```
> restart;with(plots):#with(RealDomain):
```

Solution suggestion problem 300-12

We were asked to find an expression - for a situation describing two films of ZnO on top of each other, one with the isotope ^{70}Zn, and where we seek the diffusion profile of ^{70}Zn.
We will assume that we consider only diffusjon times that are so short that the diffusion zone will be mostly around the interface. It mean we assume x0>>sqrt(Dt) where x0 is the film thichness. Then we can ignore the Saphire/ZnO interface and the surface of ZnO. Then the situation would be similar to two infinitely thick materials meeiting at x=x0.

We assume the profile is a step function initially, and that the small spread observed is the resolution (or diffusion at growth temperature)

We assume we can use the superposition principle.
We divide the ^{70}ZnO material into thin slices (with thickness dx).
..one slize at each x1 where there is ^{70}ZnO material initially. We find the diffusion profile for each thin slice and sum them up. The thin slice contribution is similar to drive in distribution except that the slice is not on the surface. So we only get half the concentration at each depth in the case at hand. The diffusion profile from atoms at the depth x1 is thus given by

```
> C1(x,t)=Q/sqrt(4*Pi*Dd*t)*exp(-((x-x1)^2)/4/Dd/t);
```

$$C1(x,t) = \frac{1}{2}\,\frac{Q\,\mathrm{e}^{-\frac{1}{4}\frac{(x-x1)^2}{Dd\,t}}}{\sqrt{\pi\,Dd\,t}}$$

Here Dd is the diffusivity (D is a predifined operatort in Maple)
t is the diffusion time Q is defined by the initial distribution where the # atoms pr area between x1 and x1+dx1 is 1/2NZnO*dx

```
> C1(x,t)*dx1=1/2*1/2*NZnO*dx1/sqrt(4*Pi*Dd*t)*exp(-((x-x1)^2)
  /4/Dd/t);
```

$$C1(x,t)\,dx1 = \frac{1}{8}\,\frac{NZnO\,dx1\,\mathrm{e}^{-\frac{1}{4}\frac{(x-x1)^2}{Dd\,t}}}{\sqrt{\pi\,Dd\,t}}$$

You can set that equation into the diffusion equation and see that it fits, and you can see the integral is always the same as the total amount from the slab. We dont do that right now

We can now integrate up C1(x,t)dx1 from x1 equal minus infinity to x1=x0 to sum up all contributions

```
> C(x,t)=int(C1(x1,x,t),x1=-infinity..x0);
```

$$C(x,t) = \int_{-\infty}^{x0} C1(x1,x,t)\,\mathrm{d}x1$$

```
> C(x,t)='int((1/8)*NZnO*exp(-(1/4)*(x-x1)^2/(Dd*t))/sqrt(Pi*Dd*t),
  x1=-infinity..x0)';
```

$$C(x,t) = \int_{-\infty}^{x0} \frac{1}{8}\,\frac{NZnO\,\mathrm{e}^{-\frac{1}{4}\frac{(x-x1)^2}{Dd\,t}}}{\sqrt{\pi\,Dd\,t}}\,\mathrm{d}x1$$

We will get

```
> C(x,t)=1/4*N[ZnO]*erfc((x-x0)/2/sqrt(Dd*t));
```

$$C(x,t) = \frac{1}{4} N_{ZnO} \operatorname{erfc}\left(\frac{1}{2} \frac{x - x0}{\sqrt{Dd\, t}} \right)$$

