Transfer Equations:
An Attempt to Pose an Optimization Problem

Project for CE291
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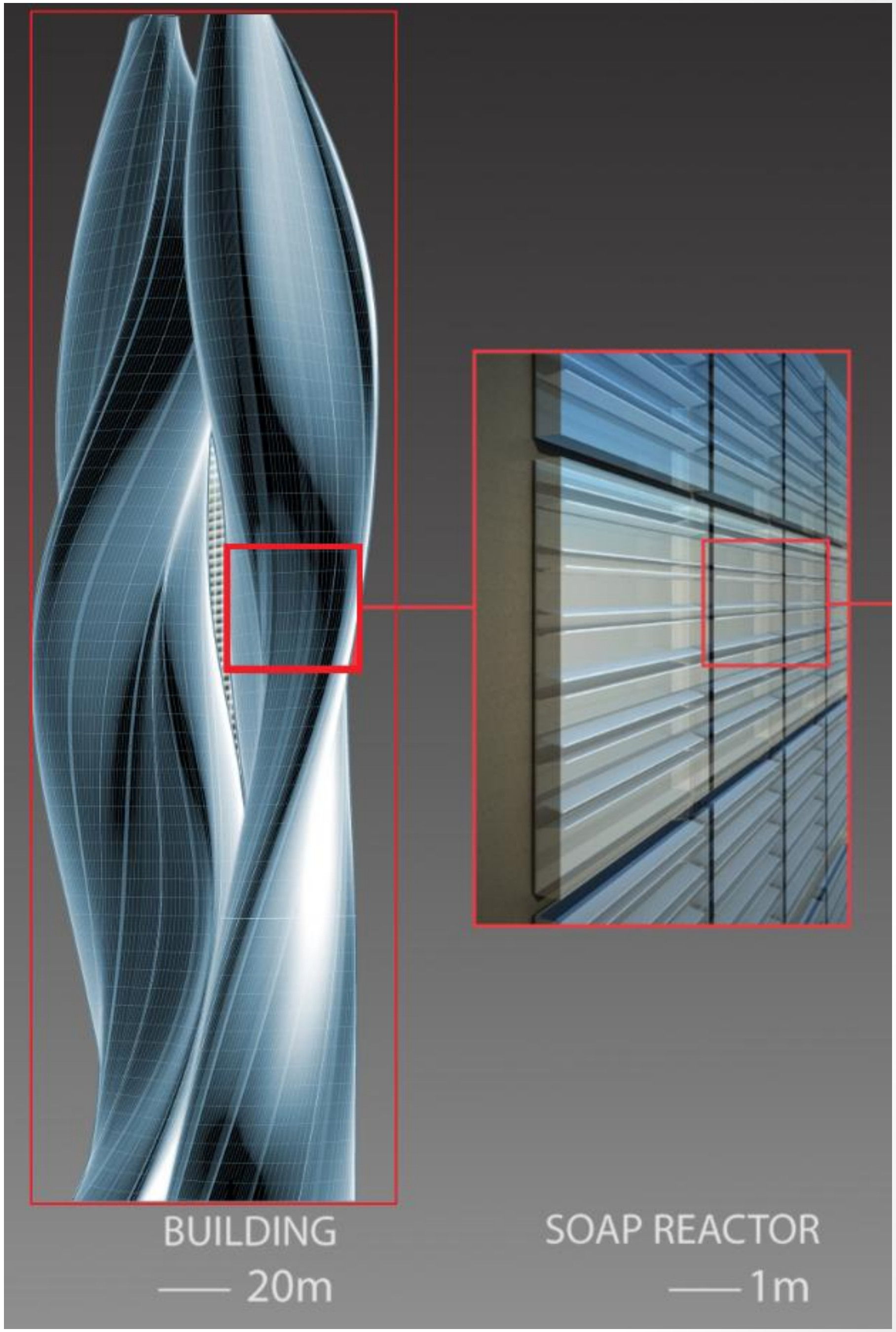
Background

