MATHEMATICAL MODELING

IMA Summer Program for Graduate Students
August 3–28, 1992

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Forward

Mathematical modeling involves understanding the physics of the problem, setting up the equations, simplifying, solving analytically or numerically, then checking the physical implications of the mathematical results, and proceeding to improve the model.

The only way to learn mathematical modeling is by doing it. Working with a group seems a good way to begin. Indeed, there are often many blind spots, or missing pieces of information when setting up the model. Bringing together several minds to bear upon the problem alleviates the frustrations or self doubts that beginners may feel.

The IMA summer program in Mathematical Modeling extended over a period of 4 weeks (August 3-28, 1992).

The goals were:

1. To expose the students to mathematical modeling of problems which come from industry and engineering sciences, and to impact on them the excitement of solving real-world problems.

2. To create an environment whereby the students will get to know each other and develop contacts that will enhance their future research.

Each Monday morning 3 problems were posed to the whole class with brief general background. Then the students were organized into 3 teams and each team concentrated on one of the problems, for the rest of the week. The students developed a mathematical model with guidance only as needed. Then they worked on the mathematical analysis of the problem and obtained numerical results. Each team was guided by a tutor.

By Friday afternoon of each week, the teams reported to the whole class on their progress and possible future directions for research.
There were 3 new problems each week. Thirty students participated in the program (several from Canada and Europe); they were selected from a larger pool of applicants.

We wish to thank the tutors for their efforts and for the excitement they elicited from the students.

We are grateful to the Sloan Foundation for supporting this program.

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Problem 1:  Blood flow in the leg veins
Presented by Mary Brewster

(Based on a problem posed by Dr. Alan Koslow, M.D., to the RPI Math-in-
Industry Workshop, 1990.) Blood flow in the leg veins is driven by
external pressure from muscle contraction, which collapses the vein in an
upward-sweeping motion during walking. A standing person would
experience random muscle contractions which alone are not sufficient to
drive the blood upward. A set of valves, usually about 15 in number, aids
circulation by preventing backflow in the veins. If these valves are
damaged—a condition known as deep venous thrombosis—circulatory
effectiveness must be maintained through frequent walking, or wearing of
a pressure stocking. Without such measures, blood pools in the lower
extremities causing high pressures within the veins (which is very
painful), and over extended periods of time, distension of the vein as it
loses its elasticity (varicose veins). Modern surgical procedures allow
artificial valves to be implanted. Surgeons would like to know how many
valves should be implanted to restore near-normal circulatory
effectiveness.

* Develop a model for calculating the influence of the number of valves
on the effectiveness of a random muscle pump in a standing person.

Bibliography

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Kamm, R.D., "Flow through collapsible tubes," in Handbook of
Bioengineering, ed. R. Skalak, S. Chien, pp. 23.1-23.19, New York, McGraw-
Hill, and references therein.
Fluid Mechanics of Circulatory System

PULMONARY SYSTEM

ARTERIES

CAPILLARIES

VEINS
Problem 2: Water pollution from electricity generating stations
Presented by Colin Please

Electricity generating power stations need to get rid of about 2kW of low grade heat for every 1kW of electricity generated. There are two common methods of disposing of this large amount of heat. First water can be evaporated in cooling towers so that the heat goes into the atmosphere. Secondly water can be taken from a nearby river heated by about 10 deg C and then returned to the river.

If a new power station is proposed the second option of using a nearby river is usually identified as the cheaper option. It is therefore necessary to predict the possible environmental impact of discharging this heated water into the river. A mathematical model is therefore needed to determine the possible temperature increases within the river.

--- from the oral presentation ---

\[ \text{efficiency} = \frac{\text{electric energy out}}{\text{thermal energy in}} \approx \frac{T_{\text{max}} - T_{\text{min}}}{T_{\text{max}}}. \]

Typically:

\[ T_{\text{min}} \approx 300^\circ K \]
\[ T_{\text{max}} \approx 600^\circ K \]
\[ \text{max efficiency} \approx \frac{600 - 300}{600} = 50\%. \]
BASIC ELECTRICITY
GENERATION

COMPRESSOR.

CONDENSER

TURBINE

HEATING

COOLING.

GENERATOR.
Problem 3: Handling thin sheets of moving materials
Presented by Julian Cole

Various aspects of the problem of handling thin sheets of moving materials will be considered. This type of problem occurs in the handling of paper, as sheets of newsprint for example, or in handling of photographic film or the manufacture of plastic sheets. The general type of physics needed to study this problem is mechanics, in particular continuum mechanics.

General equations need to be formulated to study the motion of these sheets. The description should include inertia and some of the elastic forces. Equations useful for both large and small deflection need to be found. Boundary conditions have to be specified corresponding to various physical situations. Friction and shear stress on rollers and other handling devices have to be analyzed.

Phenomena of interest include wave propagation in the sheets, stability of the sheets, formation of wrinkles, evolution of wrinkles during processing, creation of folds and tears.
Notes from the oral presentation

Continuum Mechanics

(i) inertia -

(ii) impulse - momentum

\[ \overrightarrow{F} dt = d(m \overrightarrow{v}) \]

(iii) action - reaction.

General Approach

3D Equations —

Simplified Approach 1D
Web Handling

Problem Areas
Flutter, Instability
Resonance

Tension in various segments
steady, unsteady

Wrinkles
u = horizontal displacement
v = vertical displacement
T \sin \theta = vertical stress
T \cos \theta = horizontal stress

\rho_0 = \text{density} = \text{mass/length}

\frac{\partial^2 u}{\partial t^2} = \frac{\partial}{\partial \xi} (T \cos \theta)

\frac{\partial^2 v}{\partial t^2} = \frac{\partial}{\partial \xi} (T \sin \theta)
strain = \frac{\text{change in length}}{\text{original length}}

\ell = \sqrt{\left(1 + \frac{\partial u}{\partial \xi}\right)^2 + \left(\frac{\partial v}{\partial \xi}\right)^2} \, d\xi

\varepsilon = \sqrt{\left(1 + \frac{\partial u}{\partial \xi}\right)^2 + \left(\frac{\partial v}{\partial \xi}\right)^2} - 1
Linearly Elastic E

\[ T = T_0 + E\varepsilon \]

\[ \{T\} = \text{force} = \frac{KM}{S^2} \]

\[ \rho_0 \frac{\partial^2 u}{\partial t^2} = \frac{\partial}{\partial \xi} \left( T \cos \theta \right) (+F_x) \]

\[ \rho_0 \frac{\partial^2 v}{\partial t^2} = \frac{\partial}{\partial \xi} \left( T \sin \theta \right) (+F_y) \]

\[ \sin \theta = \frac{\partial v / \partial \xi}{\sqrt{\left(1 + \frac{\partial u}{\partial \xi}\right)^2 + \left(\frac{\partial v}{\partial \xi}\right)^2}} \]

\[ \cos \theta = \frac{1 + \partial u / \partial \xi}{\sqrt{\left(1 + \frac{\partial u}{\partial \xi}\right)^2 + \left(\frac{\partial v}{\partial \xi}\right)^2}} \]

\[ v \ll L, \varepsilon \ll 1, \; \text{small strains} \]

\[ v = v_0 + \cdots \]

\[ \rho_0 \frac{\partial^2 v_0}{\partial t^2} = T_0 \frac{\partial^2 v_0}{\partial \xi^2} = T_0 \frac{\partial^2 v_0}{\partial x^2} \]

\[ \{T_0\} = \frac{KM}{S^2}, \{\rho_0\} = \frac{K}{M} \]

\[ \{T_0/\rho_0\} = \frac{M^2}{S^2}, c_0 = \sqrt{\frac{T_0}{\rho_0}} \]
\[ v = \sin \frac{n\pi x}{L} \cos \omega_n t \quad \omega_n = \frac{n\pi c_0}{L} \]

\[ \sin \omega_n t \]

waves \quad v_0 = F(x - c_0 t) + G(x + c_0 t)
Problem 4: Evaluating the danger from deflagration or explosion of gas
Presented by Mary Brewster

One of the most dramatic accidents resulting from a cryogenic fuel spill is the tragic explosion of liquefied petroleum gas (LPG) that occurred near Brenham, Texas on April 7, 1992. (LPG is a mixture of ethane and propane.) The New York Times reports

In the still morning air a substantial quantity of the gas is believed to have collected at the bottom of a small valley where it was ignited.... A seismograph at Rice University in Houston measured the blast at between 3.5 and 4 on the Richter scale, about the power of a small earthquake.

Explosions of this type require a mixture of combustible fuel and oxygen. How much of the fuel is burnt in premixed combustion depends on the equivalence ratio, $\phi$, which is proportional to the ratio of mole fractions of fuel and oxygen, and is equal to 1 when the mixture is stoichiometric. If a large amount of fuel is burnt in a partially-confined space, the rise in temperature causes an overpressure. The resulting shock wave was the primary cause of the casualties, (1 death, 13 injured) and property damage in the Brenham explosion.

