Modelling heat diffusion from magnetic nanoparticles to the surrounding tissue

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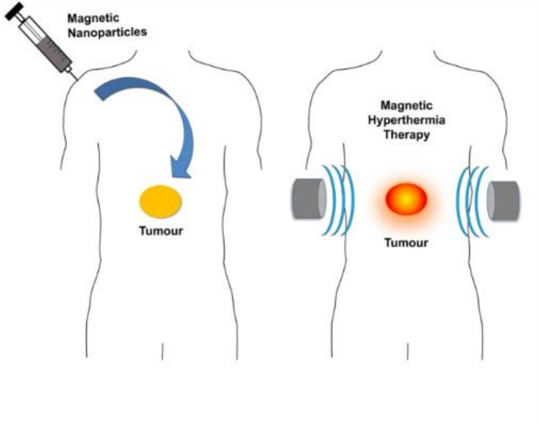
Magnetic Hyperthermia

What is magnetic hyperthermia

- Type of thermal cancer treatment that takes advantage of the heat generated by magnetic nanoparticles
- Mangetic nanoparticles can trasnform electromagnetic energy into heat



Pennes' Bioheat Equation

- Used as a standard model for predicting temperature distributions in living tissue for over 50 years

$$\rho c \frac{\partial T}{\partial t} = k \left(\frac{\partial^2 T}{\partial x^2} + \frac{\partial^2 T}{\partial y^2} + \frac{\partial^2 T}{\partial z^2} \right) + \rho_{blood} c_{blood} w (T_a - T) + Q_{met} + Q_i(x, y, z, t) \quad (1)$$

ρ is the density of the tissue

c is the specific heat capacity of the tissue

k is the tissue thermal conductivity

T is the local tissue temperature

T_a is the arterial blood temperature

ω is the local tissue-blood perfusion rate

Q_{met} tissue metabolic rate

Pennes' Bioheat Equation Shortcomings

- Thermal equilibrium doesn't occur in the capillaries, as Pennes assumed
- Doesn't take into account the directionality of blood perfusion between vessels and tissue
- Basically doesn't account for some of the significant features of the circulatory system

1D Heat Diffusion Model

Simplified the equation to 1 dimension to make the problem easier:

$$\frac{\partial T}{\partial t} = \frac{k}{\rho c}\frac{\partial^2 T}{\partial x^2} + \frac{\rho_{blood} c_{blood} w}{\rho c}(T_a - T) + Q_{met} + Q_i(x,t) \quad (2)$$

$$\frac{\partial T}{\partial t} = a\frac{\partial^2 T}{\partial x^2} + C_1(T_a - T) + C_2(x,t) + C_3 \quad (3)$$

We now arrive at the simplest possible equation for the system:

$$\frac{\partial T(x,t)}{\partial t} = a\frac{\partial^2 T(x,t)}{\partial x^2} \quad (4)$$

Testing the model

Input function:

$$f_0 = \sin\left(\frac{\pi x}{L}\right) \tag{5}$$

Analytic solution to this:

$$f(x,t) = \sin\left(\frac{\pi x}{L}\right)\exp\left(-\frac{\alpha \pi^2 t}{L^2}\right) \tag{6}$$

