The following is the analytical solution for the diffusion in composite spherical geometry: (For more details refer to "Lithium Intercalation in Core-Shell Materials–Theoretical Analysis")

```
> restart:with(plots):Digits:=15:with(RootFinding):with(IntegrationTools):
>
```

User defined parameters:

Description of parameters: beta^2=D2/D1, alpha=R1/R2, kappa=c1*/c2*,delta=current density

```
> constants:=[beta=5,alpha=0.4,gamma=1000,kappa=1.5,delta=-.25];
```

$$constants := [\beta = 5, \alpha = 0.4, \gamma = 1000, \kappa = 1.5, \delta = -0.25]$$

Number of eigenvalues to be used (Higher the better!!!)

```
> NN:=20:
>
>
```

Solution

```
> param1:=[theta[n]=alpha*lambda[n]*beta,phi[n]=lambda[n]*(alpha-1)];
```

$$param1 := [\theta_n = \alpha \lambda_n \beta, \phi_n = \lambda_n (\alpha - 1)]$$

```
> param2:=[theta[n]=alpha*lambda*beta,phi[n]=lambda*(alpha-1)];
```

$$param2 := [\theta_n = \alpha \lambda \beta, \phi_n = \lambda (\alpha - 1)]$$

Eigenvalue Equation

```
> eigeneqn:=subs(param2,(1/gamma+beta^2*alpha^2*lambda^2+1/gamma*alpha*lambda^2-alpha*kappa+beta^2*alpha)*sin(theta[n])*sin(phi[n])+(-beta^2*alpha^2*lambda+beta^2*alpha*lambda-alpha*lambda*kappa+1/gamma*lambda-1/gamma*lambda*alpha)*cos(phi[n])*sin(theta[n])+(beta*alpha^2*lambda*kappa-1/gamma*beta*lambda*alpha-1/gamma*beta*lambda^3*alpha^2)*sin(phi[n])*cos(theta[n])+(beta*alpha^2*lambda^2*kappa+1/gamma*beta*lambda^2*alpha^2-1/gamma*beta*lambda^2*alpha)*cos(theta[n])*cos(phi[n]));
```

$$eigeneqn := \left(\frac{1}{\gamma} + \beta^2 \alpha^2 \lambda^2 + \frac{\alpha \lambda^2}{\gamma} - \alpha \kappa + \beta^2 \alpha\right) \sin(\alpha \lambda \beta) \sin(\lambda (\alpha - 1)) + \left(-\beta^2 \alpha^2 \lambda + \beta^2 \alpha \lambda - \alpha \lambda \kappa + \frac{\lambda}{\gamma} - \frac{\lambda \alpha}{\gamma}\right) \cos(\lambda (\alpha - 1)) \sin(\alpha \lambda \beta) + \left(\beta \alpha^2 \lambda \kappa - \frac{\beta \lambda \alpha}{\gamma} - \frac{\beta \lambda^3 \alpha^2}{\gamma}\right) \sin(\lambda (\alpha - 1)) \cos(\alpha \lambda \beta) + \left(\beta \alpha^2 \lambda^2 \kappa + \frac{\beta \lambda^2 \alpha^2}{\gamma} - \frac{\beta \lambda^2 \alpha}{\gamma}\right) \cos(\alpha \lambda \beta) \cos(\lambda (\alpha - 1))$$

Function to return Eigenequation (necessary for using Nextzero function of Maple) The following eqution is hardcoded (copy pasted from above), this is the only way I can make the nextzero work.

```
> KKK:=lambda->(1/gamma+beta^2*alpha^2*lambda^2+1/gamma*alpha*lambda^2-alpha*kappa+beta^2*alpha)*sin(alpha*lambda*beta)*sin(lambda*(alpha-1))+(-beta^2*alpha^2*lambda+beta^2*alpha*lambda-alpha*lambda*kappa+1/gamma*lambda-1/gamma*lambda*alpha)*cos(lambda*(alpha-1))*sin(alpha*lambda*beta)+(beta*alpha^2*lambda*kappa-1/gamma*beta*lambda*alpha-1/gamma*beta*lambda^3*alpha^2)*sin(lambda*(alpha-1))*cos(alpha*lambda*beta)+(beta*alpha^2*lambda^2*kappa+1/gamma*beta*lambda^2*alpha^2-1/gamma*beta*lambda^2*alpha)*cos(alpha*lambda*beta)*cos(lambda*(alpha-1));
```