Two significant factors that control the risk in such a situation are (1) the amount of heat that could be released by a combustion event, and (2) the probability that ignition will occur. If we suppose that ignition is uniformly likely in time, then an estimate of the risk is

$$ R = \int_0^\infty Q(t) \, dt $$

where $Q(t)$ is the potential heat release from premixed combustion at time $t$.

We assume at the initial time $t = 0$, a small valley is filled with a propane-air mixture at equivalence ratio $\phi_0$. Wind of constant speed $U$ blows across the top of the valley. Determine the sensitivity of the risk $R$ to the wind speed $U$ as a function of $\phi_0$. 
Bibliography

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Mathematics in Major Accident Risk Assessment, ed. by R.A. Cox, Clarendon Press, 1989,

and references therein.

Problem 5: Radionuclide contaminants in an aquifer
Presented by Donald Cohen

Disposing of radioactive waste by burial in remote regions assumes environmental stability for extremely long times during which the waste either decays to low (hopefully non-toxic or acceptable) levels or changes through a natural chemical chain to (again hopefully) harmless daughter elements. Half-lives of these processes are measured in tens, hundreds, or even thousands of years. Both percolation through soils and transport through aquifers are major pathways for introducing contaminants into the environment.

Even small changes in aquifer flow rate (and direction) can cause significant changes in the discharge and migration over long periods of time, and over periods of interest for high level waste there is no doubt that the groundwater flow rate will certainly undergo change. For example, even a relatively minor seismic incident such as a small offset fault can introduce groundwater into a disposal site where it will cause leaching from some small number of ruptured or devitrified containers. Normal seasonal fluctuations, periods of excessively dry or flood-like times, or even long term land development a considerable distance away will alter previously assumed stable situations. Clearly, it would be nice to have some reliable theoretical estimates of the effect of various changes on the amount of waste which enters the environment. We shall attempt to produce such estimates at first incorporating only the primary mechanisms of diffusion, transport, and radioactive or chemical decay. Perhaps, we can
progress to studying models incorporating additional physical and environmental mechanisms.

Problem 6: High temperature corrosion of alloys
Presented by Patrick Hagan

Modern engineering alloys are able to withstand corrosive environments at high temperatures due to their ability to form a continuous layer of a protective metal oxide at the alloy surface (a protective external oxide scale) which separates the metal from the harsh environment. Corrosive agents from the environment, such as carbon and oxygen, and metal atoms from the alloy can only diffuse very, very slowly through a protective metal oxide. Thus if an alloy forms a continuous layer of such an oxide, it will effectively protect the alloy from further corrosion. However, when an alloy is exposed to an oxidizing environment, it can oxidize in either of two modes. Under some conditions it will oxidize externally, and the metal oxide forms as a protective oxide layer on the alloys surface. Under other conditions it will oxidize internally, and the oxide forms as small particles dispersed within the alloy. If an alloy oxidizes internally, so that no protective scale is formed, then it will continue to corrode, and corrosive failure often ensues within a matter of minutes.

We need to develop a quantitative model for high-temperature oxidation of metal alloys. This model should

1. predict the conditions under which alloys oxidize internally, and under which they oxidize externally;
2. make experimentally testable predictions.

For simplicity we should start by considering only binary alloys, composed of metals A and B. We should also only consider environments in which only one of the metals (say, B) forms an oxide (say, BO).
Problem 7: Flame propagation  
Presented by A.K. Kapila

There are many contexts in which flame propagation under conditions of varying pressure is of importance; the internal combustion engine being but one example. Construct a one-dimensional, planar model of flame propagation in a closed container, and study, in particular, the effect of varying the volume of the vessel through motion of one of the end walls.

Notes from the oral presentation

In combustion the reactant concentration $Y$ becomes a product $P$; $Y$ satisfies a differential equation

$$
\mathcal{L}(Y) = -D Y e^{-E/RT}
$$

(*)

$$
= -D^* Y \exp \left[ \frac{E}{R} \left( \frac{1}{T^*} - \frac{1}{T} \right) \right]
$$

where $E$ is the activation energy, $D \approx O(1)$ and $\frac{E}{R} \gg 1$.

The case $T > T^*$ is called detonation and the case $T < T^*$ is called deflagration or flame.

When $T \sim T^*$ then the chemistry is significant.

The model (*) is called Arrhenius kinetics.
Problem 8: Filtration fluid dynamics
Presented by Donald Drew

The behavior of filter devices depends on the fluid and filtrant flowing in them, the porosity of the filter materials, and the geometry of the filter and the container. Often, the filter material is pleated so as to expose a large area to the flow. The problem is complicated by the change in efficiency of the filter as the filtrant clogs the filter. The proposed problem focuses on the fluid dynamics of the fluid flowing in the filter. If the pleats are such that the flow channel is narrow, and if the flow is sufficiently slow, the lubrication flow model can be used to describe the velocity field and the pressure. Flow through the filter can be described by assuming that the velocity through the filter is proportional to the pressure difference. Once expressions for the flow have been obtained, several practical questions can be addressed. Clogging can be described by assuming that the porosity is a function of the total flux through the filter, which is given as the time integral of the velocity. The shape of the pleat can be chosen to maximize the life of the filter, or to minimize the work done in filtering a certain amount of fluid.
Problem 9:  Analyze the dynamics of an irregular shaped die.
Presented by Joseph Keller

What is the probability distribution of the possible outcomes?

Problem 10:  Modeling automobile bumpers
Presented by Donald Drew

An automobile bumper is required to withstand a collision of 2.5 miles per hour with no damage to the bumper or the automobile. This is tested by hitting the bumper of an automobile, in neutral with the brakes released, with a pendulum having a mass equal to that of the automobile, released from such a height that its velocity at the impact point, at the bottom of the swing is 2.5 miles per hour. The first part of the modeling is to determine the response of the automobile-bumper-pendulum system, treating the bumper as a linear spring. Then the "spring constant" can be determined by analyzing the bumper as a beam. Then the bumper can be optimized subject to the constraint that it does not deform enough to sustain damage, and also does not deform enough to damage the automobile body.

Problem 11:  Flow improvements in hydrofractured reservoirs
Presented by Patrick Hagan

A common problem in the oil industry is the discovery of oil or gas in tight (low permeability) formations. This problem is often surmounted by hydrofracturing the well. In this process, the borehole is perforated along a vertical segment at the same depths as the gas bearing strata, and a fracturing fluid is pumped down the borehole at extremely high pressures. This high-pressure fluid fractures the formation, usually creating a (roughly) straight fracture centered at the borehole (see fig. 1a). The fracture is usually held open by "packers" -- sand or gravel that flows into the fracture along with the fluid. Typically the vertical extent of the fracture roughly matches the top and bottom of the gas bearing strata (see fig. 1b), that is, the top and bottom of the permeable layer. Although these fractures are very thin, usually no more than a few milimeters across, the permeability within the fractures is radically larger than the permeability of the surrounding formation.
Advances in hydrofracturing technique promise to yield wider, longer, and more permeable fracture. It appears possible to generate multiple fractures. Here we wish to know the payoff in terms of the increased productivity of the well.

Steady state

*Problem 1.* How does the productivity (flow rate per unit time through the borehole) change due to hydrofracturing? How does it depend on the width, length, and permeability of the fracture?

*Problem 2.* How does increasing the number of fractures change the productivity?

*Problem 3.* How does the productivity increase (due to hydrofracturing) if the rock surrounding the borehole has been severely damaged (*i.e.*, the permeability is drastically reduced near the borehole)?

Transient

*Problem 4.* Suppose we measure the pressure vs flowrate of the well. What parameters about the hydrofracturing can we determine from the measurement?
Problem 12: Motion of the thermobile
Presented by A. Kapila

The thermobile is a simple mechanical device, consisting of a Nitinol wire wrapped around a pair of pulleys. Nitinol is a Nickel-Titanium alloy, possessing a memory effect caused by a temperature-induced transition in its electronic structure. When deformed plastically at room temperature, the alloy retains its shape, but returns to its undeformed state when heated above the transition temperature.

When the "driver" pulley of the thermobile is dipped into hot water, a gentle tapping of the device sets the pulleys into motion. Construct a model for the operation of the device. Determine the maximum amount of mechanical energy that the wire is capable of delivering, and examine the efficiency of the heat-to-work conversion.
STUDENTS' REPORTS
Students' Report

# 1
A Model for Venous Blood Flow in the Legs

IMA Summer Program for Graduate Students Mathematical Modeling

Week 1, Group 1
August 3-7, 1992

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Section I: Introduction and Assumptions

Introduction

Blood flow through the veins in the leg is driven by the external pressure of muscles contracting. This pressure acts to collapse the vein, forcing the blood up the vein back towards the heart. When a person stands still, there is little contraction and valves are needed within the leg to prevent blood from rushing back down the length of the leg and “pooling” at the feet. This could be lethal within a matter of a few minutes or a few hours [2]. The average human being has fifteen valves in the leg to aid in circulation by preventing blood from going very far down the leg, so that even small muscle contractions are sufficient to maintain circulation. It is possible, however, for these valves to become damaged. The latest medical tools available are artificial valves that could be implanted in their place, and this model has been created to assist surgeons in determining how many valves should be implanted along a vein in the leg to attain an acceptable level of circulatory efficiency.

