The following is the analytical solution for the diffusion in composite cylindrical 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=2,alpha=0.5,gamma=1000,kappa=2,delta=-.25];
```

$$constants := [\beta = 2, \alpha = 0.5, \gamma = 1000, \kappa = 2, \delta = -0.25]$$

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)];
```

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

Eigenvalue Equation

```
> eigeneqn:=(-BesselJ(1,lambda*alpha)*BesselY(1,lambda)*beta^3*lambda+BesselY(1,lambda*alpha)*BesselJ(1,lambda)*beta^3*lambda)*BesselJ(0,beta*lambda*alpha)+(-beta^2*kappa*lambda*BesselJ(1,lambda)*BesselY(0,lambda*alpha)+beta^2*kappa*lambda*BesselY(1,lambda)*BesselJ(0,lambda*alpha)+(-BesselJ(1,lambda*alpha)*BesselY(1,lambda)*beta^2*lambda^2+BesselY(1,lambda*alpha)*BesselJ(1,lambda)*beta^2*lambda^2)/gamma)*BesselJ(1,beta*lambda*alpha);
```

$$eigeneqn := (-\mathrm{BesselJ}(1, \lambda \alpha)\, \mathrm{BesselY}(1, \lambda)\, \beta^3 \lambda + \mathrm{BesselY}(1, \lambda \alpha)\, \mathrm{BesselJ}(1, \lambda)\, \beta^3 \lambda)\, \mathrm{BesselJ}(0, \beta \lambda \alpha) + \left(-\beta^2 \kappa \lambda\, \mathrm{BesselJ}(1, \lambda)\, \mathrm{BesselY}(0, \lambda \alpha) + \beta^2 \kappa \lambda\, \mathrm{BesselY}(1, \lambda)\, \mathrm{BesselJ}(0, \lambda \alpha) + \frac{-\mathrm{BesselJ}(1, \lambda \alpha)\, \mathrm{BesselY}(1, \lambda)\, \beta^2 \lambda^2 + \mathrm{BesselY}(1, \lambda \alpha)\, \mathrm{BesselJ}(1, \lambda)\, \beta^2 \lambda^2}{\gamma}\right) \mathrm{BesselJ}(1, \beta \lambda \alpha)$$

Function to return Eigenequation (necessary for using Nextzero function of Maple)

```
> KKK:=lambda->(-BesselJ(1,lambda*alpha)*BesselY(1,lambda)*beta^3*lambda+BesselY(1,lambda*alpha)*BesselJ(1,lambda)*beta^3*lambda)*BesselJ(0,beta*lambda*alpha)+(-beta^2*kappa*lambda*BesselJ(1,lambda)*BesselY(0,lambda*alpha)+beta^2*kappa*lambda*BesselY(1,lambda)*BesselJ(0,lambda*alpha)+(-BesselJ(1,lambda*alpha)*BesselY(1,lambda)*bet
```

```
a^2*lambda^2+BesselY(1,lambda*alpha)*BesselJ(1,lambda)*beta^2*lamb
da^2)/gamma)*BesselJ(1,beta*lambda*alpha);
```

$$KKK := \lambda \to \left(-\mathrm{BesselJ}(1, \lambda\,\alpha)\,\mathrm{BesselY}(1, \lambda)\,\beta^3\,\lambda + \mathrm{BesselY}(1, \lambda\,\alpha)\,\mathrm{BesselJ}(1, \lambda)\,\beta^3\,\lambda\right)\mathrm{BesselJ}(0, \beta\,\lambda\,\alpha) + \left(-\beta^2\,\kappa\,\lambda\,\mathrm{BesselJ}(1, \lambda)\,\mathrm{BesselY}(0, \lambda\,\alpha) + \beta^2\,\kappa\,\lambda\,\mathrm{BesselY}(1, \lambda)\,\mathrm{BesselJ}(0, \lambda\,\alpha) + \frac{-\mathrm{BesselJ}(1, \lambda\,\alpha)\,\mathrm{BesselY}(1, \lambda)\,\beta^2\,\lambda^2 + \mathrm{BesselY}(1, \lambda\,\alpha)\,\mathrm{BesselJ}(1, \lambda)\,\beta^2\,\lambda^2}{\gamma}\right)\mathrm{BesselJ}(1, \beta\,\lambda\,\alpha)$$

```
> #;
```

```
> Aneqn:=A[n]=2*BesselJ(1,beta*lambda[n]*alpha)*delta*kappa/lambda[n
]^2/Pi/(1/2*(-BesselJ(1,lambda[n]*alpha)*BesselY(1,lambda[n])*beta
*lambda[n]+BesselY(1,lambda[n]*alpha)*BesselJ(1,lambda[n])*beta*la
mbda[n])^2*alpha^2*(BesselJ(0,beta*lambda[n]*alpha)^2+BesselJ(1,be
ta*lambda[n]*alpha)^2)+BesselJ(1,beta*lambda[n]*alpha)^2*lambda[n]
^2*kappa*((1/2*BesselJ(0,lambda[n])^2-1/2*alpha^2*BesselJ(1,lambda
[n]*alpha)^2-1/2*alpha^2*BesselJ(0,lambda[n]*alpha)^2)*BesselY(1,l
ambda[n])^2+(BesselY(0,lambda[n]*alpha)*BesselJ(0,lambda[n]*alpha)
*alpha^2+BesselJ(1,lambda[n]*alpha)*BesselY(1,lambda[n]*alpha)*alp
ha^2-BesselY(0,lambda[n])*BesselJ(0,lambda[n]))*BesselJ(1,lambda[n
])*BesselY(1,lambda[n])+(-1/2*alpha^2*BesselY(1,lambda[n]*alpha)^2
+1/2*BesselY(0,lambda[n])^2-1/2*alpha^2*BesselY(0,lambda[n]*alpha)
^2)*BesselJ(1,lambda[n])^2));
```