$$KKK := \lambda \to \left(\frac{1}{\gamma} + \beta^2\alpha^2\lambda^2 + \frac{\alpha\lambda^2}{\gamma} - \alpha\kappa + \beta^2\alpha\right)\sin(\alpha\lambda\beta)\sin(\lambda(\alpha-1)) + \left(-\beta^2\alpha^2\lambda + \beta^2\alpha\lambda - \alpha\lambda\kappa + \frac{\lambda}{\gamma} - \frac{\lambda\alpha}{\gamma}\right)\cos(\lambda(\alpha-1))\sin(\alpha\lambda\beta) + \left(\beta\alpha^2\lambda\kappa - \frac{\beta\lambda\alpha}{\gamma} - \frac{\beta\lambda^3\alpha^2}{\gamma}\right)\sin(\lambda(\alpha-1))\cos(\alpha\lambda\beta) + \left(\beta\alpha^2\lambda^2\kappa + \frac{\beta\lambda^2\alpha^2}{\gamma} - \frac{\beta\lambda^2\alpha}{\gamma}\right)\cos(\alpha\lambda\beta)\cos(\lambda(\alpha-1))$$

```
> ChiParam:=
  [

  chi[1] = cos(theta[n])*theta[n]-sin(theta[n]),
  chi[2] = phi[n]*cos(phi[n])+(-alpha*lambda[n]^2-1)*sin(phi[n]),
  chi[3] = -theta[n]+cos(theta[n])*sin(theta[n]),
  chi[4] =
  cos(phi[n])*sin(phi[n])*(-lambda[n]^2+1)+2*lambda[n]*cos(phi[n])^2-phi[n]*lambda[n]^2+(-alpha-1)*lambda[n]

  ];
```

$$ChiParam := [\chi_1 = \cos(\theta_n)\theta_n - \sin(\theta_n), \chi_2 = \phi_n\cos(\phi_n) + (-\alpha\lambda_n^2 - 1)\sin(\phi_n), \chi_3 = -\theta_n + \cos(\theta_n)\sin(\theta_n), \chi_4 = \cos(\phi_n)\sin(\phi_n)(-\lambda_n^2 + 1) + 2\lambda_n\cos(\phi_n)^2 - \phi_n\lambda_n^2 + (-\alpha-1)\lambda_n]$$

```
>
> Aeqn:=A[n] =
  2*chi[1]*delta*kappa*lambda[n]/(beta^3*chi[2]^2*chi[3]-kappa*chi[1]^2*chi[4]);
```

$$Aeqn := A_n = \frac{2\chi_1\delta\kappa\lambda_n}{\beta^3\chi_2^2\chi_3 - \kappa\chi_1^2\chi_4}$$

```
> OtherParam:=[

  k[1] = -3*kappa*delta/(alpha^3*kappa-alpha^3+1),
  k[2] = -3*delta/(alpha^3*kappa-alpha^3+1),

  a[1] =
  1/10*(-5*alpha^5*beta^2-3*alpha^5+(3*alpha^5*beta^2+5*alpha^5-15*a
  lpha^3+10*alpha^2)*kappa+15*alpha^3-15*alpha^2+5*alpha^2*beta^2+3)
  *delta*kappa/(alpha^3*kappa-alpha^3+1)^2+1/10*(10*alpha^4-10*alpha
  )*delta*kappa/(alpha^3*kappa-alpha^3+1)^2/gamma,

  a[2] =
  -1/10/(alpha^6*kappa^2+(-2*alpha^6+2*alpha^3)*kappa+alpha^6-2*alph
  a^3+1)*(10*kappa^2*alpha^5+((2*beta^2-30)*alpha^5+15*alpha^3)*kapp
  a+18*alpha^5-15*alpha^3-3)*delta+1/(alpha^6*kappa^2+(-2*alpha^6+2*
  alpha^3)*kappa+alpha^6-2*alpha^3+1)*kappa*alpha^4*delta/gamma
  ];
```