Assumptions

Due to the variety of variables involved and the time constraint of the seminar, assumptions had to be made involving various physical properties of this system, the leg. Probably the largest assumption is that we only need consider one-dimensional flow. This is reasonable since compared to the amount of blood moving up and down the leg, there is actually very little motion that is not parallel to the walls. Since we are looking at a vein, blood flow can be considered laminar and axisymmetric [1]. The flow of blood through the capillaries has damped out the pulses found in arteries. We shall also only consider the effects of contractions of the thigh and calf muscles since they are the largest muscles in the leg. A standard contraction will be parabolic in shape (smooth, even contraction) and we will leave the strength and length of contractions and time between contractions to be random, therefore including patients with differing levels of activity. We shall assume a maximum pressure value in the foot of 90 mmHg when a person is standing completely still and all valves are open [2]. For computing efficiency, pressure within the vein of 150 mmH2O will be considered optimal [1].

As a starting point, we assume that the defect lies in a single major vein which runs vertically through the length of the leg from the ankle to the hip. This vein is considered to be a collapsible tube which carries approximately a third of the blood out of the leg. We will assume a distribution of capillaries along the length of the leg, proportional to the muscle tissue mass. The local cross-sectional area of the vein is assumed to be a function of distance from the foot and time. Longitudinal uniformities in the vein wall are assumed to be such that a local “tube law” is applicable at each cross-section [4]. The particular form of the tube law that we use was motivated by experimental data and the requirement
that a zero transmural pressure difference corresponds to the neutral cross-sectional area. An additional assumption made was that the local cross-sectional area cannot exceed the neutral value by more than a factor of two.

To close off the system, one valve was placed below the ankle and one at the hip. The behaviour of each valve is independent of the others and we will assume there is no breakage. Each valve will be considered to be completely open or completely closed. Readings show the density of blood hardly varies, implying incompressibility. Due to the high shear rate within the blood flow, we will assume blood acts as a Newtonian fluid [5], so that the standard Navier-Stokes equations can be used.
Section II: Nomenclature

In order to model our problem of venous blood flow in the leg, we begin by modeling the rest state as a cylinder. We then introduce the following quantities:

- \(a_{\pm}\): Riemann invariants of the hyperbolic system.
- \(\tilde{A}(\tilde{z}, \tilde{t})\): cross-sectional area of the vein at height \(\tilde{z}\) and time \(\tilde{t}\). To be directly calculated from equations. Units cm\(^2\).
- \(A_0\): rest cross-sectional area of the vein, value \(\pi/4\) cm\(^2\).
- \(B\): matrix operator used in computer simulation.
- \(c_{\pm}\): eigenvalues of \(B\).
- \(F\): vector used in computer simulation.
- \(\tilde{g}_P(\tilde{\Phi}_{ext})\), \(\tilde{g}_d(\tilde{t}_d), \tilde{g}_\Delta(\Delta \tilde{t}_d)\): probability density functions used to determine argument parameters.
- \(\tilde{G}_P(\tilde{\Phi}_{ext})\), \(\tilde{G}_d(\tilde{t}_d), \tilde{G}_\Delta(\Delta \tilde{t}_d)\): probability mass functions used to determine argument parameters.
- \(k\): conversion factor used in dimensional tube law, value 1 mmHg.
- \(l\): length of the vein, value 100 cm.
- \(\tilde{p}(\tilde{z}, \tilde{t})\): internal pressure on venous wall caused by fluid dynamics inside vein. To be calculated directly from equations. Units g·cm/sec\(^2\).
- \(\tilde{p}_a\): ankle pressure (used for efficiency calculations), value 150 mmH\(_2\)O.
- \(\tilde{P}_{ext}(\tilde{z}, \tilde{t})\): external pressure on venous wall caused by muscular contraction. Units g·cm/sec\(^2\).
- \(\tilde{p}_h\): hip pressure boundary condition (needed for computational purposes), value 111 mmH\(_2\)O.
- \(\tilde{q}\): nonmuscular influx density of blood through capillaries. Units cm\(^2\)/sec.
- \(\tilde{Q}_c(\tilde{z})\): influx density of blood through capillaries. Units cm\(^2\)/sec. Given input function.
- \(\tilde{q}_f\): maximum amplitude of foot blood influx. Units cm\(^3\)/sec.
- \(\tilde{Q}_f(\tilde{t})\): influx of blood through valve at foot as a result of foot pumping action. Units cm\(^3\)/sec. Given input function.
- \(\tilde{Q}_r(\tilde{z})\): average influx density of blood, namely

\[
\frac{1}{l} \int_{0}^{l} \tilde{Q}_c(\tilde{z}) d\tilde{z}.
\]

- \(\tilde{r}\): radial measurement of vein interior. Units: cm.
- \(R\): rest radius of the vein, value 0.5 cm.
- \(\tilde{t}\): time. Units: sec.
- \(\tilde{t}_d\): duration of muscular compression. Units: sec.
- \(\tilde{t}_i\): time at which \(i\)th muscular compression begins. Units: sec.
\( \tilde{T}_i \): time at which \( i \)th foot input begins. Units: sec.
\( \bar{u}(\bar{z}, \bar{t}) \): averaged vertical velocity of blood at height \( \bar{z} \) and time \( \bar{t} \), namely

\[
\frac{1}{\bar{A}(\bar{z}, \bar{t})} \int_{\bar{A}(\bar{z}, \bar{t})} U(\bar{r}, \bar{z}, \bar{t}) \ d\bar{A}.
\]

\( \bar{U}(\bar{r}, \bar{z}, \bar{t}) \): vertical velocity of blood at radius \( \bar{r} \), height \( \bar{z} \) and time \( \bar{t} \).
\( x_\pm \): left eigenvectors of \( B \).
\( y \): vector of nondimensionalized area and velocity.
\( \bar{z} \): height above foot valve input level. Units: cm.
\( \bar{z}_i \): height above foot valve input level of ankle (\( i = 1 \)), top part of calf (\( i = 2 \)), lower part of thigh (\( i = 3 \)), and upper part of thigh (\( i = 4 \)). Units: cm.
\( \alpha \): nondimensional parameter used in equations:

\[
\alpha = \frac{lQ_r^2}{g A_0^2}.
\]

\( \beta \): nondimensional parameter used in equations:

\[
\beta = \frac{8\pi l Q_r \nu}{g A_0^2}.
\]

\( \gamma \): derivative of the nondimensional tube law with respect to nondimensionalized area.
\( \nu \): viscosity of blood, value 0.006 cm\(^2\)/sec.
\( \rho \): density of blood, value 1 g/cm\(^3\).

Nondimensionalized variables will have no tildes.
Section III: Governing Equations

The governing equations used are:

1. the tube law:

\[ \tilde{P}_{ext}(\tilde{z}, \tilde{t}) - \tilde{p}(\tilde{z}, \tilde{t}) = k \left( \frac{1}{A^{3/2}} - \frac{1}{2 - A} \right) \]

(3.1)

2. the conservation of mass (continuity equation):

flow in = increase in volume + flow out

(3.2)

3. the Navier-Stokes equation for an incompressible fluid with no bulk viscosity:

\[ \pi \frac{\partial \nu}{\partial \tilde{t}} + (\nu \cdot \nabla) \nu = -\frac{1}{\rho} \nabla \tilde{p} + \nu \nabla^2 \nu + g. \]

(3.3)

The conservation of mass on an infinitesimal slice is:

\[ \int_{\tilde{A}(\tilde{z}, \tilde{t})} U(\tilde{r}, \tilde{z}, \tilde{t}) \, d\tilde{A} + \tilde{Q}_c(\tilde{z}) \Delta \tilde{z} = \frac{\partial \tilde{A}(\tilde{z}, \tilde{t})}{\partial \tilde{t}} \Delta \tilde{z} + \int_{\tilde{A}(\tilde{z} + \Delta \tilde{z}, \tilde{t})} U(\tilde{r}, \tilde{z} + \Delta \tilde{z}, \tilde{t}) \, d\tilde{A}. \]

(3.4)

Dividing by \( \Delta \tilde{z} \) and letting \( \Delta \tilde{z} \) tend to zero yields

\[ \frac{\partial}{\partial \tilde{z}} \left[ \int_{\tilde{A}(\tilde{z}, \tilde{t})} U(\tilde{r}, \tilde{z}, \tilde{t}) \, d\tilde{A} \right] + \frac{\partial \tilde{A}}{\partial \tilde{t}} = \tilde{Q}_c(\tilde{z}) \]

and by the definition of \( \tilde{u} \) we get

\[ \frac{\partial (\tilde{A} \tilde{u})}{\partial \tilde{z}} + \frac{\partial \tilde{A}}{\partial \tilde{t}} = \tilde{Q}_c(\tilde{z}). \]

