

semicont

Reactores em estado Transiente

Arranque e Paragem

Reactores semi-contínuos

Reactor de volume variável com reacção de 1ª ordem.

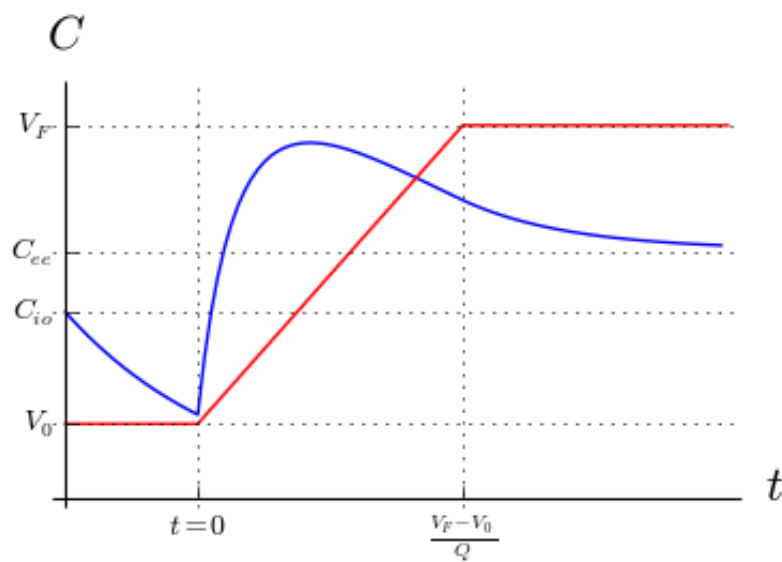
```
reset()
C=var('C')
Q=0.2
Vo=0.2
Ci=0.5
Ce=2
k=0.4

def V(t):
    if t<2:
        return Vo
    else:
        V=Vo+Q*(t-2)
        if V<1:
            return V
        else:
            return 1

t=srange(0,10,0.1)
C=range(len(t))

for i in range(len(t)):
    if t[i] <2.1:
        C[i]=Ci*exp(-k*t[i])
    else:
        C[i]=(C[i-1]*V(t[i])+(Q*(Ce-C[i-1])-k*C[i-1]*V(t[i]))*0.1)/V(t[i]))

p=line(zip(t,C),figsize=4,fontsize=10,ymax=1.1,ymin=0,axes_labels=
['t$', 'C$'],gridlines='minor',ticks=[[0,2,6],
[0,Ci,Vo,1,0.66]],tick_formatter=[['','t=0$','$\\frac{V_F-V_0}{Q}$'],
['$0$', '$C_{io}$', '$V_0$', '$V_F$', '$C_{ee}$']])
p+=plot(V,0,10,color='red')
show(p)
```