We can check that this obeys the diffusion equation, We define it as function fC

```
> fC:=(x,t)->1/4*N[ZnO]*erfc((x-x0)/2/sqrt(Dd*t));
```

$$fC := (x,t) \rightarrow \frac{1}{4} N_{ZnO} \operatorname{erfc}\left(\frac{1}{2} \frac{x - x0}{\sqrt{Dd\, t}} \right)$$

```
> diffeq:=diff(C(x,t),t)=Dd*diff(diff(C(x,t),x),x);
```

$$diffeq := \frac{\partial}{\partial t} C(x,t) = Dd \left(\frac{\partial^2}{\partial x^2} C(x,t) \right)$$

```
> eval(subs(C(x,t)=fC(x,t),diffeq));
```

$$\frac{1}{8} \frac{N_{ZnO}\, \mathrm{e}^{-\frac{1}{4} \frac{(x-x0)^2}{Dd\, t}} (x - x0)\, Dd}{\sqrt{\pi}\, (Dd\, t)^{3/2}} = \frac{1}{8} \frac{N_{ZnO} (x - x0)\, \mathrm{e}^{-\frac{1}{4} \frac{(x-x0)^2}{Dd\, t}}}{\sqrt{\pi}\, t \sqrt{Dd\, t}}$$

```
> simplify(lhs(%)-rhs(%));
```

$$0$$

So left hand side is equal to the right hand side, and the expression is a solution of the diffusion equation.

Lets check that the initial condition is OK by checking fC for (0<x<x0 and x>x0

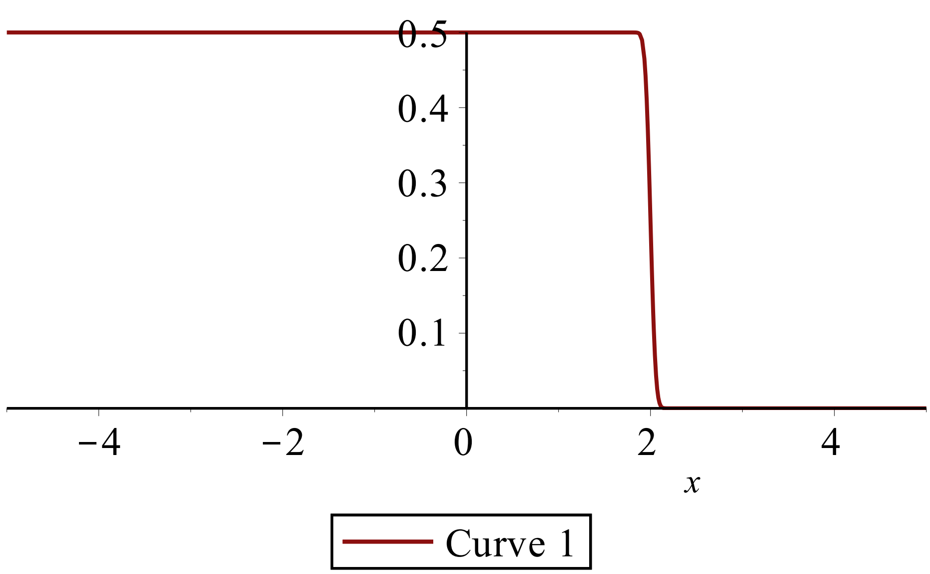
```
> evalf(subs({x0=1,x=-1000,t=1,Dd=1},fC(x,t)),2);evalf(subs({x0=1,x=
  1000,t=1,Dd=1},fC(x,t)),1);
```

$$0.50\, N_{ZnO}$$

$$6.\ 10^{-108578}\, N_{ZnO}$$

We see the concenrtration is 0.5*NZnO as it should below x0 and the second number is practically 0

