CS 131 Case Studies

RVLC

May 18, 2017

2nd Semester 2016-2017

1 GREENHOUSE GASES AND RAINWATER (needs Bisection)

It is well documented that the atmospheric levels of several so-called "greenhouse" gases have been increasing over the past 50 years. For example, Fig. 5.10 shows data for the partial pressure of carbon dioxide (CO2) collected at Mauna Loa, Hawaii from 1958 through 2008. The trend in these data can be nicely fit with a quadratic polynomial,

$$p_{CO_2} = 0.012226(t-1983)^2 + 1.418542(t-1983) + 342.38309 \tag{1}$$

where $p_{CO_2} = CO_2$ partial pressure (ppm). These data indicate that levels have increased a little over 22% over the period from 315 to 386 ppm.

One question that we can address is how this trend is affecting the pH of rainwater. Outside of urban and industrial areas, it is well documented that carbon dioxide is the primary determinant of the pH of the rain. pH is the measure of the activity of hydrogen ions and, therefore, its acidity or alkalinity. For dilute aqueous solutions, it can be computed as

$$pH = -log_{10}[H^+] \tag{2}$$

where $[H^+]$ is the molar concentration of hydrogen ions.

The following five equations govern the chemistry of rainwater:

$$K_1 = 10^6 \frac{[H^+][HCO_3^-]}{K_H p_{CO_2}} \tag{3}$$

$$K_2 = \frac{[H^+][CO_3^{-2}]}{[HCO_3^-]} \tag{4}$$

$$K_w = [H^+][OH^-] \tag{5}$$

$$c_T = \frac{K_H p_{CO_2}}{10^6} + [HCO_3^-] + [CO_3^{2-}] \tag{6}$$

$$0 = [HCO_3^-] + 2[CO_3^{2-}] \tag{7}$$

where K_H = Henry's constant, and K_1, K_2, and K_w are equilibrium coefficients. The five unknowns are c_T = total inorganic carbon, $[HCO^{3-}]$ = bicarbonate, $[CO_3^{2-}]$ = carbonate, $[H^+]$ = hydrogen ion, and $[OH^-]$ = hydroxyl ion. Notice how the partial pressure of CO_2 shows up in Eqs. 3 and 6.

Use these equations to compute the pH of rainwater given that $K_H = 10^{-1.46}$, $K_1 = 10^{-6.3}$, $K_2 = 10^{-10.3}$, and $K_w = 10^{-14}$. Compare the results in 1958 when the p_{CO2} was 315 and in 2008 when it was 386 ppm. When selecting a numerical method for your computation, consider the following:

- You know with certainty that the pH of rain in pristine areas always falls between 2 and 12.
- You also know that pH can only be measured to two places of decimal precision.

2 PIPE FRICTION (needs NewtonRoot)

Determining fluid flow through pipes and tubes has great relevance in many areas of engineering and science. In engineering, typical applications include the flow of liquids and gases through pipelines and cooling systems. Scientists are interested in topics ranging from flow in blood vessels to nutrient transmission through a plants vascular system.

The resistance to flow in such conduits is parameterized by a dimensionless number called the *friction factor*. For turbulent flow, the *Colebrook equation* provides a means to calculate the friction factor:

$$0 = \frac{1}{\sqrt{f}} + 2.0 \log \left(\frac{\varepsilon}{3.7D} + \frac{2.51}{\mathrm{Re}\sqrt{f}} \right) \tag{8}$$

where ε = the roughness (m), D = diameter (m), and Re = the *Reynolds number*:

$$\mathrm{Re} = \frac{\rho V D}{\mu}$$

where ρ = the fluids density (kg/m^3), V = its velocity (m/s), and μ = dynamic viscosity $(N \cdot s/m^2)$. In addition to appearing in Eq. 8, the Reynolds number also serves as the criterion for whether flow is turbulent (Re > 4000).

In this case study, we will illustrate how the numerical methods can be employed to determine f for air flow through a smooth, thin tube. For this case, the parameters are ρ =1.23 kg/m^3, μ=1.79×105 $N \cdot s/m^2$, D=0.005 m, V=40

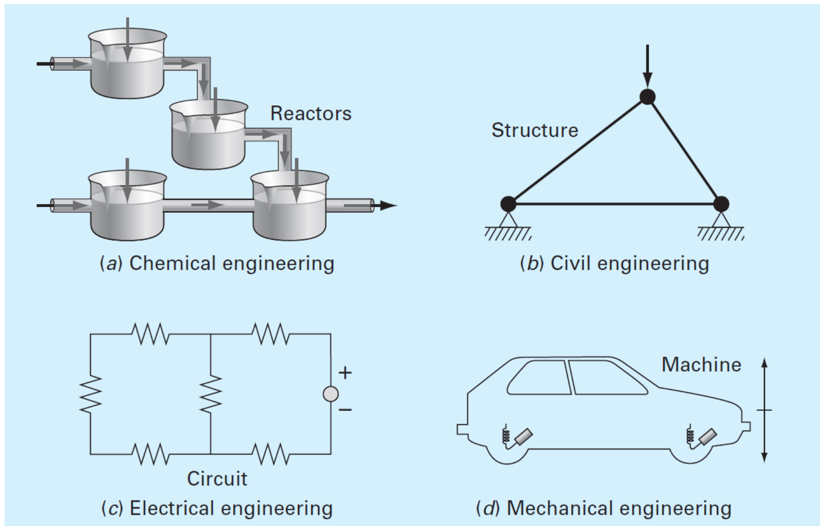

Figure 1: Models

m/s and $\varepsilon = 0.0015$ mm. Note that friction factors range from about 0.008 to 0.08. In addition, an explicit formulation called the *Swamee-Jain equation* provides an approximate estimate:

$$f \approx \frac{1.325}{\left[\ln\left(\frac{\varepsilon}{3.7D} + \frac{5.74}{\mathrm{R}e^{0.9}}\right)\right]^2} \tag{9}$$

3 CURRENTS AND VOLTAGES IN CIRCUITS (needs Gauss Seidel)

There are some models that are associated to conservation laws that figure prominently in engineering. As in Fig. 1, each model represents a system of interacting elements. Consequently, steady-state balances derived from the conservation laws yield systems of simultaneous equations. In many cases, such systems are linear and hence can be expressed in matrix form. The present case study focuses on one such application: circuit analysis.

A common problem in electrical engineering involves determining the currents and voltages at various locations in resistor circuits. These problems are solved using *Kirchhoff s current* and *voltage laws*. The *current* (or node) *law* states that the algebraic sum of all currents entering a node must be zero (Fig. 2), or

$$\Sigma\xi - \Sigma iR = 0$$

where ξ is the emf (electromotive force) of the voltage sources, and R is the

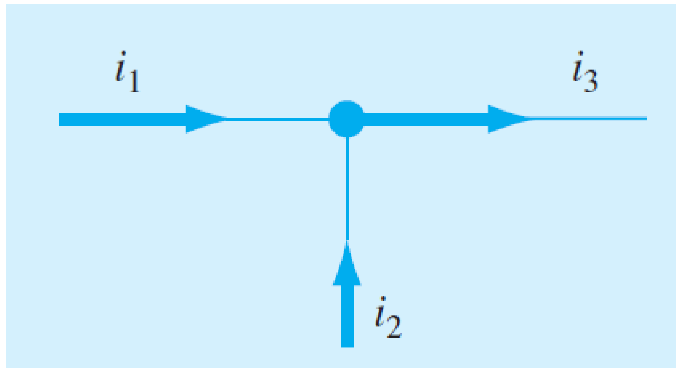

Figure 2: KCL

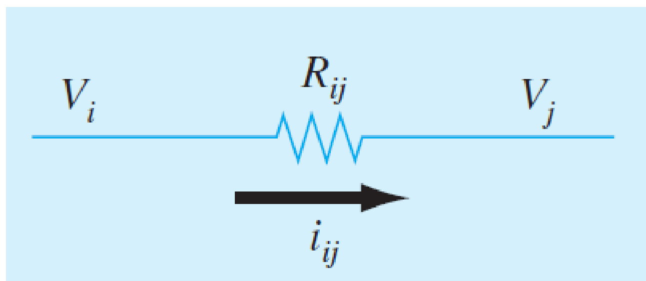

Figure 3: Ohm's Law

resistance of any resistors on the loop. Note that the second term derives from *Ohms law* (Fig. 3), which states that the voltage drop across an ideal resistor is equal to the product of the current and the resistance. Kirchhoffs voltage rule is an expression of the *conservation of energy.*

4 MODEL OF A HEATED ROD (needs Gauss with Pivot)

Linear algebraic equations can arise when modeling distributed systems. For example, Fig. 4 shows a long, thin rod positioned between two walls that are held at constant temperatures. Heat flows through the rod as well as between the rod and the surrounding air. For the steady-state case, a differential equation based on heat conservation can be written for such a system as

$$\frac{d^2T}{dx^2} + h_T(T_a - T) = 0 \tag{10}$$

where T = temperature ($°C$), x = distance along the rod (m), h_T = a heat

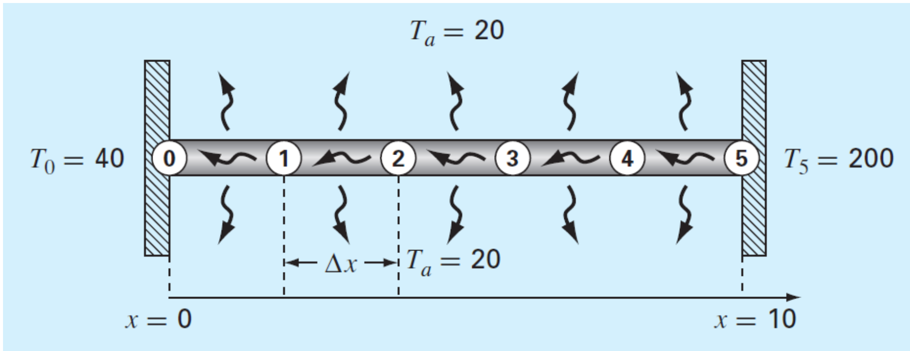

Figure 4: A noninsulated uniform rod positioned between two walls of constant but different temperature. The finite-difference representation employs four interior nodes.

transfer coefficient between the rod and the surrounding air (m^{-2}), and T_a = the air temperature ($°C$).