$$Aneqn := A_n = 2\,\mathrm{BesselJ}(1, \alpha\,\lambda_n\,\beta)\,\delta\,\kappa \Big/ \Bigg(\lambda_n^{\,2}\,\pi\,\bigg(\frac{1}{2}\left(-\mathrm{BesselJ}(1, \lambda_n\,\alpha)\,\mathrm{BesselY}(1, \lambda_n)\,\beta\,\lambda_n + \mathrm{BesselY}(1, \lambda_n\,\alpha)\,\mathrm{BesselJ}(1, \lambda_n)\,\beta\,\lambda_n\right)^2\alpha^2\left(\mathrm{BesselJ}(0, \alpha\,\lambda_n\,\beta)^2 + \mathrm{BesselJ}(1, \alpha\,\lambda_n\,\beta)^2\right) + \mathrm{BesselJ}(1, \alpha\,\lambda_n\,\beta)^2\,\lambda_n^{\,2}\,\kappa\Big(\left(\frac{1}{2}\mathrm{BesselJ}(0, \lambda_n)^2 - \frac{1}{2}\alpha^2\,\mathrm{BesselJ}(1, \lambda_n\,\alpha)^2 - \frac{1}{2}\alpha^2\,\mathrm{BesselJ}(0, \lambda_n\,\alpha)^2\right)\mathrm{BesselY}(1, \lambda_n)^2 + \big(\mathrm{BesselY}(0, \lambda_n\,\alpha)\,\mathrm{BesselJ}(0, \lambda_n\,\alpha)\,\alpha^2 + \mathrm{BesselJ}(1, \lambda_n\,\alpha)\,\mathrm{BesselY}(1, \lambda_n\,\alpha)\,\alpha^2 - \mathrm{BesselY}(0, \lambda_n)\,\mathrm{BesselJ}(0, \lambda_n)\big)\,\mathrm{BesselJ}(1, \lambda_n)\,\mathrm{BesselY}(1, \lambda_n) + \left(-\frac{1}{2}\alpha^2\,\mathrm{BesselY}(1, \lambda_n\,\alpha)^2 + \frac{1}{2}\mathrm{BesselY}(0, \lambda_n)^2 - \frac{1}{2}\alpha^2\,\mathrm{BesselY}(0, \lambda_n\,\alpha)^2\right)\mathrm{BesselJ}(1, \lambda_n)^2\Big)\bigg)\Bigg)$$

```
> OtherParam:=[
k[1] = -2*kappa*delta/(alpha^2*kappa-alpha^2+1),
k[2] = -2*delta/(alpha^2*kappa-alpha^2+1),
```

```
a[1]=
-1/4*((-alpha^4*beta^2-2*alpha^4+4*ln(alpha)*alpha^2+2*alpha^2)*ka
ppa+alpha^4-4*ln(alpha)*alpha^2+2*alpha^4*beta^2-1-2*alpha^2*beta^
2)*delta*kappa/(alpha^2*kappa-alpha^2+1)^2-1/4*(-4*alpha^3+4*alpha
)*delta*kappa/(alpha^2*kappa-alpha^2+1)^2/gamma,

a[2]=
1/4*1/(alpha^4*kappa^2+(-2*alpha^4+2*alpha^2)*kappa+alpha^4-2*alph
a^2+1)*(4*ln(alpha)*alpha^4*kappa^2+((-beta^2-8*ln(alpha)+4)*alpha
^4-2*alpha^2)*kappa+(4*ln(alpha)-3)*alpha^4+1+2*alpha^2)*delta+1/(
alpha^4*kappa^2+(-2*alpha^4+2*alpha^2)*kappa+alpha^4-2*alpha^2+1)*
alpha^3*kappa*delta/gamma];
```