System

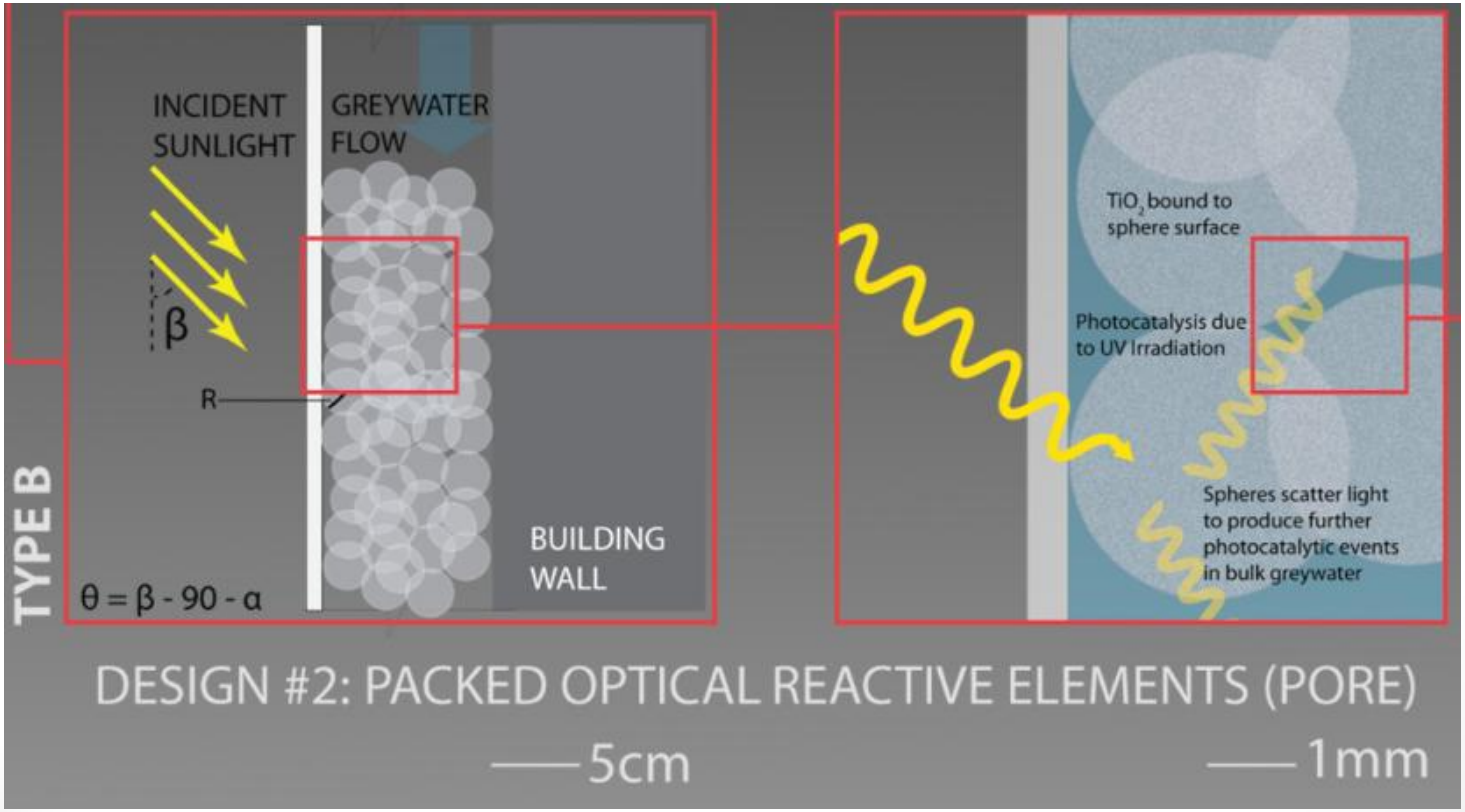
Solar Disinfection of Greywater

- The goal of this study is to define the mass transfer in a solar activated porous media batch reactor
- This is a multiphysics problem defined through multiple Partial Differential Equations



