

Assignment 3:

1. Derive the heat (diffusion) equation.
2. Derive a finite difference expression for the heat equation.
3. Use  $D = 10^{-5}$  and simulate diffusion in a 12-cm long, 1-D domain. Use  $C(0,t) = 1$  at the lhs boundary. Because we wish to compare with the analytical solution

$$C = \operatorname{erfc}\left[\frac{x}{\sqrt{4Dt}}\right] \text{ (which assumes an infinite domain with } C(\infty,t) = 0\text{), we must}$$

- limit our investigation to a similar numerical solution and the right boundary ideally won't affect the solution (i.e., put it far from any 'action'). Solve for the concentration profiles at 10,000, 100,000, and 200,000 seconds using a spreadsheet solution of the fully explicit numerical algorithm, Mathematica, and the analytical solution. Plot the analytical solution as a solid line and plot the numerical solution as open symbols on the same chart.
4. Do 3 again for  $D = 5 * 10^{-5}$ .
  5. Here is another analytical solution for diffusion:

$$C = \frac{C_0}{2} \left[ \operatorname{erf} \frac{h-x}{\sqrt{4Dt}} + \operatorname{erf} \frac{h+x}{\sqrt{4Dt}} \right]$$

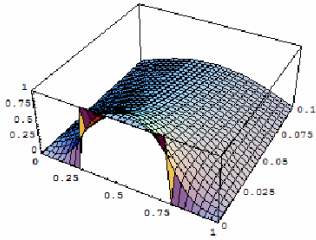
The  $h$  is the half-width of an initial source centered at  $x = 0$ . The error function (erf) can be found in Excell. The boundary conditions are at infinity. Use an explicit spreadsheet and Mathematica to numerically solve for the concentration profiles at 100, 2000, and 11000 seconds in a domain from -500 to +500 cm with  $D = 1/6 \text{ cm}^2 \text{ s}$  for  $h = 10 \text{ cm}$  and  $C_0 = 1$ . That is, the initial condition is  $C(x < -10, 0) = 0$ ,  $C(-10 < x < 10, 0) = 1$ , and  $C(x > 10, 0) = 0$ . Compare the results to the numerical solution.

Here is some Mathematica code that should help get you started.

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In[1]:= Remove["Global`*"]
solution = NDSolve[{D[f[x, t], t] == D[f[x, t], x, x], f[x, 0] == UnitStep[x - 0.25] - UnitStep[x - 0.75], f[0, t] == 0, f[1, t] == 0}, f, {x, 0, 1}, {t, 0, .1}]
Remove::rmnm : There are no symbols matching "Global`*". More_
NDSolve::mxsst : Using maximum number of grid points 10000 allowed by the MaxPoints or MinStepSize options for independent variable x. More_
Out[2]:= {{f -> InterpolatingFunction[{{0., 1.}, {0., 0.1}}, <>]}}
In[3]:= Plot3D[Evaluate[f[x, t] /. First[solution]], {x, 0, 1}, {t, 0, 0.1}, PlotRange -> {0, 1}, PlotPoints -> 30]

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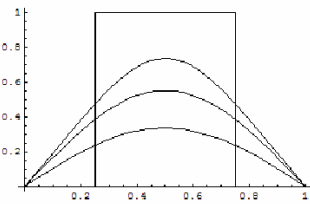
Out[3]:= - SurfaceGraphics -

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In[4]:= t = {0, .025, .050, .1}
Plot[Evaluate[f[x, t] /. First[solution]], {x, 0, 1}]

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Out[4]:= {0, 0.025, 0.05, 0.1}



Out[5]:= - Graphics -

- Address in your write-up the quality of the numerical solution relative to the analytical solution. Are there systematic deviations? Are there changes in the quality of the match with time or diffusion coefficient? If so, why?