$$OtherParam := \left[k_1 = -\frac{2\,\kappa\,\delta}{\alpha^2\,\kappa-\alpha^2+1},\ k_2 = -\frac{2\,\delta}{\alpha^2\,\kappa-\alpha^2+1},\ a_1 = -\frac{1}{4}\,\frac{((-\alpha^4\,\beta^2-2\,\alpha^4+4\ln(\alpha)\,\alpha^2+2\,\alpha^2)\,\kappa+\alpha^4-4\ln(\alpha)\,\alpha^2+2\,\alpha^4\,\beta^2-1-2\,\alpha^2\,\beta^2)\,\delta\,\kappa}{(\alpha^2\,\kappa-\alpha^2+1)^2} - \frac{(-4\,\alpha^3+4\,\alpha)\,\delta\,\kappa}{4\,(\alpha^2\,\kappa-\alpha^2+1)^2\,\gamma},\ a_2 = \frac{1}{4}\,\frac{(4\ln(\alpha)\,\alpha^4\,\kappa^2+((-\beta^2-8\ln(\alpha)+4)\,\alpha^4-2\,\alpha^2)\,\kappa+(4\ln(\alpha)-3)\,\alpha^4+1+2\,\alpha^2)\,\delta}{\alpha^4\,\kappa^2+(-2\,\alpha^4+2\,\alpha^2)\,\kappa+\alpha^4-2\,\alpha^2+1} + \frac{\alpha^3\,\kappa\,\delta}{(\alpha^4\,\kappa^2+(-2\,\alpha^4+2\,\alpha^2)\,\kappa+\alpha^4-2\,\alpha^2+1)\,\gamma}\right]$$

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

Final Solution

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

```
>
> x1part1:=1/4*k[1]*beta^2*x^2+a[1]+k[1]*t;
```

$$x1part1 := \frac{1}{4}\,k_1\,\beta^2\,x^2 + a_1 + k_1\,t$$

```
> x1part2:=(-BesselJ(1,lambda[n]*alpha)*BesselY(1,lambda[n])*beta*la
mbda[n]*A[n]+BesselY(1,lambda[n]*alpha)*BesselJ(1,lambda[n])*beta*
lambda[n]*A[n])*BesselJ(0,beta*lambda[n]*x)*exp(-lambda[n]^2*t);
```

$$x1part2 := (-\mathrm{BesselJ}(1,\lambda_n\,\alpha)\,\mathrm{BesselY}(1,\lambda_n)\,\beta\,\lambda_n\,A_n + \mathrm{BesselY}(1,\lambda_n\,\alpha)\,\mathrm{BesselJ}(1,\lambda_n)\,\beta\,\lambda_n\,A_n)\,\mathrm{BesselJ}(0,\beta\,\lambda_n\,x)\,\mathbf{e}^{\left(-\lambda_n^{\,2}\,t\right)}$$

```
>
```

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

```
> x2part1:=1/4*k[2]*x^2+(-delta-1/2*k[2])*ln(x)+a[2]+k[2]*t;
```

$$x2part1 := \frac{1}{4} k_2 x^2 + \left(-\delta - \frac{1}{2} k_2\right) \ln(x) + a_2 + k_2 t$$

```
> x2part2:=(BesselJ(1,lambda[n])*BesselY(0,lambda[n]*x)-BesselY(1,la
  mbda[n])*BesselJ(0,lambda[n]*x))*A[n]*BesselJ(1,beta*lambda[n]*alp
  ha)*lambda[n]*exp(-lambda[n]^2*t);
```

$$x2part2 := (\mathrm{BesselJ}(1, \lambda_n)\, \mathrm{BesselY}(0, \lambda_n x) - \mathrm{BesselY}(1, \lambda_n)\, \mathrm{BesselJ}(0, \lambda_n x))\, A_n \, \mathrm{BesselJ}(1, \alpha \lambda_n \beta)\, \lambda_n \, \mathbf{e}^{(-\lambda_n^2 t)}$$

```
> ########################
> #Calculation of x1 and x2 expressions using numerical eigenvalues
```

