A Computational Biology Approach to pH Selective Reactions in the Extracellular Fluid of Cancer Cells Based in the Gibbs Free Energy Minimization Approach

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"""
RISE-E-BASE
Undergraduate Research Program

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#neq:
#neq[0]=h2o
#neq[1]=s2
#neq[2]=h2sliq
#neq[3]=h3o
#neq[4]=hs
#neq[5]=oh

import numpy as np
from scipy.optimize import minimize
import math as math

#Initial data:
pH=5.0
V=100
T=298.15

in_h2o=(400*(1/1))/18.0
in_h2sgas=0.0
in_s2=2.5*(10**-6)
in_h3o=(10**(-pH))*V
in_h2s=0.0
in_hs=0.0
in_oh=(10**-(14-pH))*V

sumni_S=(0*in_h2o)+(1*in_h2sgas)+(1*in_s2)+(0*in_h3o)+(1*in_h2s)+(1*in_hs
)+(0*in_oh)
sumni_H=(2*in_h2o)+(2*in_h2sgas)+(0*in_s2)+(3*in_h3o)+(2*in_h2s)+(1*in_hs
)+(1*in_oh)
sumni_O=(1*in_h2o)+(0*in_h2sgas)+(0*in_s2)+(1*in_h3o)+(0*in_h2s)+(0*in_hs
)+(1*in_oh)


#Function to be optimized:
def GT(neq):
    neq=np.array(neq)
    gibbest_h2o=-237.14 #(kJ/mol)
    gibbest_h2sgas=-33.5
    gibbest_s2=85.8
    gibbest_h3o=0
    gibbest_h2s=-27.09
    gibbest_hs=12.05
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    gibbest_oh=-157.2

    sumneq_liq=neq[0]+neq[1]+neq[2]+neq[3]+neq[4]+neq[5]
    Grxn=gibbest_h2sgas-gibbest_h2s
    K=math.exp((-Grxn*1000)/(T*8.314))
    P=K*(neq[2]/V)
    neq_gas= (V*P)/(0.08314*T)

Gtotal=(neq[0]*((1000*gibbest_h2o)+(8.314*T*np.log(neq[0]/sumneq_liq))))+
(neq_gas*((1000*gibbest_h2sgas)+(8.314*T*np.log(P))))+(neq[1]*((1000*gibb
est_s2)+(8.314*T*np.log(neq[1]/sumneq_liq))))+(neq[2]*((1000*gibbest_h2s)
+(8.314*T*np.log(neq[2]/sumneq_liq))))+(neq[3]*((1000*gibbest_h3o)+(8.314
*T*np.log(neq[3]/sumneq_liq))))+(neq[4]*((1000*gibbest_hs)+(8.314*T*np.lo
g(neq[4]/sumneq_liq))))+(neq[5]*((1000*gibbest_oh)+(8.314*T*np.log(neq[5]
/sumneq_liq))))
    Gtotal=Gtotal/10000000
    return Gtotal

#Mass Balance:
def constraint_BS(neq):
    Grxn=-33.5-(-27.09)
    K=math.exp(-Grxn/(T*8.314))
    P=K*(neq[2]/V)
    neq_gas= (V*P)/(0.08314*T)

sumneq_S=(0*neq[0])+(1*neq_gas)+(1*neq[1])+(0*neq[3])+(1*neq[2])+(1*neq[4
])+(0*neq[5])
    return sumneq_S-sumni_S

def constraint_BH(neq):
    Grxn=-33.5-(-27.09)
    K=math.exp(-Grxn/(T*8.314))
    P=K*(neq[2]/V)
    neq_gas= (V*P)/(0.08314*T)

sumneq_H=(2*neq[0])+(2*neq_gas)+(0*neq[1])+(3*neq[3])+(2*neq[2])+(1*neq[4
])+(1*neq[5])
    return sumneq_H-sumni_H

def constraint_BO(neq):
    Grxn=-33.5-(-27.09)
    K=math.exp(-Grxn/(T*8.314))
    P=K*(neq[2]/V)
    neq_gas= (V*P)/(0.08314*T)

sumneq_O=(1*neq[0])+(0*neq_gas)+(0*neq[1])+(1*neq[3])+(0*neq[2])+(0*neq[4
])+(1*neq[5])
    return sumneq_O-sumni_O

#Equilibrium constant:
def constraint_K(neq):
    ce_h3o=neq[3]/V
    ce_oh=neq[5]/V
    return (ce_oh*ce_h3o)-(10**-14)
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def constraint_k2(neq):
    k2=(neq[4]/V)*(neq[3]/V)/(neq[2]/V)
    return k2-(9.0*10**-8)

def constraint_k3(neq):
    k3=(neq[1]/V)*(neq[3]/V)/(neq[4]/V)
    return k3-(1.0*10**-13)


#Initial Guess values:
x0=[5556.5,1.36*10**-11,0.363,0.0001,0.0002,0.0000000000233]

opt={'maxiter':30000,'ftol':0.0000000000000000001}

con1={'type': 'eq', 'fun':constraint_BS}
con2={'type': 'eq', 'fun':constraint_BH}
con3={'type': 'eq', 'fun':constraint_BO}
con5={'type': 'eq', 'fun':constraint_K}
con7={'type': 'eq', 'fun':constraint_k2}
con8={'type': 'eq', 'fun':constraint_k3}
cons=[con1,con2,con3,con5,con7,con8]

sol=minimize(GT,x0,method='SLSQP',constraints=cons, options=opt)

x=sol.x
print(sol)
print('H2O moles:'+ str(x[0]))
print('S2 moles:'+ str(x[1]))
print('H2S líquido moles:'+ str(x[2]))
print('H3O moles:'+ str(x[3]))
print('HS moles:'+ str(x[4]))
print('OH moles:'+ str(x[5]))

Grxn=-33.5-(-27.09)
K=math.exp((-Grxn*1000)/(298.15*8.314))
P=K*(x[2]/100)
neq_gas= (100*P)/(0.08314*298.15)
print ('H2S gas moles:'+ str(neq_gas))
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#Results:

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In [5]: runfile('C:/Users/User/Desktop/OPTIMIZED pH=5 clean.py', wdir='C:/Users/User/Desktop')
     fun: -0.5269806400599564
     jac: array([-0.02371401,  0.00309611, -0.01033422, -0.00248226, -0.00386876,
       -0.02046534])
 message: 'Optimization terminated successfully'
    nfev: 25954
     nit: 1553
    njev: 1553
  status: 0
 success: True
       x: array([2.22222272e+01, 2.16540073e-16, 2.38210652e-06, 9.95022047e-04,
       2.15462147e-08, 1.00500286e-07])
H2O moles:22.222227199675434
S2 moles:2.165400728008947e-16
H2S líquido moles:2.3821065202653123e-06
H3O moles:0.0009950220465025916
HS moles:2.154621473740922e-08
OH moles:1.0050028574893444e-07
H2S gas moles:1.2757402115279023e-06
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