(3.5)

Assuming the velocity field has the form

\[ \nu = 0e_r + 0e_\theta + U(\tilde{r}, \tilde{z}, \tilde{t})e_{\tilde{z}} \]

the Navier-Stokes equation becomes

\[ \left( \frac{\partial \tilde{U}}{\partial \tilde{t}} + \tilde{U} \frac{\partial \tilde{U}}{\partial \tilde{z}} \right) = -\frac{1}{\rho} \frac{\partial \tilde{p}}{\partial \tilde{z}} + \nu \left[ \frac{1}{\tilde{r}} \frac{\partial}{\partial \tilde{r}} \left( \tilde{r} \frac{\partial \tilde{U}}{\partial \tilde{r}} \right) + \frac{\partial^2 \tilde{U}}{\partial \tilde{z}^2} \right] - g. \]

(3.6)
To eliminate the dependence of the solution on $\hat{r}$, we assume that the velocity profile at any time is not too different from that in a horizontal cylinder, e.g.,

$$\tilde{U}(\tilde{r}, \tilde{z}, \hat{t}) = 2 \left[ 1 - \left( \frac{\tilde{r}}{\tilde{R}} \right)^2 \right] \tilde{u}(\tilde{z}, \hat{t})$$

where the velocity profile has been normalized so that the “mean” velocity is $\tilde{u}(\tilde{z}, \hat{t})$ (see nomenclature). This estimate for a profile is rough and empirical data could provide a more accurate profile.

Using our parabolic profile, the Navier-Stokes equation becomes

$$2 \left[ 1 - \left( \frac{\tilde{r}}{\tilde{R}} \right)^2 \right] \left\{ \frac{\partial \tilde{u}}{\partial \hat{t}} + 2 \left[ 1 - \left( \frac{\tilde{r}}{\tilde{R}} \right)^2 \right] \frac{\partial \tilde{u}}{\partial \tilde{z}} \right\}$$

$$= -\frac{1}{\rho} \frac{\partial \tilde{p}}{\partial \tilde{z}} + \nu \left\{ -\frac{8}{\tilde{R}^2} \tilde{u} + 2 \left[ 1 - \left( \frac{\tilde{r}}{\tilde{R}} \right)^2 \right] \frac{\partial^2 \tilde{u}}{\partial \tilde{z}^2} \right\} - g.$$

Averaging the equation over the rest cross-sectional area, e.g. integrating over a disk of radius $\tilde{R}$ and dividing by $\pi \tilde{R}^2$, yields the final form of the Navier-Stokes equation:

$$\frac{\partial \tilde{u}}{\partial \hat{t}} + \frac{4}{3} \tilde{u} \frac{\partial \tilde{u}}{\partial \tilde{z}} = -\frac{1}{\rho} \frac{\partial \tilde{p}}{\partial \tilde{z}} - \frac{8}{\tilde{R}^2} \nu \tilde{u} + \nu \frac{\partial^2 \tilde{u}}{\partial \tilde{z}^2} - g. \quad (3.7)$$

Now we proceed to nondimensionalize our equations. To normalize $\tilde{z}$, we choose $l$, the length of our vein. To normalize $\tilde{u}$, we calculate the velocity of the fluid given only the capillary input, which we call $u_0$:

$$u_0 = \frac{1}{A_0} \int_0^l \tilde{Q}_c(\tilde{z}) \, d\tilde{z}.$$ 

Defining

$$Q_r = \frac{1}{l} \int_0^l \tilde{Q}_c(\tilde{z}) \, d\tilde{z},$$

which is the average value of $\tilde{Q}_c$ along the vein, we have

$$u_0 = \frac{l Q_r}{A_0}.$$

Since we are concerned with the velocity in the $\tilde{z}$-direction, we normalize $\hat{t}$ by $l/u_0$. We normalize $\tilde{A}$ by $A_0$, which is the area when the vein is at rest. Summarizing, we have the following:

$$z = \frac{\tilde{z}}{l}, \quad u(z, t) = \frac{\tilde{u}(\tilde{z}, \hat{t}) A_0}{l Q_r}, \quad t = \frac{\hat{t} Q_r}{A_0}, \quad A = \frac{\tilde{A}}{A_0}. \quad (3.8)$$
We normalize pressure by the maximum hydrostatic pressure of the vein with no valves:

$$P_{\text{ext}}(z,t) = \frac{\tilde{P}_{\text{ext}}(\tilde{z},\tilde{t})}{\rho g l}, \quad p(z,t) = \frac{\tilde{p}(\tilde{z},\tilde{t})}{\rho g l}$$

$$p_a = \frac{\tilde{p}_a}{\rho g l} = 0.15, \quad p_h = \frac{\tilde{p}_h}{\rho g l} = 0.11. \quad (3.9)$$

Now normalizing equation (3.5) gives us the following:

$$\frac{A_0 \cdot l Q_r}{A_0 \cdot l} \frac{\partial (Au)}{\partial z} + \frac{A_0 \cdot Q_r}{A_0} \frac{\partial A}{\partial t} = \dot{Q}_c(z)$$

$$\frac{\partial (Au)}{\partial z} + \frac{\partial A}{\partial t} = \frac{\dot{Q}_c(z)}{Q_r} \equiv Q_c(z). \quad (3.10)$$

Normalizing equation (3.7), we have

$$\frac{l Q_r \cdot Q_r}{A_0 \cdot A_0} \frac{\partial u}{\partial t} + \frac{4l^2 Q_r^2}{3A_0^2 l} \frac{\partial u}{\partial z} = \frac{\rho g l}{\rho l} \frac{\partial p}{\partial z} - \frac{8l Q_r \cdot \pi}{A_0 \cdot A_0} \nu u + \frac{\nu l Q_r}{A_0 \cdot l^2} \frac{\partial^2 u}{\partial z^2} - g$$

$$\alpha \left( \frac{\partial u}{\partial t} + \frac{4}{3} \frac{\partial u}{\partial z} \right) = - \frac{\partial p}{\partial z} - \beta u + \frac{\nu Q_r}{g l A_0} \frac{\partial^2 u}{\partial z^2} - 1, \quad (3.11)$$

where $\alpha$ and $\beta$ are defined in the nomenclature. Lastly, normalizing the "tube law:"

$$P_{\text{ext}}(z,t) - p(z,t) = \frac{(1.3332 \times 10^3 g)}{\rho g l \cdot \text{cm} \cdot \text{sec}^2} \left( \frac{1}{A^{3/2}} - \frac{1}{2 - A} \right)$$

$$P_{\text{ext}}(z,t) - p(z,t) = 1.36 \times 10^{-2} \left( \frac{1}{A^{3/2}} - \frac{1}{2 - A} \right). \quad (3.12)$$

We set our boundaries as follows:

- $z = 0$: valve at foot
- $0 < z < z_1$: no contraction of muscle (foot to ankle)
- $z_1 < z < z_2$: contraction possible from calf muscle
- $z_2 < z < z_3$: no contraction of muscle (knee)
- $z_3 < z < z_4$: contraction possible from thigh muscle
- $z_4 < z < 1$: no contraction of muscle (above thigh)
- $z = 1$: valve at thigh.
Section IV: Input

In order to continue our analysis further, we must determine the input functions $\tilde{P}_{\text{ext}}$, $\tilde{Q}_f$, and $\tilde{Q}_c$. In addition, we must determine the $\tilde{z}_i$. Taking measurements from an average person, we have

\[ \tilde{z}_1 = 8 \text{ cm}, \quad \tilde{z}_2 = 40 \text{ cm}, \quad \tilde{z}_3 = 54 \text{ cm}, \quad \tilde{z}_4 = 92 \text{ cm}. \]

Normalizing by $l$, we immediately have the following:

\[ z_1 = 0.08, \quad z_2 = 0.4, \quad z_3 = 0.54, \quad z_4 = 0.92. \]  \hspace{1cm} (4.1)

First we consider $Q_r$. We have found that the aorta, which has an area of 2.5 cm\(^2\), pumps blood at the rate of 33 cm/sec. Since all blood passes through the aorta, we then have a flux rate for the entire of the system. We estimate that 1/6 of the total blood is found in the leg, and that 10% of that amount is in the foot. Hence, we have a flux rate for the leg.

\[ \frac{2.5 \text{ cm}^2 \cdot 33 \text{ cm} \cdot 90\%}{\text{sec} \cdot 6} = 12.4 \text{ cm}^3/\text{sec} \]

We assume a system of three veins traversing the entire leg. We assume the blood flows into them equally, so to find our average density, we divide by the length of the leg to find

\[ Q_r = \frac{12.4 \text{ cm}^3}{100 \text{ cm} \cdot 3} = 4.12 \times 10^{-2} \text{ cm}^2/\text{sec}. \]

Hence we have $Q_r/A_0 = 5.25 \times 10^{-2} \text{ sec}^{-1}$.

