [g/L]
Cp  = 0.239     # Heat capacity [J/g/K]
dHr = -5.0e4    # Enthalpy of reaction [J/mol]
UA  = 5.0e4     # Heat transfer [J/min/K]
q   = 100.0     # Flowrate [L/min]
cAi = 1.0       # Inlet feed concentration [mol/L]
Ti  = 350.0     # Inlet feed temperature [K]
cA0 = 0.5       # Initial concentration [mol/L]
T0  = 350.0     # Initial temperature [K]
Tc  = 300.0     # Coolant temperature [K]

def cstr(cA0 = 0.5, T0 = 350.0):
    m     = ConcreteModel()
    m.t   = ContinuousSet(bounds=(0.0, 10.0))
    m.cA  = Var(m.t)
    m.T   = Var(m.t)
    m.dcA = DerivativeVar(m.cA)
    m.dT  = DerivativeVar(m.T)

    # Setting the initial conditions
    m.cA[0.0] = cA0
    m.T[0.0]  = T0

    k = lambda T: k0*exp(-Ea/R/T)
    m.ode1 = Constraint(m.t, rule=lambda m, t:
        V*m.dcA[t] == q*(cAi - m.cA[t]) - V*k(m.T[t])*m.cA[t])
    m.ode2 = Constraint(m.t, rule=lambda m, t:
        V*rho*Cp*m.dT[t] == q*rho*Cp*(Ti - m.T[t]) + (-dHr)*V*k(m.T[t])*m.cA[t] + UA*(Tc
- m.T[t]))

    return m
```

Simulation and Visualization

Visualization Function

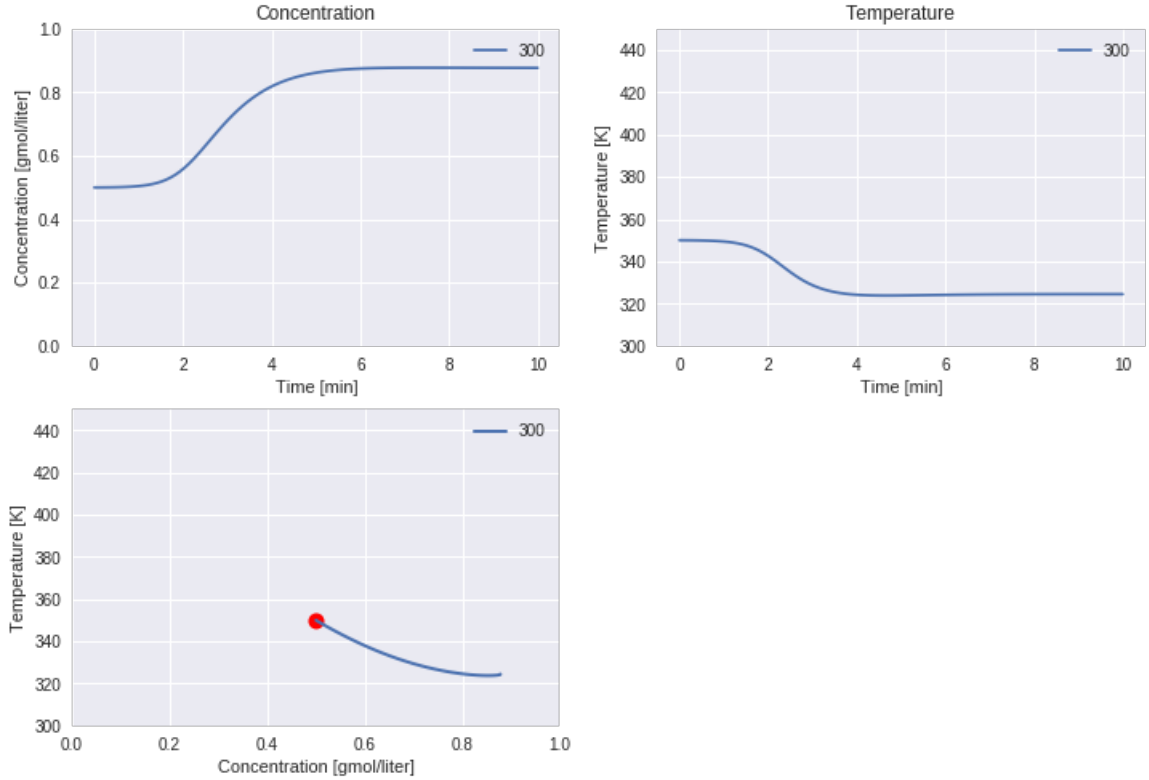
In [ ]:

```
%matplotlib inline
import matplotlib.pyplot as plt

# visualization function plots concentration and temperature
def cstr_plot(t, y, ax=[]):
    if len(ax) == 0:
        fig = plt.figure(figsize=(12,8))

        ax1 = plt.subplot(2,2,1)
        plt.xlabel('Time [min]')
        plt.ylabel('Concentration [gmol/liter]')
        plt.title('Concentration')
        plt.ylim(0,1)

        ax2 = plt.subplot(2,2,2);
        plt.xlabel('Time [min]')
        plt.ylabel('Temperature [K]');
        plt.title('Temperature')
        plt.ylim(300,450)

        ax3 = plt.subplot(2,2,3);
        plt.xlabel('Concentration [gmol/liter]')
        plt.ylabel('Temperature [K]');
        plt.xlim(0,1)
        plt.ylim(300,450)
    else:
        ax1, ax2, ax3 = ax
    ax1.plot(t, y[:,0], label=str(Tc))
    ax1.legend()
    ax2.plot(t, y[:,1], label=str(Tc))
    ax2.legend()
    ax3.plot(y[0,0],y[0,1],'r.',ms=20)
    ax3.plot(y[:,0],y[:,1], lw=2, label=str(Tc))
    ax3.legend()
    return [ax1, ax2, ax3]
```

Simulation

In [7]:

```
Tc = 300
tsim, profiles = Simulator(cstr(), package='scipy').simulate(numpoints=100)
cstr_plot(tsim, profiles);
```

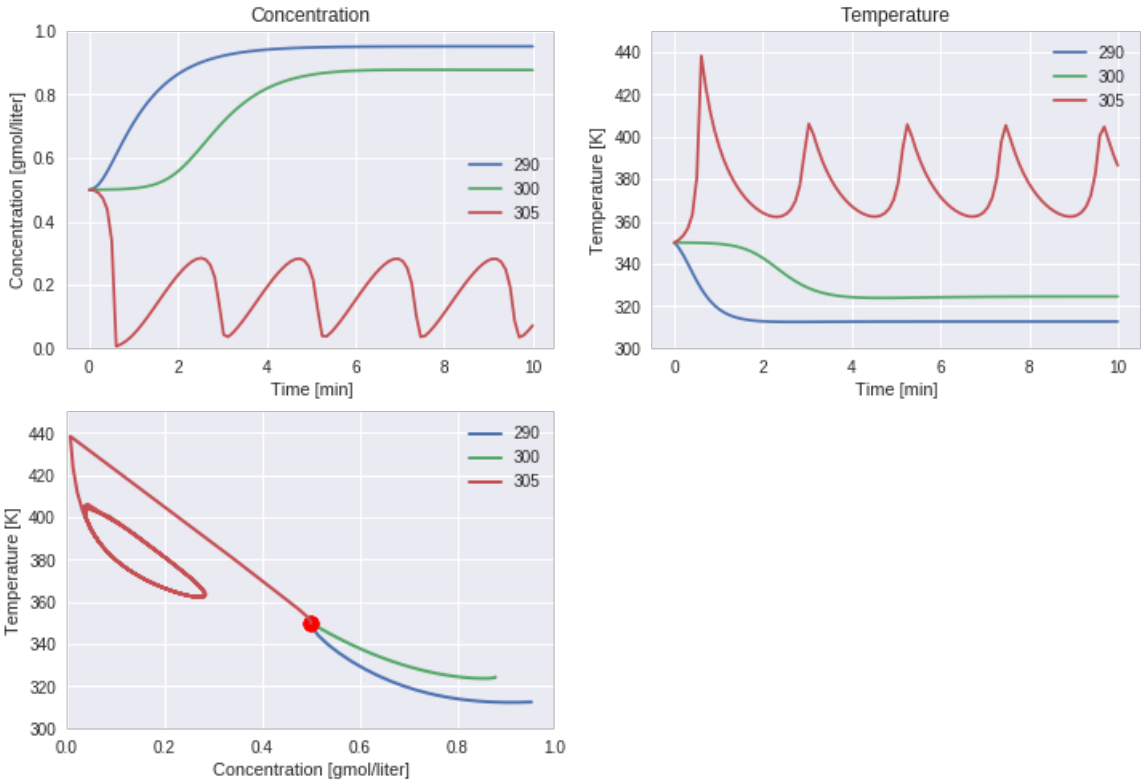


Effect of Cooling Temperature

The primary means of controlling the reactoris through temperature of the cooling water jacket. The next calculations explore the effect of plus or minus change of 5 K in cooling water temperature on reactor behavior. These simulations reproduce the behavior shown in Example 2.5 SEMD.

In [ ]:

```
ax = []
for Tc in [290, 300, 305]:
    tsim, profiles = Simulator(cstr(), package='scipy').simulate(numpoints=100)
    ax  = cstr_plot(tsim, profiles, ax)
```



In [32]:

```
#@title CSTR Simulation { run: "auto", vertical-output: true }
T_cooling = 304.4 #@param {type:"slider", min:290, max:305, step:0.1}
ax = []
Tc = T_cooling
tsim, profiles = Simulator(cstr(), package='scipy').simulate(numpoints=100)
ax  = cstr_plot(tsim, profiles, ax);
```