Given values for the parameters, forcing functions, and boundary conditions, calculus can be used to develop an analytical solution. For example, if h = 0.01, Ta = 20, T(0) = 40, and T(10) = 200, the solution is

$$T = 73.4523e^{0.1x} - 53.4523e^{-0.1x} + 20 \tag{11}$$

Although it provided a solution here, calculus does not work for all such problems. In such instances, numerical methods provide a valuable alternative. In this case study, we will use finite differences to transform this differential equation into a tridiagonal system of linear algebraic equations which can be readily solved using the numerical methods such Gaussian Elimination with Partial Pivoting.

5 INDOOR AIR POLLUTION (needs LU-Crout for Inverse)

As the name implies, indoor air pollution deals with air contamination in enclosed spaces such as homes, offices, and work areas. Suppose that you are studying the ventilation system for Bubbas Gas N Guzzle, a bus-stop restaurant located adjacent to an eight-lane expressway.

As depicted in Fig. 5, the restaurant serving area consists of two rooms for smokers and kids and one elongated room. Room 1 and section 3 have sources of carbon monoxide from smokers and a faulty grill, respectively. In addition, rooms 1 and 2 gain carbon monoxide from air intakes that unfortunately are positioned alongside the expressway.

Write steady-state mass balances for each room and solve the resulting linear algebraic equations for the concentration of carbon monoxide in each room. In

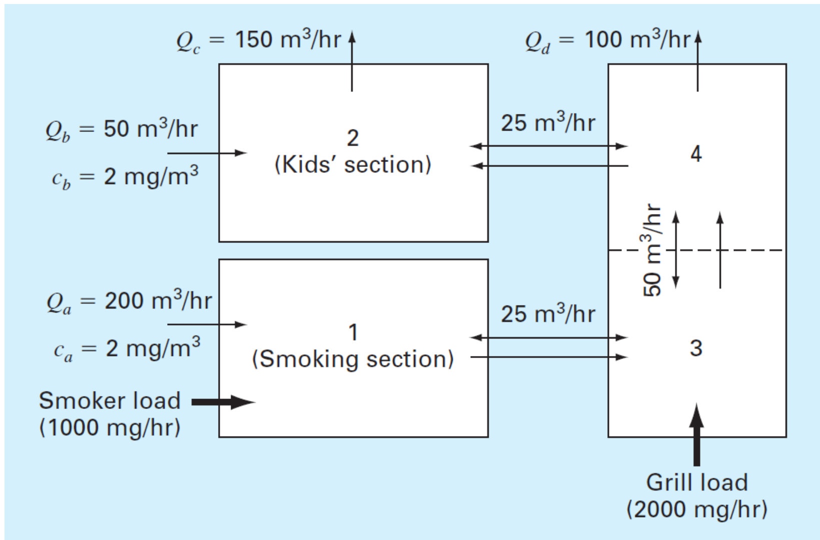

Figure 5: Overhead view of rooms in a restaurant. The one-way arrows represent volumetric airflows, whereas the two-way arrows represent diffusive mixing. The smoker and grill loads add carbon monoxide mass to the system but negligible airflow.

addition, generate the matrix inverse and use it to analyze how the various sources affect the kids room. For example, determine what percent of the carbon monoxide in the kids section is due to (1) the smokers, (2) the grill, and (3) the intake vents. In addition, compute the improvement in the kids section concentration if the carbon monoxide load is decreased by banning smoking and fixing the grill. Finally, analyze how the concentration in the kids area would change if a screen is constructed so that the mixing between areas 2 and 4 is decreased to 5 m^3/hr.

6 CHEMICAL REACTIONS (needs Newton for System of 2 Eqns)

Nonlinear systems of equations occur frequently in the characterization of chemical reactions. For example, the following chemical reactions take place in a closed system:

$$2A + B \leftrightarrow C \tag{12}$$

$$A + D \leftrightarrow C \tag{13}$$

At equilibrium, they can be characterized by

$$K_1 = \frac{c_c}{c_a^2 c_b} \tag{14}$$

$$K_2 = \frac{c_c}{c_a c_d} \tag{15}$$

where the nomenclature c_i represents the concentration of constituent i. If x_1 and x_2 are the number of moles of C that are produced due to the first and second reactions, respectively, formulate the equilibrium relationships as a pair of two simultaneous nonlinear equations. If $K_1 = 4 \times 10^{-4}$, $K_2 = 3.7 \times 10^{-2}$, $c_{a,0} = 50$, $c_{b,0} = 20$, $c_{c,0} = 5$, and $c_{d,0} = 10$, employ the Newton-Raphson method to solve these equations.