Next we consider $\tilde{P}_{\text{ext}}$. Since the muscle tissue is approximately quadratically distributed throughout the muscle, we assume that the pressure exerted by the muscle is quadratically distributed in space. Also, we assume that the pressure is quadratically distributed in time as well, since it does take some "warm-up" and "cool-down" time for the muscle. Hence, we have the following model:

\[ \tilde{P}_{\text{ext}} = \frac{16|P_{\text{ext}}|}{l_d^2(\tilde{z}_i - \tilde{z}_{i+1})^2(\tilde{z} - \tilde{z}_i)(\tilde{z}_i+1 - \tilde{z})(\tilde{t} - \tilde{t}_j)(\tilde{t}_j + \tilde{t}_d - \tilde{t})}, \quad \tilde{z}_i < \tilde{z} < \tilde{z}_{i+1}, \quad \tilde{t}_j < \tilde{t} < \tilde{t}_j + \tilde{t}_d. \]

Here $i = 1$ or 3, and $j = 1, 2, 3, \ldots$. Note that the peak value of this function comes at the middle of the muscle halfway through the duration $\tilde{t}_d$, and has value $|\tilde{P}_{\text{ext}}|$. Note also that since all of our length and time measurements appear in ratios, we may immediately nondimensionalize with only our pressure nondimensionalization, which yields the following:

\[ P_{\text{ext}} = \frac{16|P_{\text{ext}}|}{l_d^2(z_i - z_{i+1})^2(z - z_i)(z_{i+1} - z)(t - t_j)(t_j + t_d - t)}, \quad z_i < z < z_{i+1}, \quad t_j < t < t_j + t_d, \]  \hspace{1cm} (4.2)
where $|P_{\text{ext}}| = |\tilde{P}_{\text{ext}}|/\rho gl$.

Now we must determine the other parameters in the equation. We are given in [5] that pressures in the muscle over 200 mmHg are common. We assume that the thigh and calf muscles work independently. We want no negative pressures exerted and we want maximal pressures of no more than 400 mmHg, so we assume a pressure amplitude probability density distribution of the following form:

$$g_P(|\tilde{P}_{\text{ext}}|) = \frac{6|\tilde{P}_{\text{ext}}|(400 \text{ mmHg} - |\tilde{P}_{\text{ext}}|)}{(400 \text{ mmHg})^3}, \quad 0 \text{ mmHg} < |\tilde{P}_{\text{ext}}| < 400 \text{ mmHg}.$$

Note the above has a maximum at 200 mmHg. For the computer implementation, it will be more helpful to have the probability mass function, which is

$$\tilde{G}_P(|\tilde{P}_{\text{ext}}|) = \frac{2|\tilde{P}_{\text{ext}}|^2(600 \text{ mmHg} - |\tilde{P}_{\text{ext}}|)}{(400 \text{ mmHg})^3}, \quad 0 \text{ mmHg} < |\tilde{P}_{\text{ext}}| < 400 \text{ mmHg}.$$

Nondimensionalizing, we have the following:

$$G_a(|P_{\text{ext}}|) = 1.25 \times 10^{-2}|P_{\text{ext}}|^2(8.15 - |P_{\text{ext}}|), \quad 0 < |P_{\text{ext}}| < 5.43. \quad (4.3)$$

For the probability functions that determine our input conditions, we select a random number from between 0 and 1. This is the value of the probability mass function, since we are drawing from a uniform distribution. We then set our equations corresponding to the probability mass function for the desired quantity equal to our random number. We use Newton’s method to solve for the root.

Next we work on the actual duration of the compression, $\tilde{t}_d$. We assume that the average compression can take no less than 0.5 sec, and probably averages around 8 sec. Hence, we assume the following exponential distribution:

$$g_d(\tilde{t}_d) = \frac{\tilde{t}_d - 0.5 \text{ sec}}{(7.5 \text{ sec})^2} \exp \left( -\frac{\tilde{t}_d - 0.5 \text{ sec}}{7.5 \text{ sec}} \right), \quad \tilde{t}_d > 0.5 \text{ sec}.$$ 

Once again, we find the probability mass function:

$$\tilde{G}_d(\tilde{t}_d) = 1 - \frac{\tilde{t}_d + 7 \text{ sec}}{7.5 \text{ sec}} \exp \left( -\frac{\tilde{t}_d - 0.5 \text{ sec}}{7.5 \text{ sec}} \right), \quad \tilde{t}_d > 0.5 \text{ sec}.$$

Nondimensionalizing, we have the following:

$$G_d(t_d) = 1 - \frac{t_d + 3.68 \times 10^{-1}}{3.94 \times 10^{-1}} \exp \left( -\frac{t_d - 2.62 \times 10^{-2}}{3.94 \times 10^{-1}} \right), \quad t_d > 2.62 \times 10^{-2}. \quad (4.4)$$

For the duration between the compressions $\Delta \tilde{t}_j \equiv \tilde{t}_j - \tilde{t}_{j-1}$, we assume that it takes at least 1 second for the body to recover. Once again we assume a mean of 8 seconds,
which comes from the model of someone slowly shifting from leg to leg. Hence we once again use an exponential distribution:

\[ \tilde{g}_\Delta(\Delta \tilde{t}_j) = \frac{\Delta \tilde{t}_j - 1 \text{ sec}}{49 \text{ sec}^2} \exp \left( -\frac{\Delta \tilde{t}_j - 1 \text{ sec}}{7 \text{ sec}} \right), \quad \Delta \tilde{t}_j > 1. \]

Once again we find the probability mass function, which is

\[ \tilde{G}_\Delta(\Delta \tilde{t}_j) = 1 - \frac{\Delta \tilde{t}_j + 6 \text{ sec}}{7 \text{ sec}} \exp \left( -\frac{\Delta \tilde{t}_j - 1 \text{ sec}}{7 \text{ sec}} \right), \quad \Delta \tilde{t}_j > 1. \]

Nondimensionalizing, we have

\[ G_\Delta(\Delta t_j) = 1 - \frac{\Delta t_j + 6.15 \times 10^{-1}}{3.68 \times 10^{-1}} \exp \left( -\frac{\Delta t_j - 5.25 \times 10^{-2}}{3.68 \times 10^{-1}} \right), \quad \Delta t_j > 5.25 \times 10^{-2}. \]  

(4.5)

Next we work with \( \tilde{Q}_c(\tilde{z}) \). We postulate that there is some sort of steady capillary flow in the entire leg. We assume that the muscles exert more force in the center in some sort of quadratic fashion (see below), so since capillaries flow to muscle tissue, we should expect some sort of quadratic function rising from that steady flow. Since the surface area of the thigh is approximately 3 times that of the calf, we expect that the peak flow in the thigh will be 3 times that of the peak flow in the calf, which we postulate to be about 10 times that of the non-muscular areas.

Using this approach, we see that we have the following problems to consider. Letting \( \tilde{q} \) be the nonmuscular capillary flow, we have the following equation:

\[ \tilde{q}l + \int_{\tilde{z}_1}^{\tilde{z}_2} \frac{36\tilde{q}(\tilde{z} - \tilde{z}_1)(\tilde{z}_2 - \tilde{z})}{(\tilde{z}_1 - \tilde{z}_2)^2} \, d\tilde{z} + \int_{\tilde{z}_3}^{\tilde{z}_4} \frac{116\tilde{q}(\tilde{z} - \tilde{z}_3)(\tilde{z}_4 - \tilde{z})}{(\tilde{z}_3 - \tilde{z}_4)^2} \, d\tilde{z} = Q_r l. \]

Nondimensionalizing immediately, we have that

\[ 1 + 6(z_2 - z_1) + \frac{58(z_4 - z_3)}{3} = \frac{Q_r}{\tilde{q}}. \]

Using our numbers, we have

\[ \frac{\tilde{q}}{Q_r} = \frac{1}{10.27} = 9.74 \times 10^{-2}. \]

This is our nondimensionalized basic flux rate. Hence, we have the following functional form for the normalized flux density \( Q_c(z) \):

\[ Q_c(z) = \begin{cases} 
9.74 \times 10^{-2}, & 0 \leq z \leq 0.08 \\
9.74 \times 10^{-2} + 34.24(z - 0.08)(0.40 - z), & 0.08 \leq z \leq 0.40 \\
9.74 \times 10^{-2}, & 0.40 \leq z \leq 0.54 \\
9.74 \times 10^{-2} + 78.25(z - 0.54)(0.92 - z), & 0.54 \leq z \leq 0.92 \\
9.74 \times 10^{-2}, & 0.92 \leq z \leq 1.
\end{cases} \]  