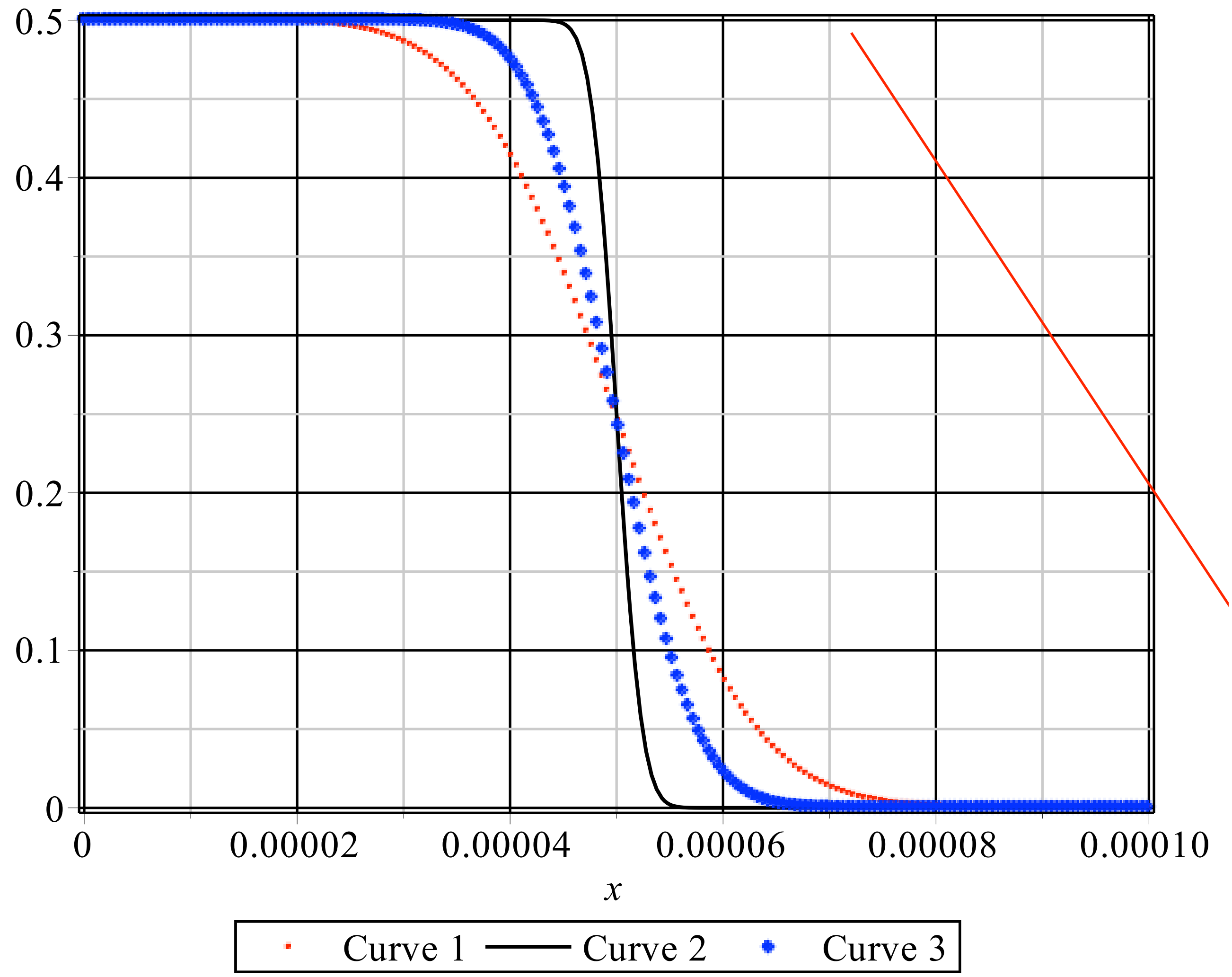
```
> plot(subs({N[ZnO]=1,Dd=1, x0=2,t=0.001},fC(x,t)),x=-5..5);
```



We see the initial conditions are OK.
We have shown what the concentration should look like.