Destilação Reactiva

$A \leftrightarrow B \uparrow$

```

reset()
Q=0.5
Vo=1
Vt=2
Ci=1
k=0.4      #cte. de velocidade
K=0.2      #cte. de equilibrio
kv=0.5     #cte. de vaporização mol_b/min

dt=0.01
tf=50
t=srange(0,tf,dt)
Np=len(t)

C=range(Np)
V=range(Np)
x=range(Np)
q=range(Np)
ng=range(Np)

C[0]=Ci
V[0]=Vo
no=Ci*Vo
q[0]=0
ng[0]=0

for i in range(len(t)):
    if i<=0:

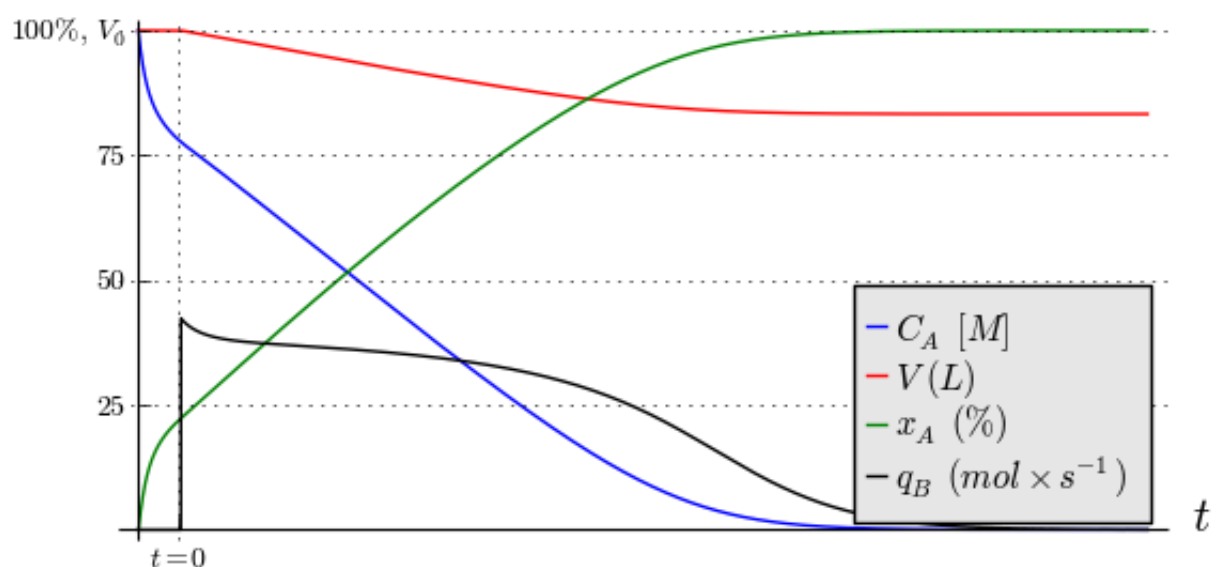
```

```

i=1
Vg=Vt-V[i-1]
if Ci-C[i-1]>0:
    Cb=Ci-C[i-1]
else:
    Cb=0
yl=Cb/Ci
yg=ng[i-1]/Vg
if t[i] <2.1:
    V[i]=Vo
    C[i]=(C[i-1]*V[i]-k*(C[i-1]-1/K*(Ci-C[i-1]))*V[i]*dt)/V[i]
    q[i]=0
    ng[i]=ng[i-1]+kv*(yl-yg)*dt
    Ci=(Ci*V[i-1]-kv*(yl-yg)*dt)/V[i-1]
else:
    ng[i]=ng[i-1]+(kv*(yl-yg)-Q*ng[i-1]/Vg)*dt
    V[i]=V[i-1]-(kv*(yl-yg)*dt)*0.2# PM/rho=0.2
    Ci=(Ci*V[i-1]-kv*(yl-yg)*dt)/V[i-1]
    C[i]=(C[i-1]*V[i-1]-k*(C[i-1]-1/K*Cb)*V[i-1]*dt)/V[i-1]
    q[i]=Q*ng[i-1]/Vg*10
x[i]=(no-C[i-1]*V[i-1])/no

p=line(zip(t,C),figsize=(6,3),fontsize=10,ymax=1,ymin=0,axes_labels=
['$t$', ''],gridlines='minor',ticks=[[0,2],
[0,0.25,0.5,0.75,Vo]],tick_formatter=[[ '','$t=0$'],['$0$','$25\
%$', '$50\ %$', '$75\ %$', '$100\%', \ V_0$']],legend_label=u'$C_A\
[M]$',
p+=line(zip(t,V),color='red',legend_label=u'$V\ (L)$')
p+=line(zip(t,x),color='green',legend_label=u'$x_A\ (\%)$')
p+=line(zip(t,q),color='black',legend_label=u'$q_B\ (mol\\times\
s^{-1})$')
show(p,legend_loc="lower right")

```



```

reset()
SAo=0.01
XBo=0.1
SAe=1
XBe=0

umax=0.1      #cte. de velocidade
K=0.1        #cte. de equilibrio
Y=0.14       #cte. de vaporização mol_b/min
D=0.04

dt=0.1
tf=60
t=srange(0,tf,dt)
Np=len(t)

S=range(Np)
X=range(Np)

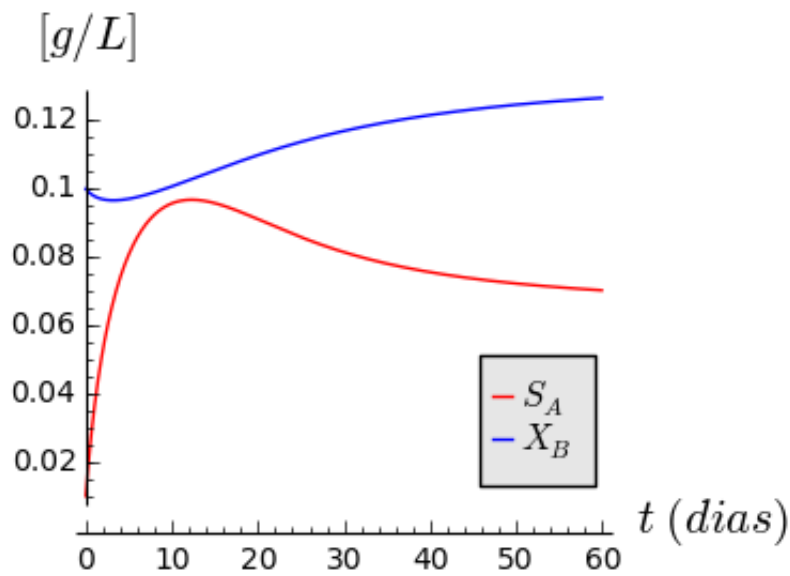
S[0]=SAo
X[0]=XBo

def nu(S):
    return umax*S/(K+S)

for i in range(len(t)):
    if i<=0:
        i=1
    Si=S[i-1]
    Xi=X[i-1]
    S[i]=Si+(D*(SAe-Si)-nu(Si)*Xi/Y)*dt
    X[i]=Xi+(D*(XBe-Xi)+nu(Si)*Xi)*dt

p=line(zip(t,S),color='red',legend_label=u'$S_A$')
p+=line(zip(t,X),figsize=(4,3),fontsize=10,axes_labels=['$t\backslash$
(dias)$','$[g/L ]$'],legend_label=u'$X_B$')
show(p,legend_loc="lower right")

