Lecture 5 - Scaling Out Dimensionless Groups

Contents

Review from Lecture 4

Last time, we showed that the construction of dimensionless groups can be illustrative for revealing important physical scaling relationships specific to a given transport problem. The goal of non-dimensionalization is two-fold:

1. Reduce the number of parameters that define the PDE and B.C.s
2. Obtain physical insight about the nature of the solution

The key ideas associated with dimensionless groups and their application to PDE's and B.C. is that we will seek to transform independent and dependent variables s.t. they are of order 1 or span the value from $[0, 1]$.

As we saw in the previous example, it is not always the case that these basic strategies work, and despite our best efforts, there sometime remain terms that are dimensionless, but can take on an arbitrary magnitude, $[0, \infty]$

Consider the previous example from Lecture 4. We defined $\eta = r/R$ and $\theta = \dfrac{k(T - T_\infty)}{R^2 h_v}$ and the resulting ODE and B.C.'s reduced to the following:

$$\frac{1}{\eta}\frac{\partial}{\partial \eta}\left(\eta \frac{\partial \theta}{\partial \eta}\right) = -1$$

$$\left.\frac{\partial \theta}{\partial \eta}\right|_{\eta=1} = -Bi\theta$$

$$\left.\frac{\partial \theta}{\partial \eta}\right|_{\eta=0} = 0$$

All terms of this differential equation are scaled except the one within the B.C. #1. The Bi have any magnitude, and therefore this equation is not "scaled" properly (i.e., the fundamental nature of the solution depends on the magnitude of the Bi).

Scaling and Order of Magnitude Analysis

Sometimes these parameters appear in the ODE itself and can greatly influence the physics. Let's consider the following example. A polymeric capsule of radius R is embedded within a fluid that has a dissolved macromolecule, A at a concentration C_∞, that undergoes a chemical reaction with the polymer such that it is transformed to a mobile species B via the following reaction:

$$A \rightarrow 2B$$

A and B are approximately the same molecular diameter so their diffusivities are about equal (i.e., $D_A = D_B$). Let's analyze the steady state solution of the concentration profiles of both species and for now let's assume that B is dilute and we consider only the homogeneous reaction **within the bead**.

Balance on Equations for Species A

Based on the above assumptions, the balance expression for A

$$\frac{DC_A}{Dt} = D_A \nabla^2 C_A + R_A$$

where $R_A = -k_f C_A$

$$\left.\frac{\partial C_A}{\partial r}\right|_{r=0} = 0$$

$$C_A|_{r=R} = C_0$$

where $C_0 = K_A C_\infty$

where K_A is the partition coefficient of species A within the bead.

Let's try to make this dimensionless:

Define: $\xi = r/R$ and $\theta = C_A/C_0$:

Choosing spherical geometry and taking the dot product along the radial dimension:

$$\frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2 \frac{\partial C_A}{\partial r}\right) - \frac{k_f}{D_A} C_A = 0$$

is transformed to:

$$\frac{1}{\xi^2}\frac{\partial}{\partial \xi}\left(\xi^2 \frac{\partial \theta}{\partial \xi}\right) - \frac{k_f R^2}{D_A}\theta = 0$$

$$\left.\frac{\partial \theta}{\partial \xi}\right|_{\xi=0} = 0$$

$$\theta|_{\xi=1} = 1$$

Ok, just like in Lecture 4, we see a dimensionless group arise based on the defined dimensionless concentrations and radial positions:

$$Da = \text{Damkohler number} = \frac{k_f R^2}{D_A} = \frac{\text{homogeneous reaction rate}}{\text{diffusion rate}}$$

The **Damkohler Number** is the dimensionless balance of homogeneous reaction against diffusion of species A throughout the sphere's volume.

Rewriting the above

$$\frac{1}{\xi^2}\frac{d}{d\xi}\left(\xi^2\frac{d\theta}{d\xi}\right) - Da\theta = 0$$

$$\left.\frac{d\theta}{d\xi}\right|_{\xi=0} = 0$$

$$\theta|_{\xi=1} = 1$$

The distinction between this problem and Lecture 4 is now clear - a parameter appears in the ODE that can take on an arbitrary value on the domain $[0, \infty]$. Looking at the two limits:

Case I: $Da \to 0$

$$\frac{1}{\xi^2}\frac{d}{d\xi}\left(\xi^2\frac{d\theta}{d\xi}\right) = 0$$

$$\left.\frac{d\theta}{d\xi}\right|_{\xi=0} = 0$$

$$\theta|_{\xi=1} = 1$$

We can solve this ODE:

Integrating once:

$\frac{d\theta}{d\xi} = \frac{C_1}{\xi^2}$ where $C_1 = 0$ in order to obery B.C. #1

Integrating again,

$\theta = C_2$

By inspection, we immediately write:

$\theta = 1$

This solution is trivial and simply states that in the limit of no reaction, the concentration within the bead is uniform everywhere and equal to C_0.

Case II: $Da \to \infty$

$$-Da\theta = 0$$

$$\left.\frac{d\theta}{d\xi}\right|_{\xi=0} = 0$$

$$\theta|_{\xi=1} = 1$$

The solution is:

$\theta = 0$

This solution makes physical sense. If the reaction is infinitely fast, then there should be no A remaining within the sphere's volume. Unfortunately, because the concentration must vary from 0 to C_0, there must be a thin region near the sphere's surface where the change in concentration occurs. This **boundary layer** should become thinner and thinner as the $Da >> 1$

Let's solve for the general case:

$$\frac{1}{\xi^2}\frac{d}{d\xi}\left(\xi^2\frac{d\theta}{d\xi}\right) - Da\theta = 0$$

$$\left.\frac{d\theta}{d\xi}\right|_{\xi=0} = 0$$

$$\theta|_{\xi=1} = 1$$

This ODE is a version of modified spherical Bessel's equation (Appendix B.5), which has the form:

$\frac{1}{x^2}\frac{d}{dx}\left(x^2\frac{dy}{dx}\right) - m^2 y = 0$ when $n = 0$

and the general solution is:

$$y(x) = A\frac{sinh(mx)}{mx} + B\frac{cosh(mx)}{mx}$$

Note: that this form is preferred as the domain size is finite.

Important identities of these functions are:

$lim_{x\to 0}\frac{sinh(mx)}{mx} = 1$ and $lim_{x\to 0}\frac{d}{dx}\left(\frac{sinh(mx)}{mx}\right) = 0$

and

$lim_{x\to 0}\frac{cosh(mx)}{mx} = \infty$ and $lim_{x\to 0}\frac{d}{dx}\left(\frac{cosh(mx)}{mx}\right) = \infty$

Based on B.C. #1, B=0

$$\theta = A\frac{sinh(Da^{0.5}\xi)}{Da^{0.5}\xi}$$

Using B.C. #2,

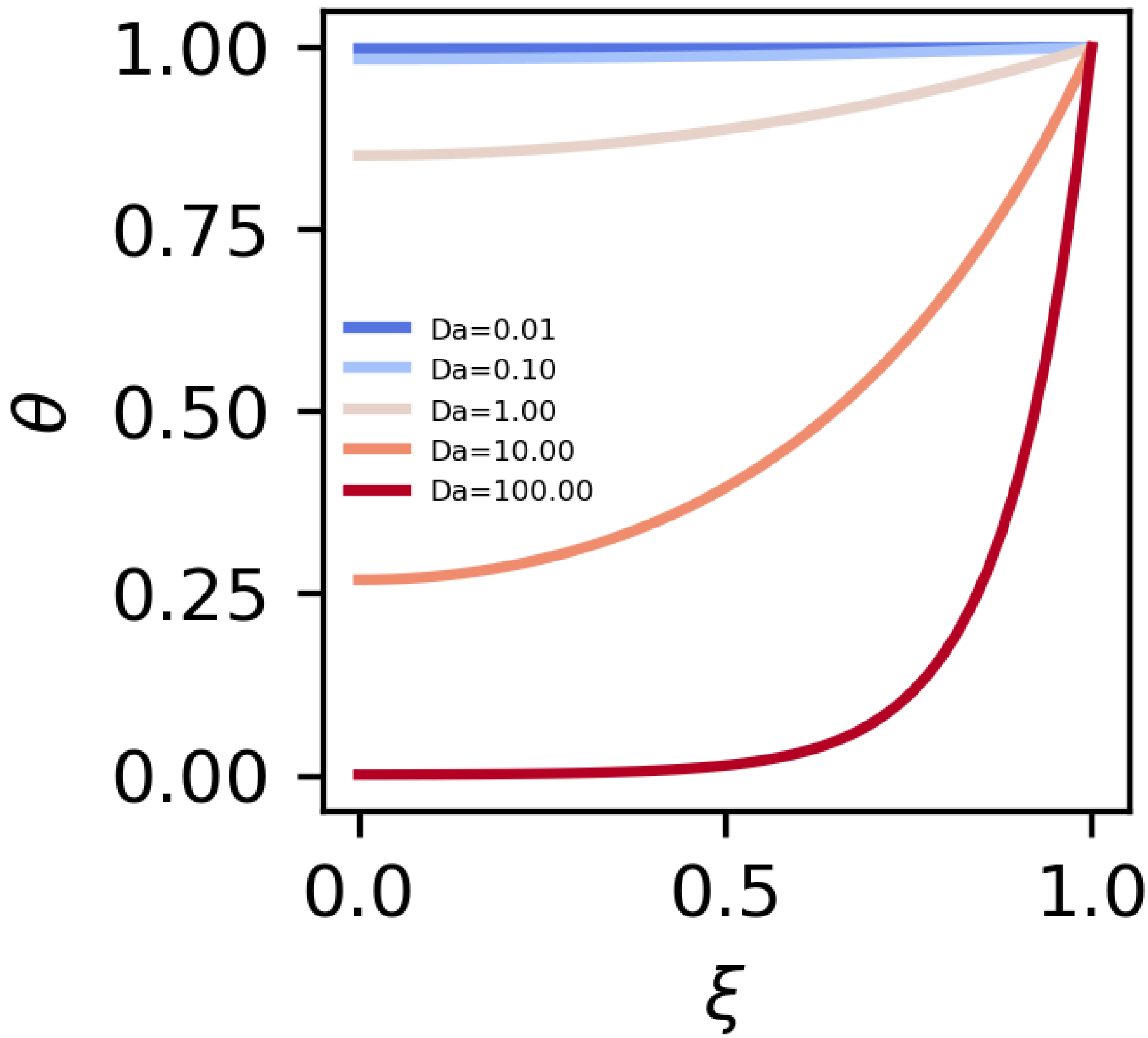
$1 = A\frac{sinh(Da^{0.5})}{Da^{0.5}}$ and $A = \frac{Da^{0.5}}{sinh(Da^{0.5})}$

rearranging we arrive at the final solution:

$$\theta = \frac{sinh\left(Da^{0.5}\xi\right)}{sinh\left(Da^{0.5}\right)\xi}$$

Let's plot the result

```
import matplotlib.pyplot as plt
import numpy as np
from numpy import sinh
import matplotlib.cm as cm


def fun(xi,Da):

    z=xi*Da**0.5

    ans=np.ones(len(xi))

    ##ndivision by zero is undefined
    mask=xi!=0
    ans[mask]=sinh(z[mask])/(xi[mask]*sinh(Da**0.5))

    ##handle the exception
    mask=xi==0
    ans[mask]=Da**0.5/sinh(Da**0.5)

    return ans

xi=np.linspace(0,1)

# Generate a colormap
colors = cm.coolwarm(np.linspace(0.1, 1, 5))

plt.figure(dpi=300,figsize=(2,2))
for Da,color in zip([0.01,0.1,1,10,100],colors):

    plt.plot(xi,fun(xi,Da),label='Da=%3.2f'%Da,color=color)

plt.ylabel(r'$\theta$')
plt.xlabel(r'$\xi$')

plt.legend(fontsize=4,frameon=False)
plt.show()
```



1.00
0.75
0.50
0.25
0.00
θ
Da=0.01
Da=0.10
Da=1.00
Da=10.00
Da=100.00
0.0
0.5
1.0
ξ