(4.6)
Lastly, we work with $Q_f(t)$. Using the arguments above when we found $Q_r$, we have a flow rate into the foot:

$$\frac{2.5 \text{ cm}^2 \cdot 33 \text{ cm} \cdot 10\%}{\text{sec} \cdot 6} = 1.38 \text{ cm}^3/\text{sec}.$$ 

We consider the foot to be a reservoir from which we can always siphon a small fraction of its blood. We assume average spacing of 8 seconds between steps to get an average volume of blood that should be pumped out of the foot in one step. Now, there are 3 veins, so we have

$$\frac{1.38 \text{ cm}^3 \cdot 8}{\text{sec} \cdot 3} = 3.67 \text{ cm}^3.$$ 

We hypothesize that an average step lasts for approximately 1/2 second. We also postulate a parabolic shape for the rate. Hence, letting $\ddot{q}_f$ be some constant, we require that

$$\int_0^{0.5 \text{ sec}} \frac{16\ddot{q}_f \ddot{t}(0.5 \text{ sec} - \ddot{t})}{\text{sec}^2} = 3.67 \text{ cm}^3$$

Using our normalization, we have

$$\frac{\ddot{q}_f \cdot \text{sec}}{3lQ_r} = \frac{3.67 \text{ cm}^3 \cdot \text{sec}}{1.236 \times 10^{-1} \text{ cm}^2 \cdot 100 \text{ cm}}$$

$$\frac{\ddot{q}_f}{lQ_r} = 0.297.$$ 

This once again gives our normalized flow rate. Then our normalized function becomes the following:

$$Q_f(t) = 4.75(t - T_i)(0.5 + T_i - t), \quad (4.7)$$

where $T_i \ (i = 1, 2, 3, \ldots)$ is the start time of the $i$th pump. To model the $\Delta T_i$, we use the same function as for the $\Delta t_i$, since we are assuming shifting from leg to leg, which would not change the lag time. Hence we have

$$G_T(\Delta T_i) = 1 - \frac{\Delta T_i + 3.15 \times 10^{-1}}{3.68 \times 10^{-1}} \exp\left(-\frac{\Delta T_i - 5.25 \times 10^{-2}}{3.68 \times 10^{-1}}\right), \quad \Delta T_i > 5.25 \times 10^{-2}. \quad (4.8)$$

Now that we have calculated our parameters, we may actually attach values to equation (3.11). Doing so, we have the following:

$$\frac{100 \text{ cm} \cdot (4.12 \times 10^{-2} \text{ cm}^2)^2 \cdot \text{sec}^2 \cdot 256}{981 \text{ cm} \cdot \pi^4 \text{cm}^4} \left(\frac{\partial u}{\partial t} + \frac{4}{3}u \frac{\partial u}{\partial z}\right) = -\frac{\partial p}{\partial z}$$

$$- \frac{8\pi \cdot 100 \text{ cm} \cdot 4.12 \times 10^{-2} \text{ cm}^2 \cdot 6 \times 10^{-3} \text{ cm}^2 \cdot \text{sec}^2 \cdot 256}{981 \text{ cm} \cdot \pi^4 \text{ cm}^4} u + \frac{6 \times 10^{-3} \text{ cm}^2 \cdot 4.12 \times 10^{-2} \text{ cm}^2 \cdot 16 \frac{\partial^2 u}{\partial z^2} - 1}{981 \text{ cm} \cdot 100 \text{ cm} \cdot \pi^2 \text{ cm}^2}$$
\[ 4.55 \times 10^{-4} \left( \frac{\partial u}{\partial t} + \frac{4}{3} u \frac{\partial u}{\partial z} \right) = -\frac{\partial p}{\partial z} - 1.66 \times 10^{-3} u + 4.09 \times 10^{-9} \frac{\partial^2 u}{\partial z^2} - 1. \quad (4.9) \]

As a first guess, we consider the diffusive term in equation (4.9) to be insignificant, so we have the following equation:

\[ 4.55 \times 10^{-4} \left( \frac{\partial u}{\partial t} + \frac{4}{3} u \frac{\partial u}{\partial z} \right) = -\frac{\partial p}{\partial z} - 1.66 \times 10^{-3} u - 1. \quad (4.10) \]

The system of three equations [(3.10), (3.12), and (4.10)] with their attendant input functions is what we are trying to solve.

Lastly, we have the conditions at the valves. If a valve is closed, trivially \( u = 0 \) above and below it. This is in essence two conditions. If a valve is open, both \( u \) and \( P \) must be continuous across it. Once again, we have two conditions.

To determine if an open valve should be closed, we check the value of \( u \) at the valve. If it is less than 0, we close the valve, since we want no backflow. To determine if a closed valve should be opened, we check the pressure below and above the valve. If the pressure below the valve is greater than the pressure above the valve, then we open it.
Probability Density Function
for Amplitude of Compression Wave
(Peak is at 200 mmHg)
Probability Density Function for Duration of Muscle Compressions (Peak is at 8 sec)
Probability Density Function
for Waiting Times Between Muscle
Compressions and Foot-Pump Inputs
(Peak is at 8 sec)
Section V: Computer Simulation

The Characteristic Method

In order to solve our problem numerically, we use the characteristic method [6]. First we replace \( p \) in equation (3.11) using the tube law (3.12) and divide the whole equation by \( \alpha \). Then, neglecting our diffusive term and letting \( y = (A, u) \), our system becomes

\[
\frac{\partial y}{\partial t} + B \frac{\partial y}{\partial z} + F = 0, \text{ where}
\]

\[
B = \begin{bmatrix} u & A \\ \gamma/\alpha & 4u/3 \end{bmatrix}, \quad F = \begin{bmatrix} -Q_e(z) \\ (\partial P_{ext}/\partial z + \beta u + 1)/\alpha \end{bmatrix}, \text{ and}
\]

\[
\gamma = k \left( \frac{3}{2A^{5/2}} + \frac{1}{(2 - A)^2} \right). \tag{5.2b}
\]

Since our system is hyperbolic, \( B \) has two real eigenvalues \( c_+ \) and \( c_- \), given by

\[
c_{\pm} = \frac{7u}{6} \pm \frac{1}{2} \sqrt{\frac{u^2}{9} + \frac{4A\gamma}{\alpha}} \tag{5.3}
\]

with their corresponding left eigenvectors \( x_{\pm} \). Then the Riemann invariants \( a_{\pm} = \langle x_{\pm}, y \rangle \) are given by

\[
\frac{da_{\pm}}{dt} + \langle x_{\pm}, F \rangle = 0 \text{ on } \frac{dz}{dt} = c_{\pm}, \tag{5.4}
\]

where \(|c_{\pm}|\) is the local "speed of sound."

The leg (z-axis) is subdivided into equal segments. Values are calculated on a grid subdividing each segment. The characteristic method is used to calculate boundary conditions at the valves.

Computing Algorithm

1. Assume we know \( u, A, \) and \( p \) everywhere.
2. For each open valve, if \( u < 0 \) at the valve, then close it. For each closed valve, if \( p_{\text{below}} > p_{\text{above}} \), open it.
3. Use conservative central differencing in space and explicit Euler in time to update all interior points. An open valve is considered to be an interior point.
4. Use characteristic relations and the boundary condition \( u = 0 \) to update values at the closed valves.
5. For the boundary condition at the foot, if there is no flux, we use \( u = 0 \). If there is a flux, we use the characteristic relations and \( uA = Q_f \).
6. For the boundary condition at the hip, if the valve is closed, we have $u = 0$, so we can calculate $A$ (from the characteristic relations). Otherwise, the pressure is $p_h$, and we may calculate $u$. From the tube law, we calculate $A$, and from the characteristic relations we obtain $u$.

7. Compute $p$ everywhere using the tube law.

8. Go to line 1.
Random Input Generated by Computer Simulation for Normalized Thigh Pressure
Random Input Generated by Computer Simulation for Foot Pump Flux
Section VI: Future Research

There are many areas that could be further explored to attain a more accurate model. The assumption of one-dimensional flow could be expanded to include two or three dimensions. Also, the major veins in the legs are branched together, which needs to be taken into account. Shear rates vary, making it important to consider blood as a non-Newtonian fluid. The values inputed and assumed for maxima and minima are average numbers for an average person, and can vary greatly depending on the individual's health, age, and other factors. There is also wave propagation and possible blood turbulence that will appear in more than one dimension. A more accurate version of the tube law could also be employed for the specific case being considered [3,4].
Section VII: References


Students' Report
#2
IMA Summer Program for Graduate Students

Mathematical Modeling

Positioning of a Power Plant

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1 FORMULATION OF PROBLEM

1 Formulation of Problem

The Northern States Power Company wants to build a 1000 MW power station on the Mississippi river at Minneapolis taking 25 m$^3$/s water from the river and using a direct cooling system. This will mean that the water is taken out of the river at some point and will be put back in at some other point at a higher temperature.