How to find from experimental data?
They where generated by

```
> p1:=plot(subs({N[ZnO]=1,Dd=0.5e-14, x0=5e-5,t=3600*0.1},fC(x,t)),x=
  0..1e-4,color =black):p2:=plot(subs({N[ZnO]=1,Dd=0.5e-14, x0=5e-5,
  t=3600*1},fC(x,t)),x=0..1e-4,color =blue):p3:=plot(subs({N[ZnO]=1,
  Dd=0.5e-14, x0=500e-7,t=3600*3},fC(x,t)),x=0..1e-4,color =red)
  :display({p1,p2,p3});
```



When the scale goes to 0.5 at the surface, it means it is relative to N[ZnO],

So how to find the diffusivity
Strategy, read off the point where C(x,t) is equal to say 0.4, We could do that for the curves and solve the equation for C(x,t), We could repeat for other values, we could pick a lot of point and do a least sqaere curve fit.

```
> restart;with(RealDomain):
```

We have the theoretical concentration

```
> eqX:=C(x, t) = (1/4)*N[ZnO]*erfc((1/2)*(x-x0)/sqrt(Dd*t));
```

$$eqX := C(x, t) = \frac{1}{4} N_{ZnO} \operatorname{erfc}\left(\frac{1}{2} \frac{x - x0}{\sqrt{Dd\, t}}\right)$$

For the blue curve we read off C=0.4 ->x=0.000044726

```
> eqX1:=subs({C(x,t)=0.4,N[ZnO]=1,x0=5e-5,t=3600*1,x=0.000044726},
```

```
eqX);
```

$$eqX1 := 0.4 = \frac{1}{4}\,\mathrm{erfc}\left(-\frac{7.325000000\ 10^{-10}\sqrt{3600}}{\sqrt{Dd}}\right)$$

```
> Dd=evalf(solve(eqX1,Dd));
```

$$Dd = 5.453990619\ 10^{-15}$$

For the red curve we read off C=0.4 ->x=0.000041229, 4522

```
> eqX2:=subs({C(x,t)=0.4,N[ZnO]=1,x0=5e-5,t=3600*3,x=0.000041229},
  eqX);
```

$$eqX2 := 0.4 = \frac{1}{4}\,\mathrm{erfc}\left(-\frac{4.060648148\ 10^{-10}\sqrt{10800}}{\sqrt{Dd}}\right)$$

```
> Dd=evalf(solve(eqX2,Dd));
```

$$Dd = 5.028183320\ 10^{-15}$$

The diffusivity is determined to around 5e-15
which incidentally agree with the value used for generation
Reading of x=0.00004 C=0.578, blue curve

```
> eqX3:=subs({C(x,t)=0.476,N[ZnO]=1,x0=5e-5,t=3600*1,x=0.00004},eqX);
  Dd=evalf(solve(eqX3,Dd));
```

$$eqX3 := 0.476 = \frac{1}{4}\,\mathrm{erfc}\left(-\frac{1.388888889\ 10^{-9}\sqrt{3600}}{\sqrt{Dd}}\right)$$

$$Dd = 5.012646774\ 10^{-15}$$

```
> eqX4:=subs({C(x,t)=0.416,N[ZnO]=1,x0=5e-5,t=3600*3,x=0.00006},eqX)
  ;Dd=evalf(solve(eqX4,Dd));
```

$$eqX4 := 0.416 = \frac{1}{4}\,\mathrm{erfc}\left(\frac{4.629629630\ 10^{-10}\sqrt{10800}}{\sqrt{Dd}}\right)$$

$$Dd = 5.001576832\ 10^{-15}$$

We can look at the derivative

```
> diff(C(x,t),x)=evalf(subs(x=x0,diff(rhs(eqX),x))/N[ZnO]);Dd=solve
  (%,Dd);
```

$$\frac{\partial}{\partial x}\,C(x,t) = -\frac{0.1410473959}{\sqrt{Dd\,t}}$$

$$Dd = \frac{0.01989436789}{t\left(\frac{\partial}{\partial x}\,C(x,t)\right)^2}$$

Red curve Derivati dC/dx=0.5/0.00002519

```
> subs({t=3600*3, diff(C(x, t), x)=0.5/0.00002519},Dd =
  0.1989436789e-1/(t*(diff(C(x, t), x))^2));
```

$$Dd = 4.675442448\ 10^{-15}$$

Could read off any width of C slope vlu from red and blue, say for between C=0.1 and C=0.4 , Delx
plot delx^2 vs time t, slope is diffusivity