First Eigenvalue

```
> Lam[1]:=NextZero(subs(constants,lambda[n]=lambda,eval(KKK)),0.0);
```

$$Lam_1 := 2.49821996052966$$

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)]:
```

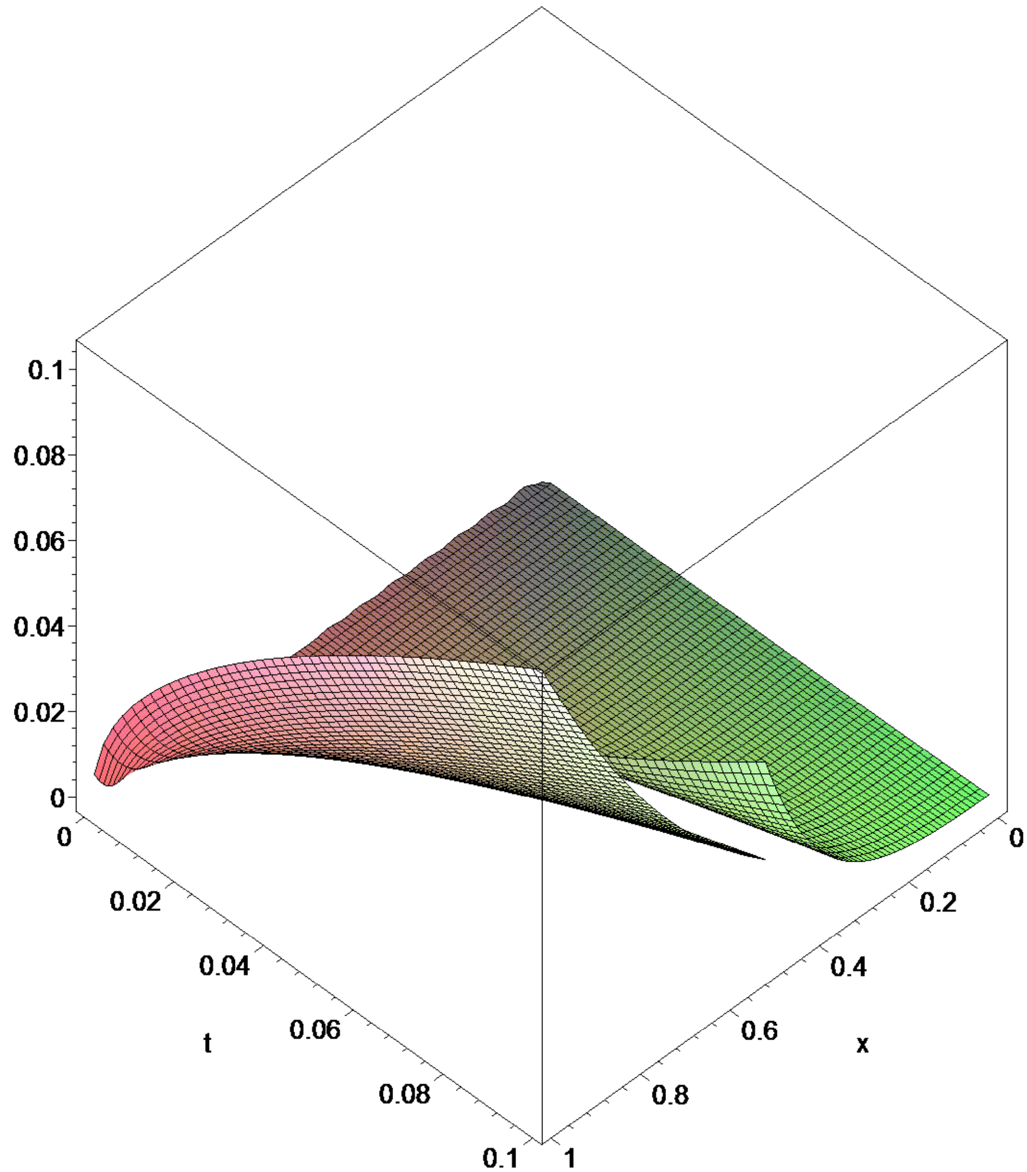
Check if the k1 k2 and a1 and a2 are calculated numerically

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

Computation of Expressions for x1 and x2

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

  NumChiparam:=[1=1];
  NumAn:=evalf(subs(param1,n=i,ListLambda,constants,NumChiparam,Aeq
  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):
>
>
```

```
> #plots of curves:
> p3:=plot(evalf(subs(t=0,expr1)),x=0..eval(alpha,constants)):p4:=plot(evalf(subs(t=0,expr2)),x=eval(alpha,constants)..1):display(p3,p4);

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