What effects will this have on the flow and temperature distributions in the river?

2 Aspects of Modeling

Pretending, as we will do, that nothing is actually known at all about the problem at hand the first thing we have to do is to consider what effects and what quantities have to be taken into account, i.e. we have to write down what we think might pertain to the problem. Some of those quantities and effects are:

- total flow in river
- proportion of flow taken out
- heat transport (by fluid flow (advection), by molecular interaction (diffusion), due to buoyancy forces, due to turbulence)
- existing temperature distribution (sunshine, snow, rain, ice, air temperature, other heat sources, water clarity)
- conduction to earth
- evaporation
- river shape/profile

At this point it is then quite clear that we will have to tidy up. One particular aspect in deciding which effects to take into account is the different timescales these effects make themselves felt in. Obviously we are not interested in variations in heat conduction to earth, since those come into effect in the scale of years and certainly not in minutes, which we think will be the timescale we are looking at. These considerations finally lead to assumptions as to what we should be looking at.

As the problem is posed in section 1, it is much too difficult to deal with directly. Thus, we must make some simplifying assumptions and reduce the main problem to various subproblems. Since the profile and shape of a river is very complicated, we will first start out by assuming that the river is an ideal channel. We will consider the subproblem of modeling fluid flow down an ideal channel by using the Navier-Stokes equations and after several assumptions, reducing these equations to the shallow water equations. We will then consider the problem of modeling fluid flow where intake and outflow pipes are added to our channel. Finally, we will model fluid flow where heat is added to our system.
3 Derivation of the Shallow Water Equations

We start out considering a subproblem, namely fluid flow in an ideal channel which is $L = 10km$ in length and with a depth of $H = 10m$ and a width of $W = 100m$.

We will assume that the water is pure and that it will have constant density $\rho$. Since we will be looking at fluid flow, we will be interested in Eulerian coordinates, i.e. at each point in space and time we will try to find a velocity vector $\mathbf{u}(x, y, z, t)$ and the pressure $p(x, y, z, t)$, thus describing fluid flow. At this point we assume further that there is a uniform distribution across the river, so that we need not consider the $z$ direction. Therefore, let

$$\mathbf{u}(x, y, t) = (u(x, y, t), v(x, y, t))$$

denote the velocity of the water and $p(x, y, t)$ the pressure. Then, conservation of mass states that

$$\frac{\partial \rho}{\partial t} = -\nabla \cdot (\rho \mathbf{u}),$$

which, since $\rho$ is constant, reduces to

$$\nabla \cdot (\mathbf{u}) = \frac{\partial u}{\partial x} + \frac{\partial v}{\partial y} = 0.$$  

We can derive further equations from the principle of conservation of momentum. This principle can in our case be written in the following form:

$$\frac{\partial \mathbf{u}}{\partial t} + (\mathbf{u} \cdot \nabla) \mathbf{u} = -\nabla \left( \frac{p}{\rho} \right) + \nu \nabla^2 \mathbf{u} + \mathbf{F},$$

where we have summarized various forces such as gravity in $\mathbf{F}$ and $\nu$ denotes kinematic viscosity. Thus, we arrive at the following system of partial differential equations:

$$\frac{\partial u}{\partial t} + u \frac{\partial u}{\partial x} + v \frac{\partial u}{\partial y} = -\frac{\partial (p/\rho)}{\partial x} + \nu \left( \frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2} \right)$$

$$\frac{\partial v}{\partial t} + u \frac{\partial v}{\partial x} + v \frac{\partial v}{\partial y} = -\frac{\partial (p/\rho)}{\partial y} + \nu \left( \frac{\partial^2 v}{\partial x^2} + \frac{\partial^2 v}{\partial y^2} \right) - g$$
The above equations are known as the Navier-Stokes equations. These will govern our problem in the bulk of the river. However, we will now have to consider boundary conditions.

Let

\[ y = \eta(x, t) \quad (f(x, y, t) = 0) \]

describe the height of the river

Then, the boundary conditions are:

\[
\begin{align*}
\frac{\partial u}{\partial t} + u \cdot \nabla f &= 0 \\
\frac{\partial f}{\partial t} + (u \cdot \nabla)f &= 0 \\
\nabla(u \cdot \tau) \cdot n &= 0 \quad \text{on} \quad y = \eta,
\end{align*}
\]

where \( \tau \) is the tangent vector, and \( n \) is the normal vector to \( y = \eta(x, t) \). The condition on the bottom of the river \((y = 0)\) is called the no-slip condition, the first condition on the surface \((y = \eta)\) is the so-called kinematic condition. This latter condition simplifies to

\[
\frac{\partial \eta}{\partial t} + u \frac{\partial \eta}{\partial x} - v = 0
\]

At this point it is worth noting that we are dealing with a free boundary problem and that we have fully posed the subproblem in physical variables that do have dimensions associated with them. This is generally not a very good idea, since in that manner we would be dealing with quantities of all kinds of magnitude. In order to avoid this, the first step therefore is to nondimensionalize our equations. Let

\[
\begin{align*}
U &= \hat{U} \\
\eta &= H \hat{\eta} \\
y &= H \hat{y} \\
x &= L \hat{x} \\
t &= T \hat{t} \\
p &= p_{\text{air}} + (\rho g H) \hat{p} \\
v &= \left( \frac{H \hat{U}}{L} \right) \hat{v}
\end{align*}
\]

With this change of variables in dimensionless form the Navier-Stokes equations become (where we resort to writing the variables without a bar again, keeping in mind that \( u(x, y, t) \) should really be \( \hat{u}(\hat{x}, \hat{y}, \hat{t}) \)):

\[
\begin{align*}
\frac{\partial u}{\partial t} + \frac{u \cdot \nabla u}{x} + \frac{\partial v}{\partial y} &= 0 \\
\frac{\partial u}{\partial t} + \frac{U}{L} \left( \frac{\partial u}{\partial x} + \frac{\partial v}{\partial y} \right) &= -gH \frac{\partial p}{\partial x} + \frac{\nu T}{H^2} \left( \frac{H}{L} \right)^2 \left( \frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2} \right) \\
\frac{\partial u}{\partial t} + \frac{H U \nu}{g L T} \left( \frac{\partial u}{\partial x} + \frac{\partial v}{\partial y} \right) &= -\frac{\partial p}{\partial y} - 1 + \frac{\nu U}{g L H} \left( \frac{H}{L} \right)^2 \left( \frac{\partial^2 v}{\partial x^2} + \frac{\partial^2 v}{\partial y^2} \right)
\end{align*}
\]
For the boundary conditions we find:

\[
\begin{aligned}
&u = 0, \quad v = 0 \quad \text{on} \quad y = 0 \\
&\frac{L}{UT} \frac{\partial \eta}{\partial t} + u \frac{\partial \eta}{\partial x} - v = 0 \\
&p = 0 \quad \text{on} \quad y = \eta \\
&- \left( \frac{H}{L} \right)^2 \frac{\partial u}{\partial x} \frac{\partial \eta}{\partial x} - \left( \frac{H}{L} \right)^4 \frac{\partial v}{\partial x} \left( \frac{\partial \eta}{\partial x} \right)^2 - \left( \frac{H}{L} \right)^4 v \frac{\partial^2 \eta}{\partial x^2} \frac{\partial \eta}{\partial x} + \frac{\partial u}{\partial y} + \left( \frac{H}{L} \right)^2 \frac{\partial v}{\partial y} \frac{\partial \eta}{\partial x} = 0
\end{aligned}
\]

Now let

\[
\frac{TU}{L} = \frac{gHT}{LU}
\]

which will make \( U \) the natural speed at which waves propagate. Then we find

\[
U = \sqrt{gH} \approx 10\text{m/s}.
\]

Also, let

\[
T = \frac{L}{U} = \frac{L}{\sqrt{gH}} \approx 17\text{min},
\]

so that \( T \) becomes the transit time, i.e. the time it would take a particle travelling at speed \( U \) to go through a portion of length \( L \) of the channel. Then we have

\[
\frac{TU}{L} = \frac{gHT}{LU} = 1.
\]

Other than that we have

\[
\frac{\nu T}{H^2} \ll 1, \quad \frac{HU}{gLT} \ll 1, \quad \frac{\nu U}{gL} \ll 1, \quad \frac{H}{L} \ll 1,
\]

since \( \nu \approx 10^{-6}\text{m}^2/\text{s} \).