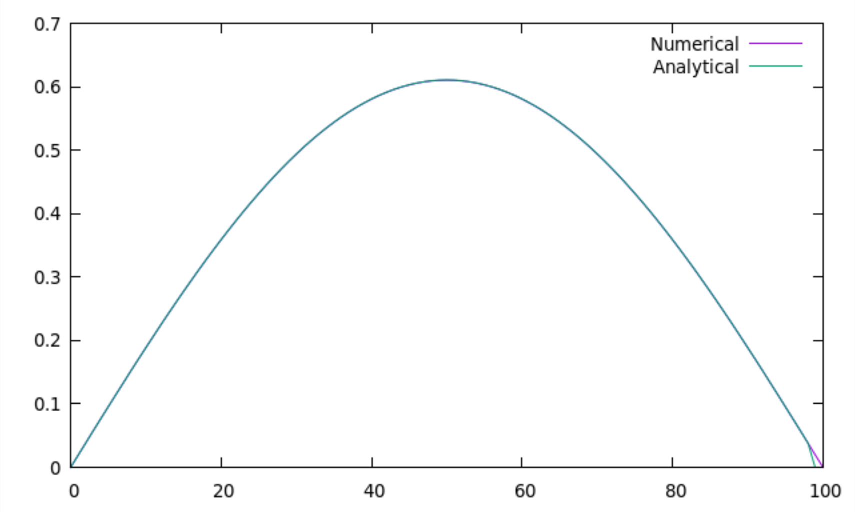
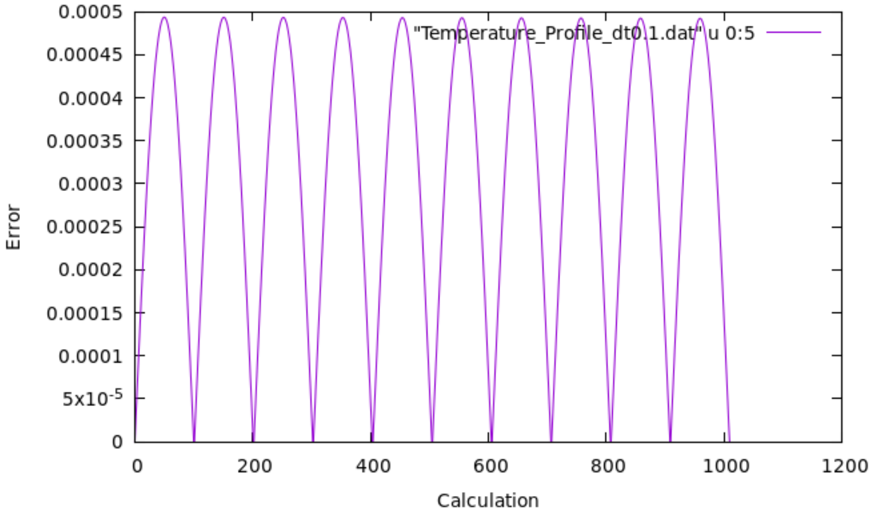


Figure 1: dt = 0.00005, dx = 0.01, N = 100, runs = 1000, time = 0.05


"Temperature_Profile_dt0.1.dat" u 0:5
Error
Calculation
0.0005
0.00045
0.0004
0.00035
0.0003
0.00025
0.0002
0.00015
0.0001
5x10-5
0
200
400
600
800
1000
1200

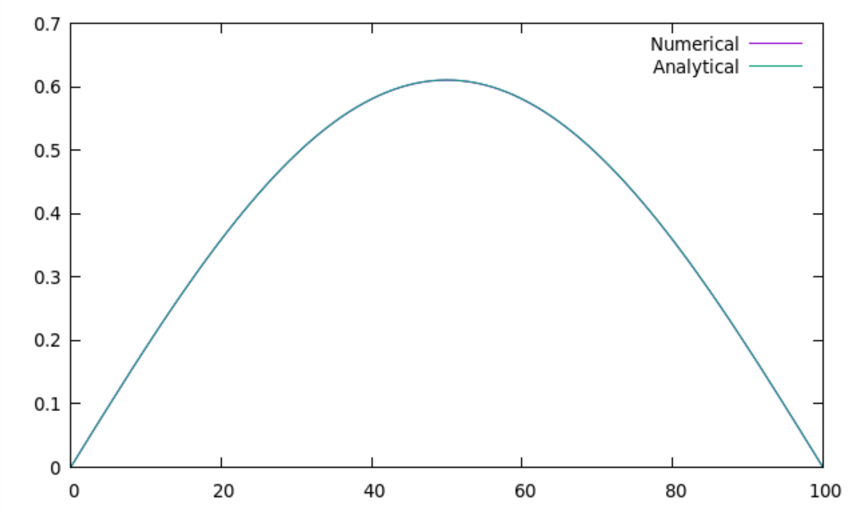
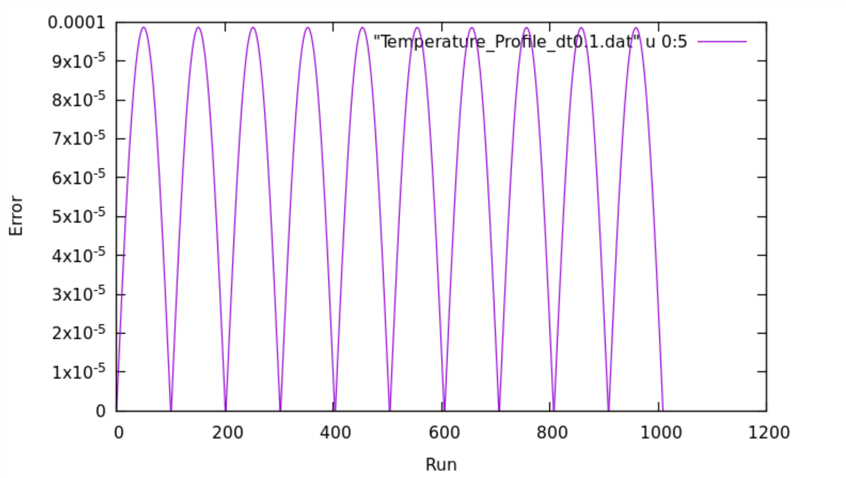


Figure 2: dt = 0.00005, dx = 0.01, N = 100, runs = 1000, time = 0.05



"Temperature_Profile_dt0.1.dat" u 0:5
0.0001
9x10-5
8x10-5
7x10-5
6x10-5
5x10-5
4x10-5
3x10-5
2x10-5
1x10-5
0
Error
0
200
400
600
800
1000
1200
Run

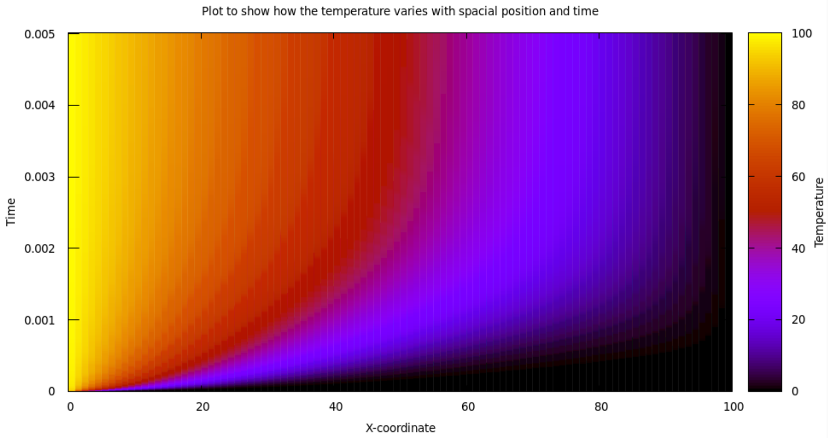
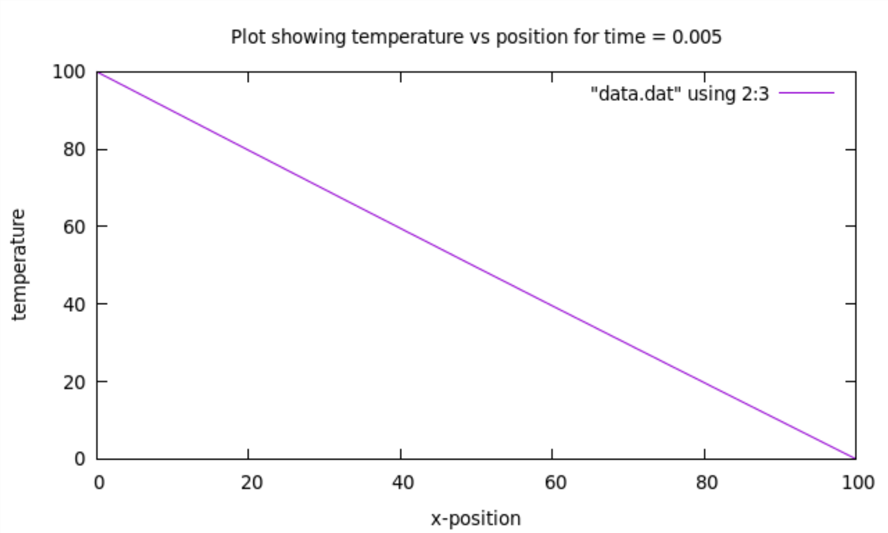


Figure 3: dt = 0.0000001, dx = 0.001, runs = 50000, time = 0.005


Plot showing temperature vs position for time = 0.005
"data.dat" using 2:3
temperature
x-position
100
80
60
40
20
0
0
20
40
60
80
100

Heat capactity of magnetite can be described by the Shomate equation:

$$C_p = A + BT + CT^2 + DT^3 + \frac{E}{T^2} \tag{7}$$

For temperatures $298K - 900K$:

$$A = 104.2096,\ B = 178.5108,\ C = 10.61510,\ D = 1.132534,$$

$$E = -0.994202$$

For temperatures $900K - 3000K$:

$$A = 200.8320,\ B = 1.586435 \times 10^{-7},\ C = -6.661682 \times 10^{-8},$$

$$D = 9.452452 \times 10^{-9},\ E = 3.186020 \times 10^{-8}$$

https://webbook.nist.gov/cgi/cbook.cgi?ID=C1309382&Mask=2&Type=JANAFS&Plot=on