```



```

reset()
Qo=0.2
Vo=0.2
Ce=2
k=0.2

dt=0.01
t=srange(0,10,dt)
Np=len(t)
A=range(Np)
B=range(Np)
V=range(Np)

A[0]=1
B[0]=0
V[0]=Vo

for i in range(Np):
    if i<1:
        i=1
    if t[i] <2.1:
        Q=0
    else:
        Q=Qo

    V[i]=V[i-1]+Q*dt
    rA=-k*A[i-1]*B[i-1]
    A[i]=A[i-1]+(rA-Q/V[i-1]*A[i-1])*dt
    B[i]=B[i-1]+(rA+Q/V[i-1]*(Ce-B[i-1]))*dt

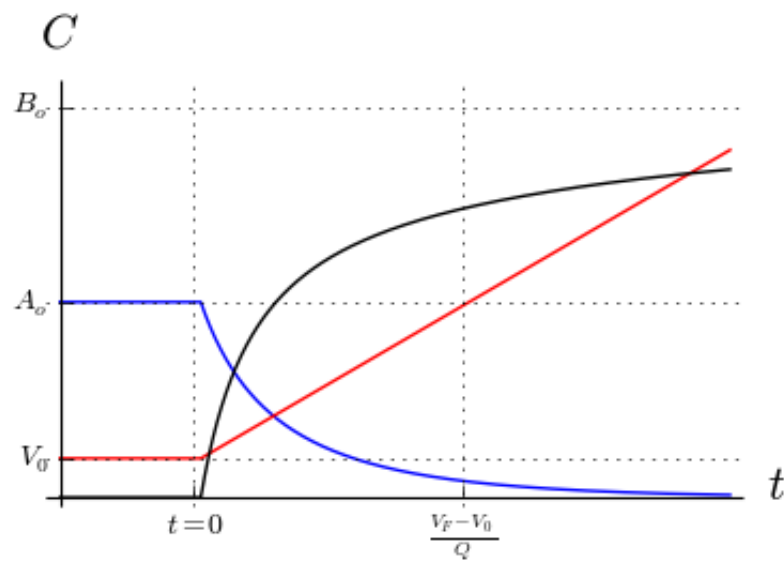
p=line(zip(t,A),figsize=4,fontsize=10,axes_labels=
['$t$', '$C$'],gridlines='minor',ticks=[[0,2,6],
[0,Vo,1,Ce]],tick_formatter=[['','$t=0$','$\\frac{V_F-V_0}{Q}$'],

```

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['$0$', '$V_0$', '$A_o$', '$B_o$']],ymax=2.1)
p+=line(zip(t,V),color='red')
p+=line(zip(t,B),color='black')
show(p)

```



```

reset()
Qo=0.02
Vo=0.5
Ce=2
kD=10
kU=10

dt=0.01
t=srange(0,10,dt)
Np=len(t)
A=range(Np)
B=range(Np)
D=range(Np)
U=range(Np)
V=range(Np)

A[0]=0.4
B[0]=0
D[0]=0
U[0]=0
V[0]=Vo

for i in range(Np):
    if i<=1:
        i=1
    V[i]=V[i-1]+Qo*dt
    if B[i-1]<=0 or A[i-1]<=0:
        rD=0
        rU=0
    else:
        rD=-kD*A[i-1]^2*B[i-1]/V[i-1]^2