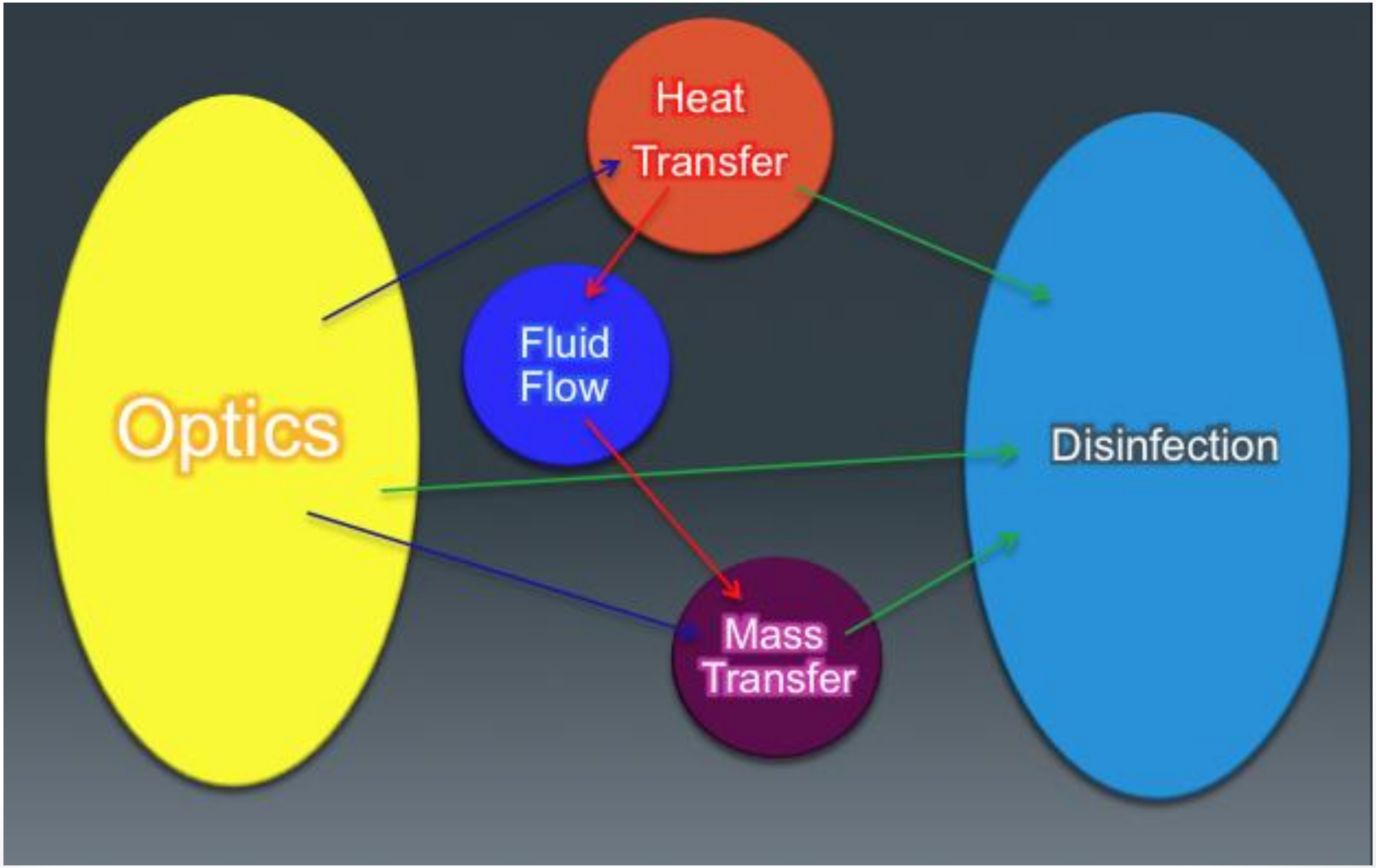
Batch Reactor with Photocatalysis

- Photocatalyst fixed to surface of porous bed
- Reacts with UV Light to produce hydroxyl radical
- Radicals kill organic contaminants as first order surface reaction



Relevant Physics

Physics Interaction



Parameters of Interest

- The defining parameters for packed bed phenomena are:

- d = diameter of packing spheres
- ε = porosity (Volume of fluid space/Total Volume) of bed

- It is worth noting that the porosity for randomly packed spheres in a bed is in the range of 0.47-0.42, any value outside of this range will significantly affect the physics of packed bed phenomena. We consider the porosity constant at 0.44 for this study