$$OtherParam := \left[k_1 = -\frac{3\,\kappa\,\delta}{\alpha^3\,\kappa - \alpha^3 + 1},\ k_2 = -\frac{3\,\delta}{\alpha^3\,\kappa - \alpha^3 + 1},\ a_1 = \frac{(-5\,\alpha^5\,\beta^2 - 3\,\alpha^5 + (3\,\alpha^5\,\beta^2 + 5\,\alpha^5 - 15\,\alpha^3 + 10\,\alpha^2)\,\kappa + 15\,\alpha^3 - 15\,\alpha^2 + 5\,\alpha^2\,\beta^2 + 3)\,\delta\,\kappa}{10\,(\alpha^3\,\kappa - \alpha^3 + 1)^2} + \frac{(10\,\alpha^4 - 10\,\alpha)\,\delta\,\kappa}{10\,(\alpha^3\,\kappa - \alpha^3 + 1)^2\,\gamma},\ a_2 = -\frac{(10\,\kappa^2\,\alpha^5 + ((2\,\beta^2 - 30)\,\alpha^5 + 15\,\alpha^3)\,\kappa + 18\,\alpha^5 - 15\,\alpha^3 - 3)\,\delta}{10\,(\alpha^6\,\kappa^2 + (-2\,\alpha^6 + 2\,\alpha^3)\,\kappa + \alpha^6 - 2\,\alpha^3 + 1)} + \frac{\kappa\,\alpha^4\,\delta}{(\alpha^6\,\kappa^2 + (-2\,\alpha^6 + 2\,\alpha^3)\,\kappa + \alpha^6 - 2\,\alpha^3 + 1)\,\gamma} \right]$$

```
> ###################
```

Final Solution

x2 #part1=without infinite sum, part2 term in the infinite sum

```
>
> x1part1:=1/6*k[1]*beta^2*x^2+a[1]+k[1]*t;
```

$$x1part1 := \frac{1}{6}\,k_1\,\beta^2\,x^2 + a_1 + k_1\,t$$

```
> x1part2:=-sin(lambda[n]*beta*x)*chi[2]*A[n]*beta^2/lambda[n]/x*exp
  (-lambda[n]^2*t);
```

$$x1part2 := -\frac{\sin(\lambda_n\,\beta\,x)\,\chi_2\,A_n\,\beta^2\,\mathbf{e}^{(-\lambda_n^{\,2}\,t)}}{\lambda_n\,x}$$

>

x2 #part1=without infinite sum, part2 term in the infinite sum

```
> x2part1:=1/6*k[2]*x^2-(-delta-1/3*k[2])/x+a[2]+k[2]*t;
```

$$x2part1 := \frac{1}{6} k_2 x^2 - \frac{-\delta - \frac{1}{3} k_2}{x} + a_2 + k_2 t$$

```
> x2part2:=-(lambda[n]*cos(x*lambda[n]-lambda[n])+sin(x*lambda[n]-la
  mbda[n]))/lambda[n]/x*chi[1]*A[n]*exp(-lambda[n]^2*t);
```

$$x2part2 := -\frac{(\lambda_n \cos(x \lambda_n - \lambda_n) + \sin(x \lambda_n - \lambda_n)) \chi_1 A_n \mathbf{e}^{\left(-\lambda_n^2 t\right)}}{\lambda_n x}$$

>

Calculation of X1 and X2 expressions using numerical eigenvalues

First Eigenvalue

```
> Lam[1]:=NextZero(subs(param1,constants,lambda[n]=lambda,eval(KKK))
  ,0);
```

$$Lam_1 := 1.58054819116320$$

All eigenvalues till NN

```
> for i from 2 to NN do
  Lam[i]:=NextZero(subs(constants,eval(KKK)),Lam[i-1]);od:
```

List of all the eigenvalues

```
> ListLambda:=[seq(lambda[i]=Lam[i],i=1..NN)]:
```

Check if the k1 k2 and a1 and a2 are calculated numerically

```
> evalf(subs(constants,OtherParam)):
```

Computation of Expressions for x1 and x2

```
> expr11:=0:expr22:=0:
  for i from 1 to NN do

  NumChiparam:=evalf(subs(param1,n=i,ListLambda,constants,ChiParam))
  ;
  NumAn:=evalf(subs(param1,n=i,ListLambda,constants,NumChiparam,Aneq
  n));

  expr11:=expr11
  +subs(param1,n=i,NumChiparam,ListLambda,NumAn,OtherParam,constants
  , x1part2):

  expr22:=expr22
```

```
+subs(param1,n=i,NumChiparam,ListLambda,NumAn,OtherParam,constants
, x2part2):
od:
> expr1:=expr11+subs(OtherParam,constants,x1part1):
> expr2:=expr22+subs(OtherParam,constants,x2part1):
> param1;
>
>
>
```

Plot of concentration curves

```
> p3:=plot(evalf(subs(t=0,expr1)),x=0..eval(alpha,constants)):p4:=pl
ot(evalf(subs(t=0,expr2)),x=eval(alpha,constants)..1):display(p3,p
4);

>
> q1:=plot3d(expr1,x=0..subs(constants,alpha),t=1/4000..0.1,axes=box
ed):
> q2:=plot3d(expr2,x=subs(constants,alpha)..1,t=1/4000..0.1,axes=box
ed):
> with(plots):
> display(q1,q2);
```

$$\mathrm{display}(q1, q2)$$

```
>
>
>
```

Stress parameter definition and equations:

```
> nondimparam := [Theta = E[1]/E[2], PI = Omega[1]/Omega[2],
Sigma[r[1]] = -(-1+nu[1])*sigma[r1](x)/Omega[1]/E[1]/c[0],
Sigma[t[1]] = -(-1+nu[1])*sigma[t1](x)/Omega[1]/E[1]/c[0],
Sigma[r[2]] = -(-1+nu[2])*sigma[r2](x)/Omega[2]/E[2]/c[0],
Sigma[t[2]] = -(-1+nu[2])*sigma[t2](x)/Omega[2]/E[2]/c[0]];
```

$$nondimparam := \left[\Theta = \frac{E_1}{E_2}, \Pi = \frac{\Omega_1}{\Omega_2}, \Sigma_{r_1} = -\frac{(-1+\nu_1)\,\sigma_{r1}(x)}{\Omega_1\,E_1\,c_0}, \Sigma_{t_1} = -\frac{(-1+\nu_1)\,\sigma_{t1}(x)}{\Omega_1\,E_1\,c_0}, \Sigma_{r_2} = -\frac{(-1+\nu_2)\,\sigma_{r2}(x)}{\Omega_2\,E_2\,c_0}, \Sigma_{t_2} = -\frac{(-1+\nu_2)\,\sigma_{t2}(x)}{\Omega_2\,E_2\,c_0}\right]$$

```
> add_param :=
[4*Theta*alpha^3*nu[2]-2*Theta*alpha^3-4*alpha^3*nu[1]+2*alpha^3-T
heta*nu[2]-Theta+4*nu[1]-2 = Delta[1],
4*Theta*alpha^3*nu[2]-2*Theta*alpha^3-alpha^3*nu[1]-alpha^3-Theta*
```

```
nu[2]-Theta+nu[1]+1 = Delta[2], 2*Theta*nu[2]-Theta-2*nu[1]+1 =
Delta[3], Theta*nu[2]+Theta-4*nu[1]+2 = Delta[4]];
```

$$add\_param := [4\,\Theta\,\alpha^3\,\nu_2 - 2\,\Theta\,\alpha^3 - 4\,\alpha^3\,\nu_1 + 2\,\alpha^3 - \Theta\,\nu_2 - \Theta + 4\,\nu_1 - 2 = \Delta_1, 4\,\Theta\,\alpha^3\,\nu_2 - 2\,\Theta\,\alpha^3 - \alpha^3\,\nu_1 - \alpha^3 - \Theta\,\nu_2 - \Theta + \nu_1 + 1 = \Delta_2, 2\,\Theta\,\nu_2 - \Theta - 2\,\nu_1 + 1 = \Delta_3, \Theta\,\nu_2 + \Theta - 4\,\nu_1 + 2 = \Delta_4]$$

```
> sigmar1eqn1 := Sigma[r[1]] =
2/3*Delta[2]/alpha^3/Delta[1]*int(z^2*x[1](z),z = 0 ..
alpha)-2/3*1/x^3*int(z^2*x[1](z),z = 0 ..
x)+2*(-1+nu[1])/Delta[1]/PI*int(z^2*x[2](z),z = alpha .. 1);
```

$$sigmar1eqn1 := \Sigma_{r_1} = \frac{2}{3}\left(\frac{\Delta_2}{\alpha^3\,\Delta_1}\int_0^{\alpha} z^2\,x_1(z)\,dz\right) - \frac{2}{3}\left(\frac{1}{x^3}\int_0^{x} z^2\,x_1(z)\,dz\right) + \frac{2\,(-1+\nu_1)}{\Delta_1\,\Pi}\int_{\alpha}^{1} z^2\,x_2(z)\,dz$$

```
> sigmat1eqn1 := Sigma[t[1]] =
2/3*Delta[2]/alpha^3/Delta[1]*int(z^2*x[1](z),z = 0 ..
alpha)+1/3*1/x^3*int(z^2*x[1](z),z = 0 ..
x)+2*(-1+nu[1])/Delta[1]/PI*int(z^2*x[2](z),z = alpha ..
1)-1/3*x[1](z);
```

$$sigmat1eqn1 := \Sigma_{t_1} = \frac{2}{3}\left(\frac{\Delta_2}{\alpha^3\,\Delta_1}\int_0^{\alpha} z^2\,x_1(z)\,dz\right) + \frac{1}{3}\left(\frac{1}{x^3}\int_0^{x} z^2\,x_1(z)\,dz\right) + \frac{2\,(-1+\nu_1)}{\Delta_1\,\Pi}\int_{\alpha}^{1} z^2\,x_2(z)\,dz - \frac{1}{3}\,x_1(z)$$

```
> sigmar2eqn1 := Sigma[r[2]] =
2*Theta*PI*(x-1)*(x^2+x+1)*(-1+nu[2])/Delta[1]/x^3*int(z^2*x[1](z)
,z = 0 ..
alpha)+2/3*(2*alpha^3*Delta[3]-x^3*Delta[4])/Delta[1]/x^3*int(z^2*
x[2](z),z = alpha .. 1)-2/3*1/x^3*int(z^2*x[2](z),z = alpha .. x);
```

$$sigmar2eqn1 := \Sigma_{r_2} = \frac{2\,\Theta\,\Pi\,(x-1)\,(x^2+x+1)\,(-1+\nu_2)}{\Delta_1\,x^3}\int_0^{\alpha} z^2\,x_1(z)\,dz + \frac{2}{3}\left(\frac{2\,\alpha^3\,\Delta_3 - x^3\,\Delta_4}{\Delta_1\,x^3}\int_{\alpha}^{1} z^2\,x_2(z)\,dz\right) - \frac{2}{3}\left(\frac{1}{x^3}\int_{\alpha}^{x} z^2\,x_2(z)\,dz\right)$$

```
> sigmat2eqn1 := Sigma[t[2]] =
Theta*(2*x^3+1)*(-1+nu[2])*PI/Delta[1]/x^3*int(z^2*x[1](z),z = 0
..
alpha)-2/3*(alpha^3*Delta[3]+x^3*Delta[4])/Delta[1]/x^3*int(z^2*x[
2](z),z = alpha .. 1)+1/3*1/x^3*int(z^2*x[2](z),z = alpha ..
x)-1/3*x[2](z);
```

$$sigmat2eqn1 := \Sigma_{t_2} = \frac{\Theta\,(2\,x^3+1)\,(-1+\nu_2)\,\Pi}{\Delta_1\,x^3}\int_0^{\alpha} z^2\,x_1(z)\,dz - \frac{2}{3}\left(\frac{\alpha^3\,\Delta_3 + x^3\,\Delta_4}{\Delta_1\,x^3}\int_{\alpha}^{1} z^2\,x_2(z)\,dz\right) + \frac{1}{3}\left(\frac{1}{x^3}\int_{\alpha}^{x} z^2\,x_2(z)\,dz\right) - \frac{1}{3}\,x_2(z)$$

```
>
>
```

Stress calculation and plots

```
> num_nondimparam:=[Theta=1,PI=1,nu[1]=0.3,nu[2]=0.3];#param22
```

$$num\_nondimparam := [\Theta = 1, \Pi = 1, \nu_1 = 0.3, \nu_2 = 0.3]$$

```
> add_param2:=[seq(rhs(add_param[i])=lhs(subs(num_nondimparam,consta
nts,add_param[i])),i=1..nops(add_param))];#param11
```

$$add\_param2 := [\Delta_1 = -2.1, \Delta_2 = -0.1344, \Delta_3 = 0., \Delta_4 = 2.1]$$

Plot at different point in time

```
> NPlots:=5:
```

Specific time when profiles will be plotted

```
> ttime:=[0.01,0.025,0.05,0.1,0.2]:
```

Style of lines in the plot (may not work)

```
> styleop:=[dash,dashdot,dot,solid,circle];
```

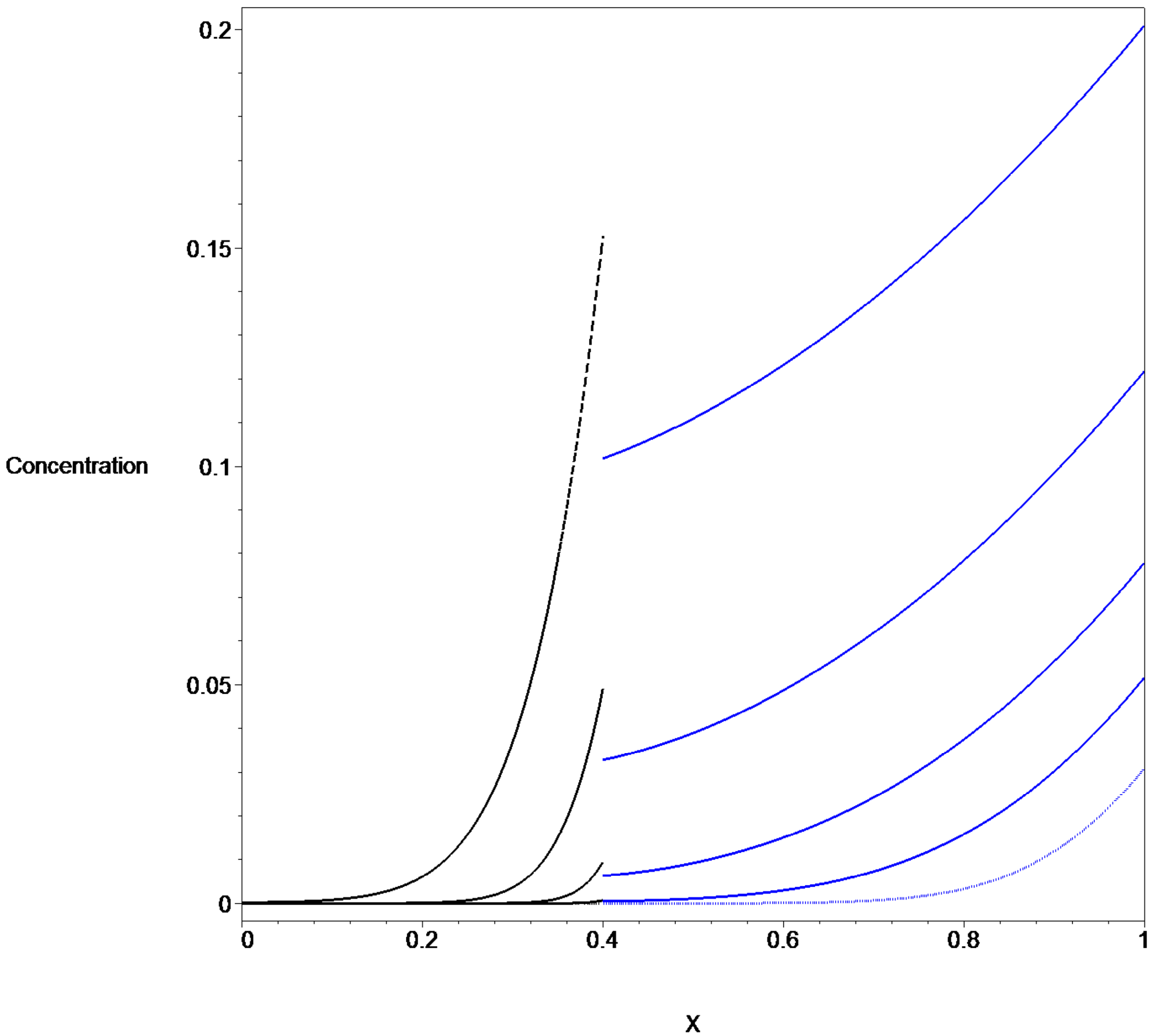
$$styleop := [dash, dashdot, dot, solid, circle]$$

```
>
> for i from 1 to NPlots do

dumexpr11:=evalf(subs(t=ttime[i],expr1)):
dumexpr22:=evalf(subs(t=ttime[i],expr2)):

px1||i:=plot(evalf(subs(t=ttime[i],expr1)),x=0..eval(alpha,constan
ts),color=black,thickness=3,linestyle = i+1):
px2||i:=plot(evalf(subs(t=ttime[i],expr2)),x=eval(alpha,constants)
..1,color=blue,thickness=3,linestyle = i+1);

#print(i);

psr1_||i:=plot(Expand(subs(add_param2,constants,num_nondimparam,su
bs(x[1](x)=dumexpr11,x[2](x)=dumexpr22,(PI*Theta)*rhs(subs(z=x,sig
mar1eqn1))))),x=0..eval(alpha,constants),color=black,thickness=3,l
inestyle = i+1):
#print(i);
psr2_||i:=plot(Expand(subs(add_param2,constants,num_nondimparam,su
```

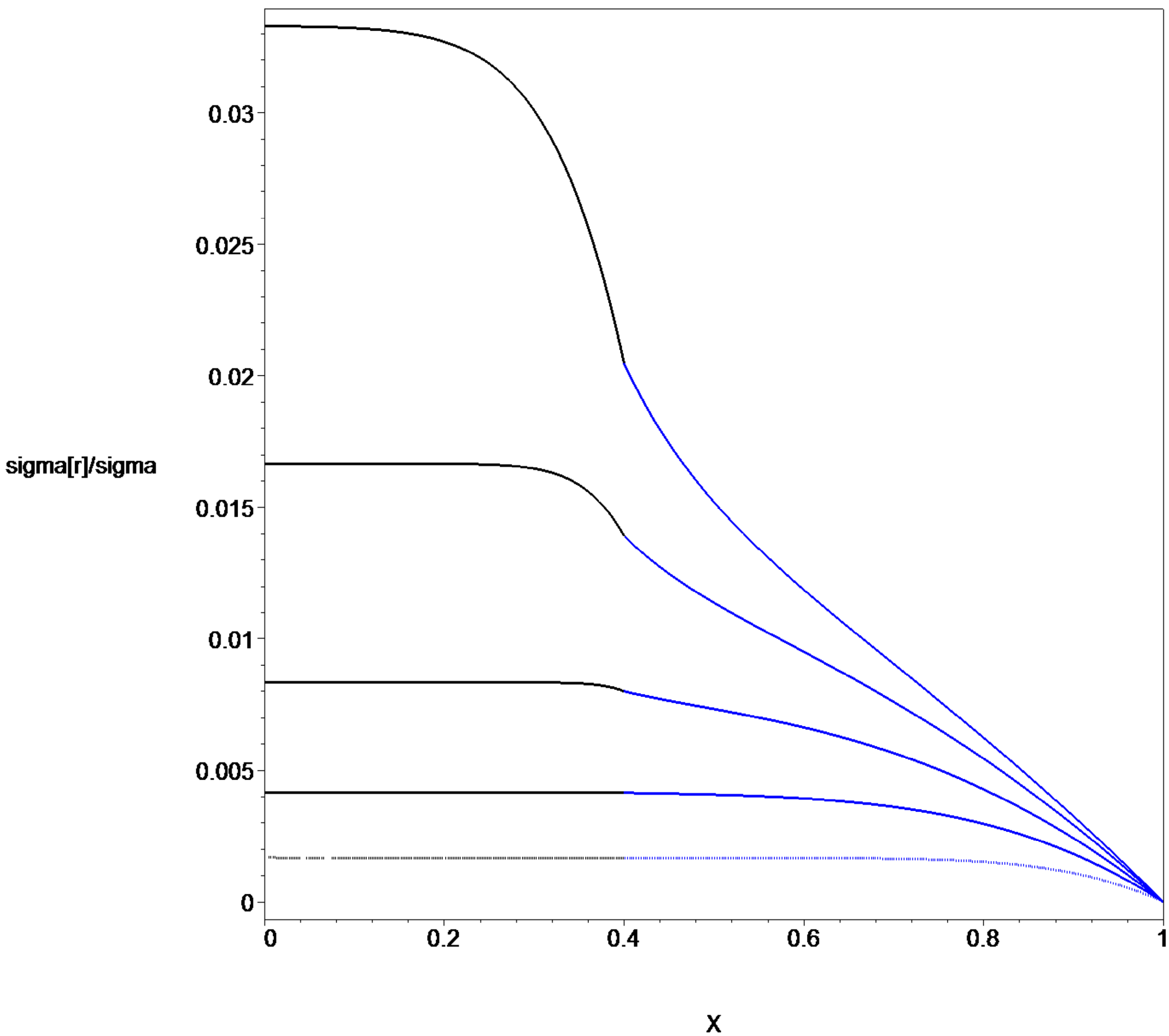
```
bs(x[1](x)=dumexpr11,x[2](x)=dumexpr22,rhs(subs(z=x,sigmar2eqn1)))
)),x=eval(alpha,constants)..1,color=blue,thickness=3,linestyle =
i+1):

#print(i);

pst1_||i:=plot(Expand(subs(add_param2,constants,num_nondimparam,su
bs(x[1](x)=dumexpr11,x[2](x)=dumexpr22,(PI*Theta)*rhs(subs(z=x,sig
mat1eqn1))))),x=0..eval(alpha,constants),color=black,thickness=3,l
inestyle = i+1):

pst2_||i:=plot(Expand(subs(add_param2,constants,num_nondimparam,su
bs(x[1](x)=dumexpr11,x[2](x)=dumexpr22,rhs(subs(z=x,sigmat2eqn1)))
)),x=eval(alpha,constants)..1,color=blue,thickness=3,linestyle =
i+1):
print(i);
od:
```

1
2
3
4
5

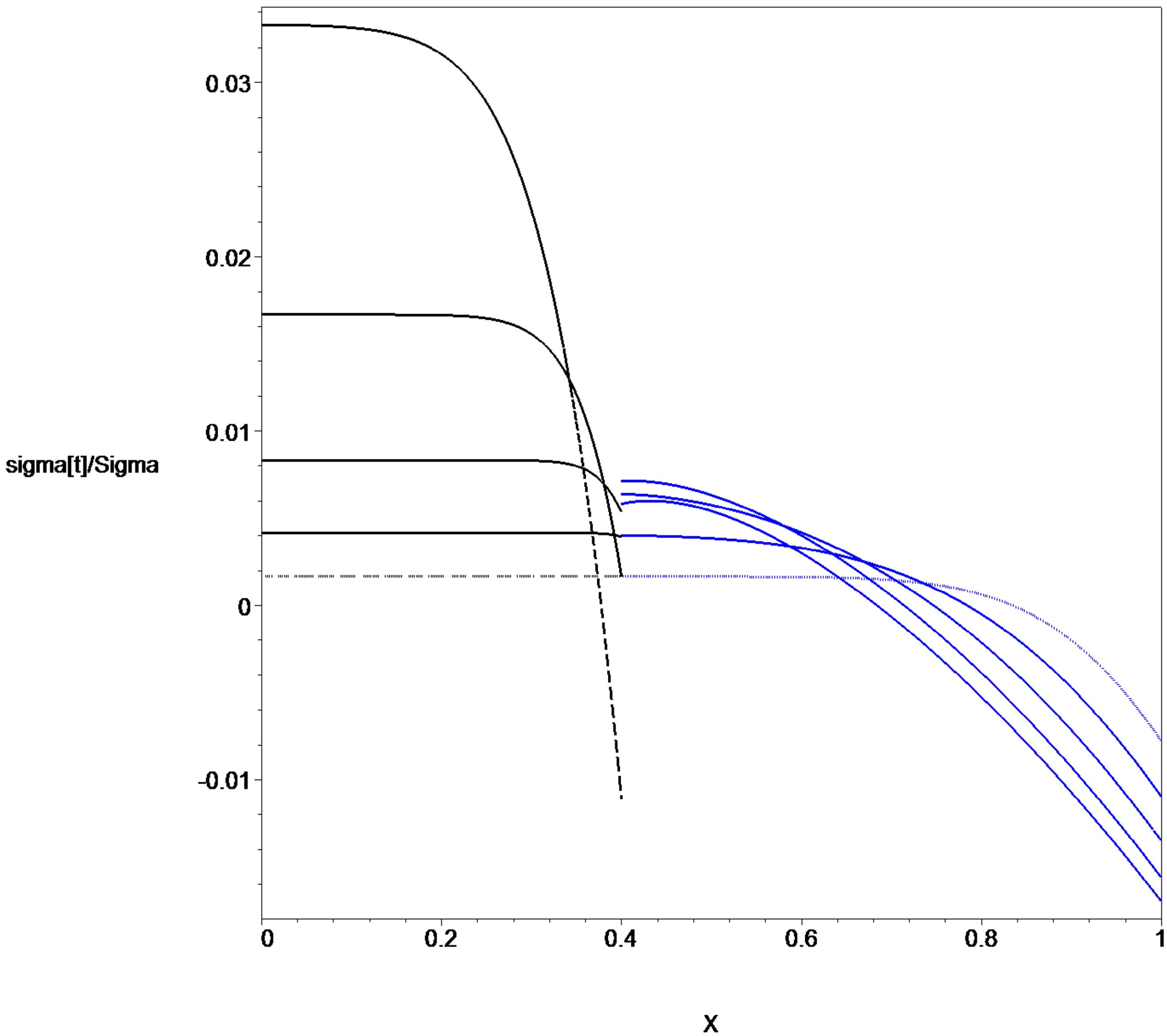
```
> i:='i':
display(seq(px1||i,i=1..NPlots),seq(px2||i,i=1..NPlots),axes=boxed
,labels=["X",Concentration],labeldirections=[horizontal,horizontal
]);
```




```
>
> #?font
> display(seq(psr1_||i,i=1..NPlots),seq(psr2_||i,i=1..NPlots),axes=b
  oxed,labels=["X",sigma[r]/sigma],labeldirections=[horizontal,horiz
  ontal]);
```




```
>
> display(seq(pst1_||i,i=1..NPlots),seq(pst2_||i,i=1..NPlots),axes=b
  oxed,labels=["X",sigma[t]/Sigma],labeldirections=[horizontal,horiz
  ontal]);
```



0.03
0.02
0.01
sigma[t]/Sigma
0
-0.01
0
0.2
0.4
0.6
0.8
1
x

>

>

>