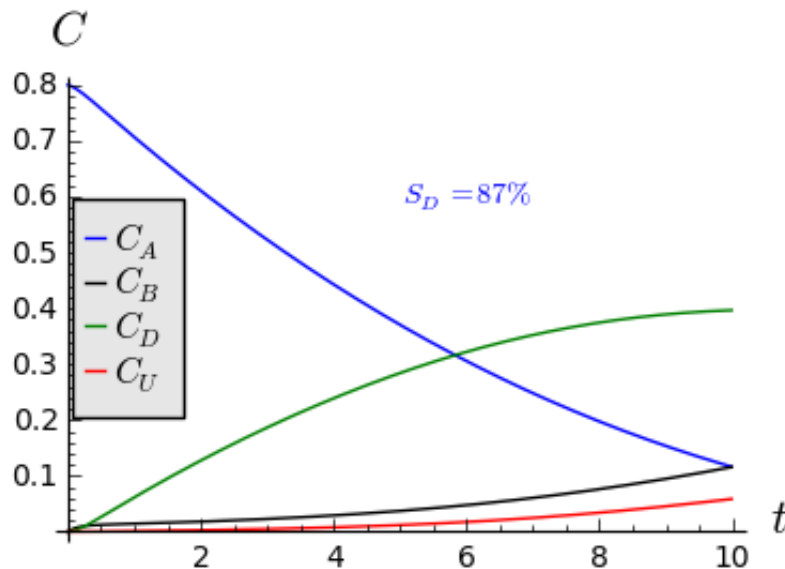
```

```

        rU=-kU*A[i-1]*B[i-1]^2/V[i-1]^2
        A[i]=A[i-1]+(rD+rU)*dt
        B[i]=B[i-1]+(rD+rU+Qo*Ce)*dt
        D[i]=D[i-1]+(-rD)*dt
        U[i]=U[i-1]+(-rU)*dt
for i in range(Np):
    A[i]=A[i]/V[i]
    B[i]=B[i]/V[i]
    D[i]=D[i]/V[i]
    U[i]=U[i]/V[i]

p=line(zip(t,A),figsize=4,fontsize=10,axes_labels=
['$t$', '$C_A$'],legend_label=u'$C_A$')
#p+=line(zip(t,V),color='gray',legend_label=u'$V$')
p+=line(zip(t,B),color='black',legend_label=u'$C_B$')
p+=line(zip(t,D),color='green',legend_label=u'$C_D$')
p+=line(zip(t,U),color='red',legend_label=u'$C_U$')
p+=text('$S_D=87\%\$',(6,0.6))
show(p)

```



```
D[Np-1]/(D[Np-1]+U[Np-1])
```

```
0.871320676104430
```

```

reset()
Qo=0
Vo=0.5
Ce=2
kD=10
kU=10

dt=0.01
t=srange(0,10,dt)
Np=len(t)
A=range(Np)
B=range(Np)
D=range(Np)

```

```

U=range(Np)
V=range(Np)

A[0]=0.4
B[0]=0.4
D[0]=0
U[0]=0
V[0]=Vo+0.02*10

for i in range(Np):
    if i<=1:
        i=1
    V[i]=V[i-1]+Qo*dt
    if B[i-1]<=0 or A[i-1]<=0:
        rD=0
        rU=0
    else:
        rD=-kD*A[i-1]^2*B[i-1]/V[i-1]^2
        rU=-kU*A[i-1]*B[i-1]^2/V[i-1]^2
    A[i]=A[i-1]+(rD+rU)*dt
    B[i]=B[i-1]+(rD+rU+Qo*Ce)*dt
    D[i]=D[i-1]+(-rD)*dt
    U[i]=U[i-1]+(-rU)*dt
for i in range(Np):
    A[i]=A[i]/V[i]
    B[i]=B[i]/V[i]
    D[i]=D[i]/V[i]
    U[i]=U[i]/V[i]

p=line(zip(t,A),figsize=4,fontsize=10,axes_labels=
['$t$', '$C_A$'],legend_label=u'$C_A$')
#p+=line(zip(t,V),color='gray',legend_label=u'$V$')
p+=line(zip(t,B),color='black',legend_label=u'$C_B$',linestyle='--')
p+=line(zip(t,D),color='green',legend_label=u'$C_D$')
p+=line(zip(t,U),color='red',legend_label=u'$C_U$',linestyle='--')
p+=text('$S_D=50\\%$',(6,0.6))
show(p)

```