- The parameter "d" shows up in all equations related to the physics and is the parameter variable we will use to investigate optimal transfer

Driving Force: Light Intensity

- Light is the source of energy in this system
- Beers Law gives us the Intensity as a function of space, time, and the diameter of the packing material

$$I(x,t,d) = I_o(t)e^{-a(d)x}$$

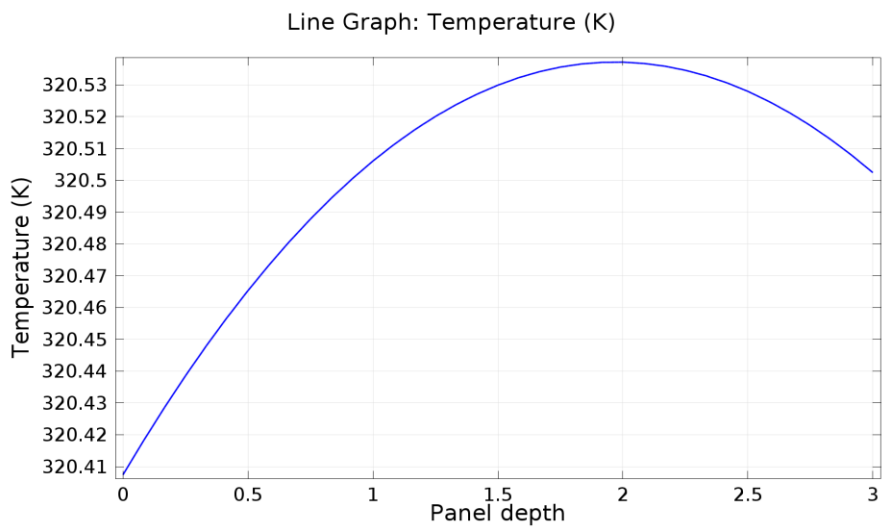
- α is the coefficient of absorption
- The light intensity through the bed decays exponentially
- This is the source of photocatalytic reactions and heating

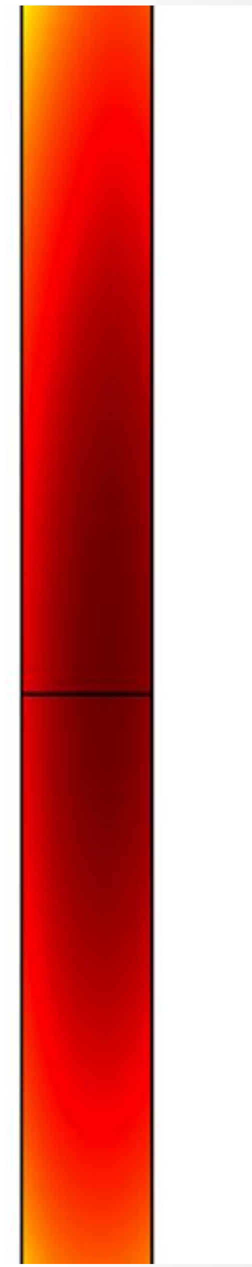
Heat Transfer

- Heat source given by light absorption
  (k is conductivity)

$$\frac{¶T}{¶t} - k(e)\frac{¶^2 T}{¶x} = q(x,d)$$

- Studies done in COMSOL with flux boundary conditions derived from free convection correlations at surfaces of panel





On Momentum and Mass Transfer

- Most challenging part of the study is to understand the effect of free convection in fluid due to differential heating
- Throughout most of the day, models show that even though absolute temperature changes, temperature profile and magnitude are constant
- Though small in absolute value, it is expected that the velocity gained by the fluid from free convection will greatly speed the process of mass transfer, so it must be characterized

Momentum Transfer

- Steady State Navier-Stokes equations

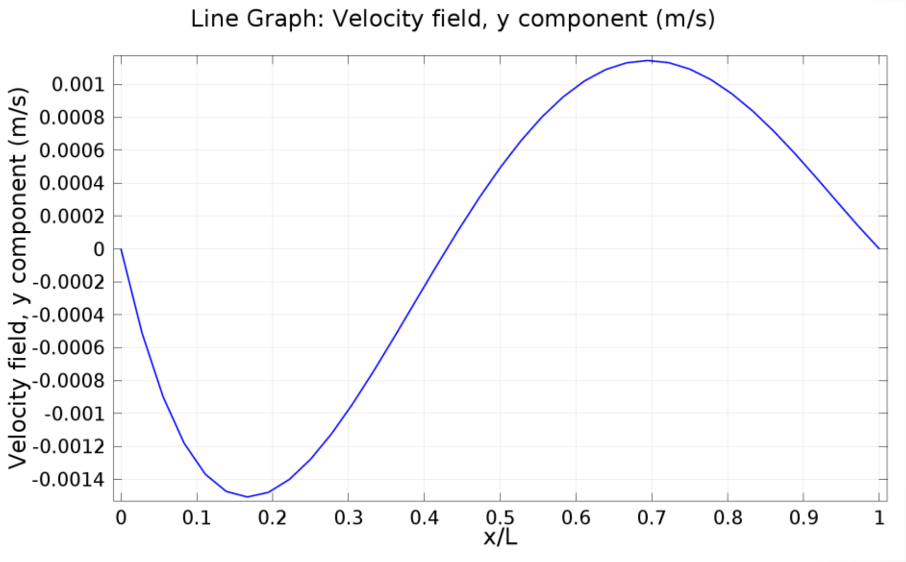
$$\rho(\mathbf{u}\cdot\nabla)\mathbf{u} = -\nabla p + \nabla\cdot\mu(\nabla\mathbf{u} + (\nabla\mathbf{u})^T) + \rho_0\mathbf{g}\beta(T - T_0)$$

$$\nabla\cdot\mathbf{u} = 0$$

- Convective acceleration = 0 in a homogenous packed bed
- ρ_og term is a Boussinesq approximation for free convection force, where (T-T_o) is the temperature profile from Heat Eq.
- Pressure gradient term related to porous media via Darcy's Law

Flow Field Assumptions

- The convective flow field will be negative in the front (left) of the panel, and positive in the rear (right) of the panel, and relatively anti-symmetric
- Panel is tall, shallow, and wide, meaning that the flow field can be defined in x,z coords
- Flow in the tall central section is in z direction only
- Fully developed, incompressible



Darcy’s Law

$$\frac{\Delta P}{h} = \left(\frac{k}{\mu}\right) v_z$$

Relates pressure drop to flow field, requires laminar regime to be valid (Re≤10)

$$k = \frac{d^2 \varepsilon^2}{180(1-\varepsilon)^2}$$

k is the permeability, a function of the packing modulus size, shape, and bed porosity, from Carman-Kozeny empirical relations

Substituting into the original and simplifying:

$$\left(\frac{\mu}{\rho g}\right) \cdot \frac{\partial^2}{\partial x^2} v_z(x) + \left(\frac{\mu}{k \rho g}\right) v_z(x) + b(T(x) - T_o) = 0$$

Buckingham Pi theorem

- Of the dimensionless relations found through Buckingham Pi, two in particular stand out as meaningful in this equation:

$$D = \frac{mv}{krg}$$

Ratio of frictional forces to gravitational forces

$$B(q(x) - 1) = b \times T_o \frac{(T(x) - T_o)}{T_o}$$

Non-Dimensionalization of Temperature function

- Using $x = \frac{X}{L}$, N-S equation becomes:

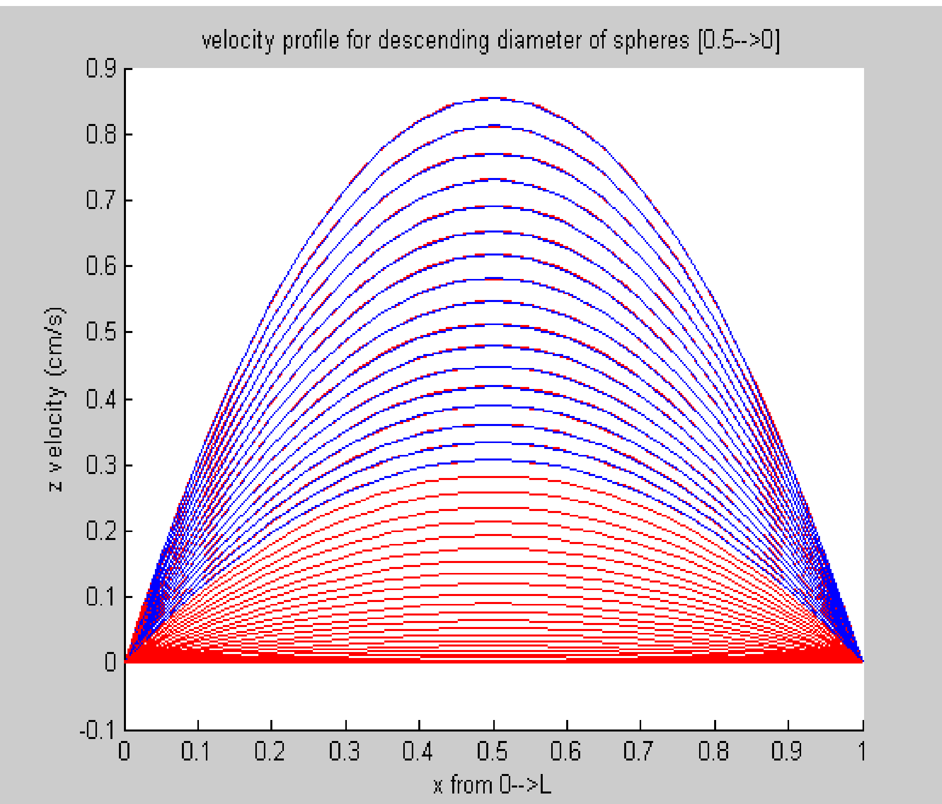
$$\frac{\partial^2 D(x)}{\partial x^2} + \left(\frac{L}{k}\right)^2 D(x) = B(q(x) - 1)$$

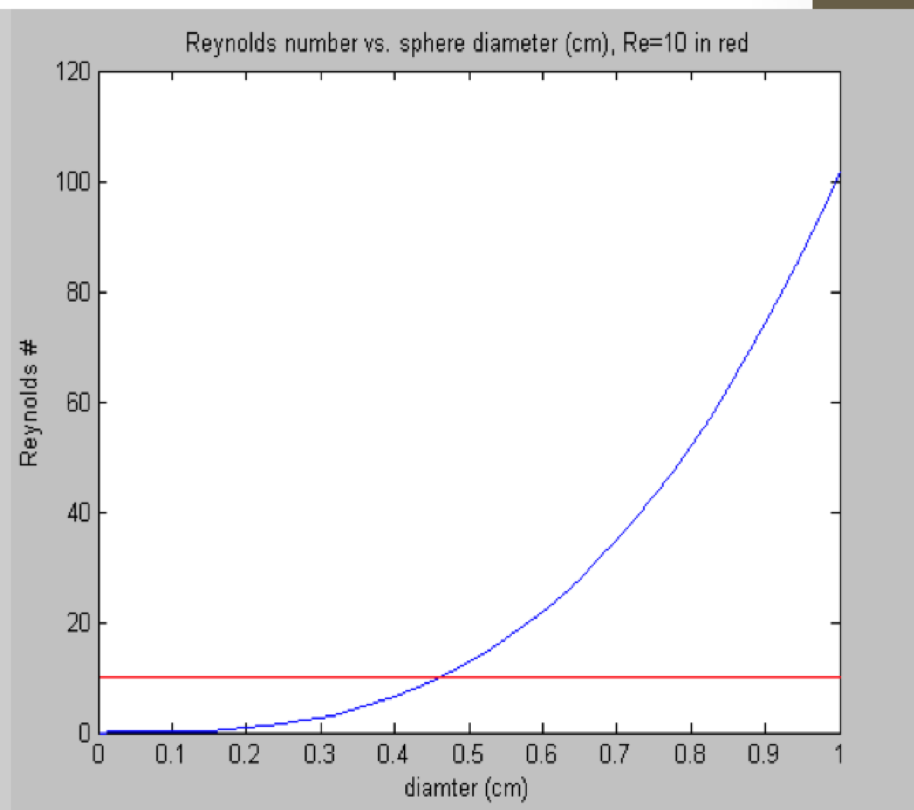
(a second order non-homogeneous ODE)

Reforming $v_z(x)$

- From the previous

$$v_z = \frac{k r g}{m} D \qquad \mathrm{Re}_{pb} = \frac{r v d}{6 m(1 - e)}$$





Mass Transfer Optimization: Posing the problem

Peclet Number:

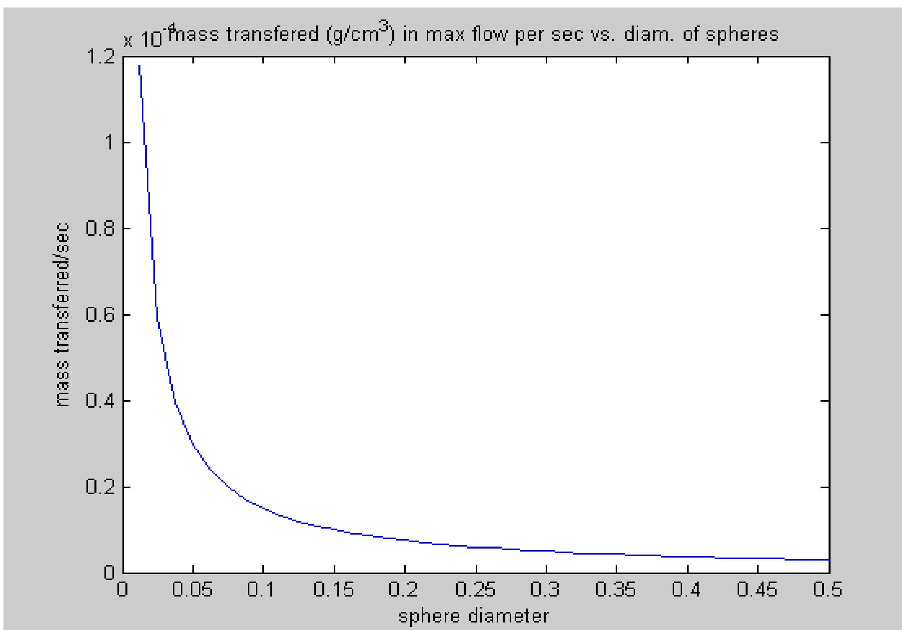
$$\frac{d \times v_z}{Dif_b}$$

- Dimensionless Peclet number defines the ratio of the convective to diffusive mass transfer time scales for beds
- For Peclet numbers above 10^3 we can expect that convection plays a significant role in mass transfer for the system
- Peclet # decreases with sphere diameter
- Peclet number > 1000 for d > 0.05 cm

Convection Diffusion Eqn.

- Concentration of bacteria at surface is 0 due to rapid surface reaction
- Mass transfer rate on the surface of the sphere comes from a boundary layer/film theory analysis:

$$W_b = 6.33 \times Dif_b \times Pec^{1/3} \times C_{b@¥}$$



An Advection-Diff. Equation for flow through packed bed

$$\frac{\partial c_b(z,t)}{\partial t} = -v_{z,avg}\frac{\partial c_b(z,t)}{\partial z} - (S_o K_c)c_b(z,t)$$

$$K_c = \frac{1.09}{\varepsilon}\frac{Dif_b}{d}\mathrm{Re}^{1/3}Sc^{1/3},\ Sc = \frac{\mu}{\rho \cdot Dif_b}$$

$$S_o = \frac{6}{d}$$

K_c is reaction coefficient

S_o is specific surface area

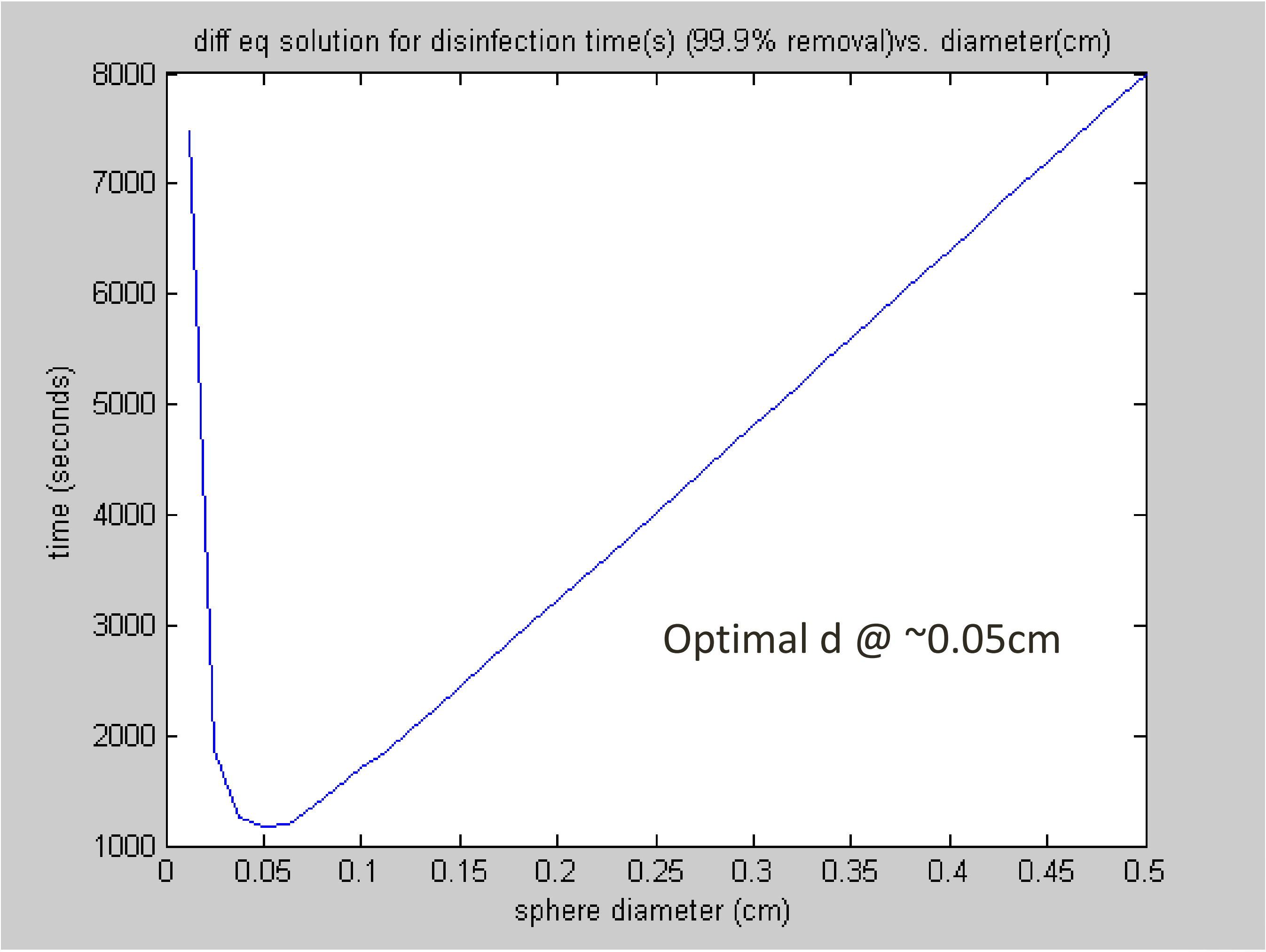
Changing variables:

$$\eta = (z - v_z t)$$

Changing variables allows for conversion into an ODE.
Solution can be found from in the form:

$$\frac{\partial c_b(\eta)}{\partial \eta} = -\frac{S_o K_c}{v_{z,\max}}c_b(\eta)$$

Plot of disinfection time vs. d



…alas, there are problems

- This study only observes what happens once the flow is developed in the primary central section of the panel
- Light intensity in media decreases with decreasing d
- Optimization of the problem then requires the incorporation of light intensity/velocity relationship to diameter of packing media in mass transfer estimate

Posing the Problem:
A task for the future…

$$Max\{W_b(c_b(v_z), v_z(d), d)\}$$

$$st: \frac{\partial c_b}{\partial h} = -f(v_z, d) \times c_b$$

$$I = I_o(t)e^{-f(d,x)}$$

$$0.02 > d > 1.0$$

$$c(0) = c_o$$