```
>
> #back check (mass conservation)
```

Integral of concentration over x int(x*c1(x),x=0..alpha)+int(x c2(x),x=alpha..1)

```
> IntC:=int(x*expr1,x=0..eval(alpha,constants))+int(x*expr2,x=eval(a
  lpha,constants)..1):
```

Integration of Flux up to that point

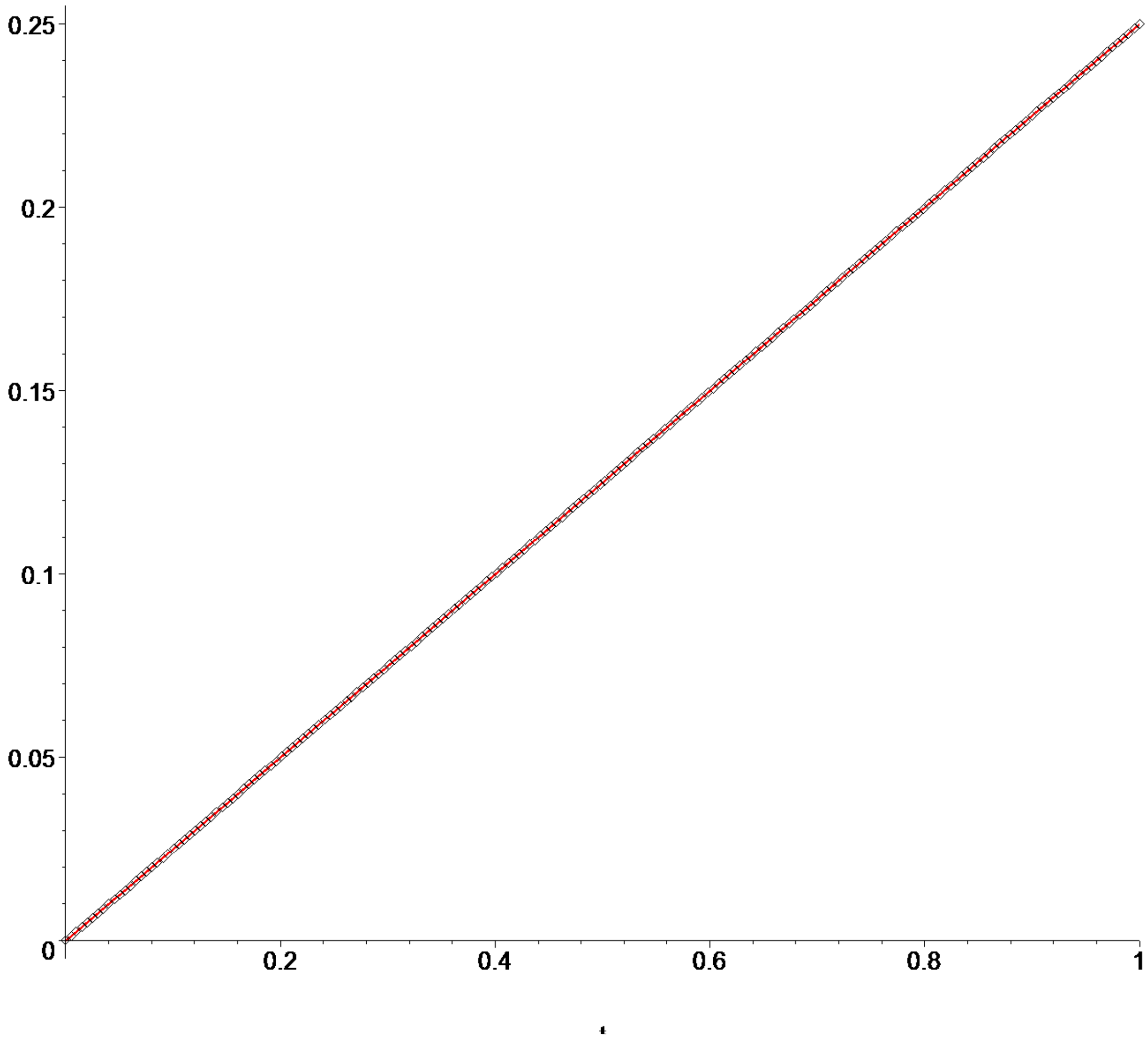
```
> IntF:=-subs(constants,delta*t);
```

$$IntF := 0.25\,t$$

```
> pp1:=plot(IntC,t=0..1,style=point,color=black,symbolsize=20):
> pp2:=plot(IntF,t=0..1,thickness=3,color=red):
```

Plot of both integration (Both plots should be identical, if not increase the number of eigenvalues to be used)

```
> display(pp1,pp2);
```




```
>
>
>
```