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Python Kinetics Code

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Simple Micro Kinetic Model for CO Oxidation :

Overall Reaction:

$$CO + \frac{1}{2}O_2 \overset{\text{Pt/Pd}}{\rightleftharpoons} CO_2$$

Note Reations in the Reaction Mechanism may be reversible or irreversible

Reaction 1: Adsorption of CO

$$CO + * \rightleftharpoons CO^*$$

Reaction 2: Adsorption of O_2

$$O_2 + * \rightleftharpoons {O_2}^*$$

Reaction 3: Dissociation of ${O_2}^*$

$${O_2}^* + * \rightleftharpoons 2O^*$$

Reaction 4: Surface Reaction of CO and O_2

$$CO^* + O^* \rightleftharpoons CO_2 + 2*$$

Modelling Proposed Reaction Mechanism :

${k_i}^j$ = Rate constant/coefficient for reaction i,
for j = {f,r} ; where f = forward reaction and r = the reverse reaction
r_i = Rate of reaction for reaction i

θ_m = Surface Coverage of species m
$\sum_{m=1}^{N} \theta_m = 1$
$= \theta_{CO} + \theta_{O_2} + \theta_O + \theta_*$

For the Irreversible Case: (Method 1)

Rate Equations:

$$r_1 = k_1^f \cdot \mathrm{P}_{CO} \cdot \theta_*$$

$$r_2 = k_2^f \cdot \mathrm{P}_{O_2} \cdot \theta_*$$

$$r_3 = k_3^f \cdot \theta_{O_2} \cdot \theta_*$$

$$r_4 = k_4^f \cdot \theta_{CO} \cdot \theta_O$$

For the Reversible Case: (Method 2)

Rate Equations:

$$r_1 = k_1^f \cdot \mathrm{P}_{CO} \cdot \theta_* - k_1^r \cdot \theta_{CO}$$

$$r_2 = k_2^f \cdot \mathrm{P}_{O_2} \cdot \theta_* - k_2^r \cdot \theta_{O_2}$$

$$r_3 = k_3^f \cdot \theta_{O_2} \cdot \theta_* - k_3^r \cdot \theta_O^2$$

$$r_4 = k_4^f \cdot \theta_{CO} \cdot \theta_O - k_4^r \cdot \mathrm{P}_{CO_2} \cdot \theta_*^2$$

The Corresponding Differential Equations corresponding to the rate of formations of the different coverages:

$$r_{\theta_{CO}} = \frac{d\theta_{CO}}{dt} = r_1 - r_4$$

$$r_{\theta_{O_2}} = \frac{d\theta_{O_2}}{dt} = r_2 - r_3$$

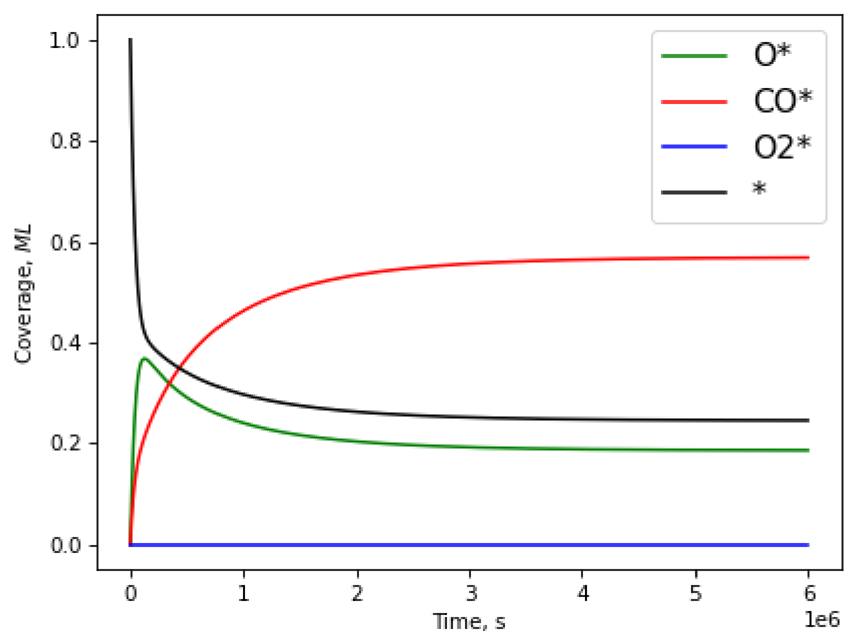
$$r_{\theta_O} = \frac{d\theta_O}{dt} = 2r_3 - r_4$$

$$r_{\theta_*} = \frac{d\theta_*}{dt} = 2r_4 - r_1 - r_2 - r_3$$

In [1]:
```
%matplotlib notebook
import matplotlib.pyplot as plt
import numpy as np


def sol(t,u,k1f,k1r,k2f,k2r,k3f,k3r,k4f,k4r,P1,P2,P3):
    # 1 = CO ; 2 = O2 ; 3 = O ; 4 = *

    #Surface Coverage
    th1 = u[0] #Theta_CO
    th2 = u[1] #Theta_O
    th3 = u[2] #Theta_O2
    th4 = u[3] #Theta_*

    #Partial Pressures
    P1 #P_CO
    P2 #P_O2
    P3 #P_CO2

    #Rates of reaction
    r1 = k1f*P1*th4 - k1r*th1
    r2 = k2f*P2*th4 - k2r*th2
    r3 = k3f*th2*(th4) - k3r*(th3**2)
    r4 = k4f*th1*th3 - k4r*P3*(th4**2)


    #Rate of change of surface coverages
    D1 = r1-r4              #Rate of Formation of CO*
    D2 = r2-r3              #Rate of Formation of O_2*
    D3 = (2*r3)-r4          #Rate of Formation of O*
    D4 = (2*r4)-r3-r2-r1    #Rate of Formation of *

    return [D1,D2,D3,D4]

# CO ; O2 ; O ; *
init = [0,0,0,1]


P = 1e-8 # 1e-8 #bar
P1 = 1e-8 #P
P2 = 1e-8 #P
P3 = 1e-8 #P

k1f = 2.00e+00
k1r = 6.65e-09
k2f = 2.31e+02
k2r = 1.15e+05
k3f = 6.13e+08
k3r = 2.14e-02
k4f = 2.85e-06
k4r = 5.00e+02

Time =np.linspace(0, 6e6, num=1000)
t_span = (Time[0], Time[-1])
from scipy.integrate import odeint, solve_ivp
solve = solve_ivp(sol,t_span,init,args=(k1f,k1r,k2f,k2r,k3f,k3r,k4f,k4r,P1,P2,P3),method='BDF', rtol = 1I
solv = np.transpose(solve.y)
Time = np.transpose(solve.t)
```

In [2]:
```
plt.plot(Time, solv[:,2], 'g-', label='O*')
plt.plot(Time, solv[:,0],'r-', label='CO*')
plt.plot(Time, solv[:,1],'b-', label='O2*')
plt.plot(Time, solv[:,3],'k-', label='*')

#plt.plot(Time, solv[:,3], label='4')
plt.xlabel('Time, s')
plt.ylabel("Coverage, $ML$")
plt.legend(fontsize=15, loc='best')
plt.show()
```

Figure 1



pan/zoom

In [ ]: