

Math 521 Lecture #5

§1.2.1: Characteristic Scales; §1.2.2: A Chemical Reactor Problem

Another procedure useful in formulating a mathematical model is that of scaling.

This procedure leads to the comparison of magnitudes of quantities and parameters and enables the neglecting of small terms.

It also can reduce the number of independent parameters present in the problem.

To motivate the idea of scaling, is time measured in seconds appropriate for glacier motion? is the unit of seconds appropriate for a nuclear reaction?

Each problem has an intrinsic **time scale** or **characteristic time** t_c that is appropriate for discernible changes.

A characteristic time for glacier motion is on the order of years, while for a nuclear reaction it is on the order of microseconds.

Sometimes there are two or more characteristic times for a problem, such as when a chemical reaction has a low concentration for a long time, only then to have a large concentration for a short time.

Once a characteristic time t_c has been identified, a new dimensionless variable \bar{t} can be defined by

$$\bar{t} = \frac{t}{t_c}.$$

For a wisely chosen t_c , the values of \bar{t} is neither too big nor too small, but rather of order unity.

Typically, after characteristic scales are chosen for each of the variables and parameters in a model, the resulting model is reformulated in dimensionless form.

This process is called **non-dimensionalization** or **scaling** the problem.

The Pi Theorem asserts that we can always non-dimensionalize a unit-free problem.

Example 1.11. The logistic growth model for a population $p(t)$ of animals at time t is

$$\frac{dp}{dt} = rp \left(1 - \frac{p}{K}\right), \quad p(0) = p_0$$

where r is the per capita growth rate (in the absence of limiting factors), and K is the carrying capacity (the number of animals the ecosystem can sustain).

To reduce this equation to non-dimensional form, we scale the time and population variables.

The time scale is formed from the one parameter that has the dimension of time in it, namely r (with dimensions of T^{-1}).

We scale time by $1/r$ through division, giving a dimensionless time variable defined by

$$\tau = \frac{t}{1/r} = rt.$$

There are two parameters involving population, namely K and p_0 .

Choosing K , we obtain a dimensionless population defined by

$$P = \frac{p}{K}.$$

By the Chain Rule, the time scale and the population scale change the derivative of the ODE as follows:

$$\frac{dp}{dt} = \frac{dp}{d\tau} \frac{d\tau}{dt} = r \frac{dp}{d\tau} = r \frac{d}{d\tau} (KP) = rK \frac{dP}{d\tau}.$$

The other side of the ODE changes as follows:

$$rp \left(1 - \frac{p}{K}\right) = rKP(1 - P).$$

The common factor of rK cancels, and we are left with

$$\frac{dP}{d\tau} = P(1 - P), \quad P(0) = \frac{p_0}{K} = P_0.$$

The original model has three parameters r , K , and p_0 , while the dimensionless model has only one.

A Chemical Reactor Problem. A chemical **C** of fixed concentration c_i (in mass per volume) enters a reactor of fixed volume V , at a constant rate flow of q (volume per time).

Initially there is a concentration c_0 of the chemical **C** in the reactor.

The mixture in the reactor is perfectly stirred, and the mixture leaves the reactor at the flow rate q .

Let $c = c(t)$ denote the concentration of the chemical **C** in the reactor at time t .

The chemical **C** is consumed by the reaction with a rate R (in mass per volume, per time).

We assume that the reaction rate doesn't depend on the temperature but that the reaction rate depends linearly only on the concentration c . (This makes the reaction isothermal.)

The perfectly stirred assumption implies that the concentration does not depend on a spatial variable.

What is the governing principle for this reactor?

The law of mass balance states that the time rate of change of the mass of the chemical in the reactor must equal the rate at which mass flows in (qc_i), minus the rate at which mass flows out (qc), plus the rate at which the mass is consumed by the reaction (VR).

This mass balance is the ODE

$$\frac{d}{dt}(Vc) = qc_i - qc - VR.$$

Notice that we included V to make the units consistent (every term has dimensions of mass per time).

We take $R = kc$ where $k > 0$ is the rate constant having the dimensions of inverse time.

We obtain a mathematical model of the reactor as the IVP

$$\frac{dc}{dt} = \frac{q(c_i - c)}{V} - kc, \quad c(0) = c_0.$$

To non-dimensionalize this model we look for characteristic times and concentrations.

The parameters c_i , c_0 , V , q , and k in the model lead to several choices of characteristic values.

We have two concentration parameters c_i and c_0 of which either one is suitable.

Define a dimensionless concentration $C = c/c_i$, so that all concentrations in the model are measured relative to c_i .

For a time scale there are two constants V/q (based on the flow rate) and k^{-1} (based on the reaction rate) formed from the parameters.

If we set T to be either V/q or k^{-1} , and define a dimensionless time variable $\tau = t/T$, we obtain by the chain rule

$$\frac{dC}{d\tau} = \frac{T}{c_i} \frac{dc}{dt} = \frac{T}{c_i} \left(\frac{q(c_i - c)}{V} - kc \right) = \frac{qT(1 - C)}{V} - kTC, \quad C(0) = \gamma$$

where $\gamma = c_0/c_i$.

For the choice of $T = V/q$, the corresponding dimensionless model is

$$\frac{dC}{d\tau} = 1 - C - \beta C, \quad C(0) = \gamma$$

where $\beta = kV/q$ is a dimensionless constant giving the ratio of the two time scales.

When $\beta \ll 1$, we may ignore the small term βC in the ODE, to get the approximation $C(\tau) = 1 + (\gamma - 1)e^{-\tau}$ which indicates that the concentration approaches that of the feed.

On the other hand, for the choice of $T = k^{-1}$, the corresponding dimensionless model is

$$\frac{dC}{d\tau} = \frac{1 - C}{\beta} - C, \quad C(0) = \gamma.$$

Multiplying the ODE through by β gives

$$\beta \frac{dC}{d\tau} = 1 - C - \beta C.$$

By ignoring the small terms when $\beta \ll 1$, we get the approximation $C = 1$, which may not satisfy the initial condition.

The second dimensionless model is more appropriate when $\beta \gg 1$, because, by ignoring the small term $(1 - C)/\beta$ we get the approximation $C(\tau) = \gamma e^{-\tau}$, indicating that the concentration decays to 0.