Taking these magnitudes into consideration we will deal with the following set of equations:

\[
\begin{aligned}
(3.1) \quad &\frac{\partial u}{\partial x} + \frac{\partial v}{\partial y} = 0 \\
(3.2) \quad &\frac{\partial u}{\partial t} + u \frac{\partial u}{\partial x} + v \frac{\partial u}{\partial y} = -\frac{\partial p}{\partial x} \quad \text{and} \quad \frac{\partial p}{\partial y} + 1 = 0 \\
(3.3) \quad &\frac{\partial \eta}{\partial t} + u \frac{\partial \eta}{\partial x} - v = 0 \\
&\quad p = 0 \quad \text{on} \quad y = \eta.
\end{aligned}
\]

Since we have

\[
\frac{gLH}{\nu U} \gg 1 \quad \text{and} \quad \frac{H}{L} \ll 1,
\]

this can be considered a shallow water problem, since the depth \( H \) is small compared to the lateral scale \( L \), or, to put it in another way, the aspect ratio \( \frac{H}{L} \) is small.
3 DERIVATION OF THE SHALLOW WATER EQUATIONS

As it is, the problem is now overprescribed. Therefore, making some further simplifying assumptions, we will no longer impose the no-slip condition on the bottom, so that we can disregard boundary layer theory and we will also think of our fluid as being inviscid. By doing this we do not consider the conditions

\[ u = 0 \text{ at } y = 0 \quad \text{and} \quad \frac{\partial u}{\partial y} = 0 \text{ at } y = \eta. \]

Now,

\[ \frac{\partial p}{\partial y} + 1 = 0 \quad \Rightarrow \quad p = -y + \eta(x, t), \]

so we will assume that the pressure depends solely on the height in the water. Since

\[ \frac{\partial p}{\partial x} = \frac{\partial \eta}{\partial x}, \]

equation (3.2) becomes

\[ \frac{\partial u}{\partial t} + u \frac{\partial u}{\partial x} + v \frac{\partial u}{\partial y} = -\frac{\partial \eta}{\partial x}. \]  

(3.4)

From equation (3.1), we get

\[ v = - \int_0^y \frac{\partial u}{\partial x} \, dy + g(x, t), \]

and by applying the boundary condition \( v = 0 \text{ at } y = 0 \), we obtain

\[ v = - \int_0^y \frac{\partial u}{\partial x} \, dy. \]

Substituting the above \( v \) into equation (3.4), we obtain

\[ \frac{\partial u}{\partial t} + u \frac{\partial u}{\partial x} - \frac{\partial u}{\partial y} \int_0^y \frac{\partial u}{\partial x} \, dy = -\frac{\partial \eta}{\partial x}. \]

Also, boundary condition (3.3) becomes

\[ \frac{\partial \eta}{\partial t} + u \frac{\partial \eta}{\partial x} + \int_0^\eta \frac{\partial u}{\partial x} \, dy = 0 \quad \text{on} \quad y = \eta. \]

Thus we end up with

\[ \frac{\partial u}{\partial t} + u \frac{\partial u}{\partial x} - \frac{\partial u}{\partial y} \int_0^y \frac{\partial u}{\partial x} \, dy = -\frac{\partial \eta}{\partial x}, \]

\[ \frac{\partial \eta}{\partial t} + u \frac{\partial \eta}{\partial x} + \int_0^\eta \frac{\partial u}{\partial x} \, dy = 0 \quad \text{on} \quad y = \eta. \]

We will now assume that we are dealing with plug flow; i.e. we assume \( u \) to be independent of \( y \) at all times, so that \( u(x, y, t) = u(x, t) \). Then the last set of equations reduces to

\[ \frac{\partial u}{\partial t} + u \frac{\partial u}{\partial x} = -\frac{\partial \eta}{\partial x}, \]

\[ \frac{\partial \eta}{\partial t} + u \frac{\partial \eta}{\partial x} + \frac{\partial u}{\partial x} = 0. \]
These equations are the actual shallow water equations. Note that these form a hyperbolic system of nonlinear partial differential equations. So, we have now reduced our initial problem, which was a free boundary problem to a kind of problem we might have some hope to be able to treat.

We will use the above equations in the next analysis where we add the input and outflow pipes.

Now, assuming a steady state,

\[
\frac{\partial u}{\partial x} + \frac{\partial \eta}{\partial x} = 0
\]

\[
\frac{\partial \eta}{\partial x} + u \frac{\partial u}{\partial x} = 0
\]

Thus \( u \) and \( \eta \) will be constants.

For the shallow water equations we perform a perturbation analysis and set

\[
u(x, t) = u_0 + \epsilon \tilde{u}(x, t) \]

\[
\eta(x, t) = \eta_0 + \epsilon \tilde{\eta}(x, t)
\]

Plugging these into the shallow water equations (not in the steady-state), results in

\[
\frac{\partial \tilde{u}}{\partial t} + u_0 \frac{\partial \tilde{u}}{\partial x} = -\frac{\partial \tilde{\eta}}{\partial x}
\]

\[
\frac{\partial \tilde{\eta}}{\partial t} + u_0 \frac{\partial \tilde{\eta}}{\partial x} + \eta_0 \frac{\partial \tilde{u}}{\partial x} = 0
\]

For this system of PDE with constant coefficients, which is just another form of the wave equation, it has been known since D'Alembert that the general solution is of the form

\[
\tilde{\eta}(x, t) = H(x + at)
\]

\[
\tilde{u}(x, t) = F(x + at).
\]

This yields

\[
(a + u_0)F' + H' = 0
\]

\[
\eta_0 F' + (a + u_0)H' = 0
\]

which implies that

\[
a_{1/2} = -u_0 \pm \sqrt{\eta_0}.
\]

Therefore the first order approximation to our solution is

\[
u(x, t) = u_0 + \epsilon \left( F(x + a_1 t) + F(x + a_2 t) \right)
\]

\[
\eta(x, t) = \eta_0 + \epsilon \left( H(x + a_1 t) + H(x + a_2 t) \right)
\]

Since \( u_0 \) is very small, \( a_1 \) and \( a_2 \) will have different signs. This in turn implies that in our ideal channel waves go in two different directions.
4 Adding a Power Plant (No Heat Yet!)

Now that we have a model for fluid flow in an ideal channel, we can add an intake pipe and an outflow pipe to our channel. Since the river velocity in the \( z \)-direction can be assumed to be slower than the velocity in the \( y \)-direction of the water coming in and out of the pipes, we will assume that our intake pipe \( x_{in} \) and outflow pipe \( x_{out} \) will be sheet sources and sheet sinks.

\[
\begin{array}{ccc}
I & II & III \\
\hline
x_{in} & x_{in} & x
\end{array}
\]

Let \( x_{in} \) be the \( z \)-coordinate where approximately 1/3 of the volume is taken into the power plant and let \( x_{out} \) be the \( x \)-coordinate where the same volume of water is added to the river. In the regions I, II, and III, the shallow water equations are used. Assuming a steady state, \( u \) will be a constant in each region. In the intake and outflow regions, conservation of mass and conservation of momentum must hold.

For a fixed control volume,

\[
\int_{\partial \Omega} \rho u \cdot n dS = -\frac{\partial}{\partial t} \int_{\Omega} \rho dV
\]

is the integral form of the conservation of mass equation, \( u \) is the vector \((u, v)\), and \( n \) is the normal vector. The left hand side is the net mass flow out of the control surface, and the right hand side is the time rate of decrease of mass inside the control volume. The right hand side is zero for steady flow. The left hand side is

\[
(4.1) \quad -\rho W u^- \eta^- + \rho W u^+ \eta^+ + \rho Q W
\]

for the intake region. For the outflow region \( Q \) is replaced by \(-Q\). Here,

- \( W \) is the width of the canal
- \( Q \) is the total flow divided by the width
- \( u^-, \eta^- \) refer to the velocity and height just before the intake (or outflow)
- \( u^+, \eta^+ \) refer to the velocity and height just after the intake (or outflow)

Thus equation (4.1) becomes

\[
\begin{align*}
0 &= u^- \eta^- - u^+ \eta^+ - Q \quad \text{(intake)} \\
0 &= u^- \eta^- - u^+ \eta^+ + Q \quad \text{(outflow)}
\end{align*}
\]

For a fixed control volume

\[
\frac{\partial}{\partial t} \int_{\Omega} \rho u dV = \int_{\partial \Omega} \rho u n dS - \int_{\partial \Omega} \rho u (u \cdot n) dS
\]
is the integral form of the conservation of momentum equation (for inviscid flow). The left hand side is the rate of change of total momentum in the control volume which equals zero in the steady state. The first term on the right hand side is the momentum due to the pressure change.

\[ W\left[ \int_{0}^{\eta^-} [p_{\text{air}} + \rho g(\eta^- - y)]dy + \int_{0}^{\eta^+} [p_{\text{air}} + \rho g(\eta^+ - y)]dy + \int_{\eta^+}^{\eta^-} p_{\text{air}}dy \right] = \frac{W\rho g}{2} [(\eta^+)^2 - (\eta^-)^2] \]

The second term is the amount of flux through the control volume, and is equal to

\[ W\rho (u^-)\eta^- - W\rho (u^+)\eta^+ - \rho (\frac{u^- + u^+}{2})QW \]

for the intake region. For the outflow region, the pipe is assumed to be straight up, thus there is no third term. Thus

\[ \left(-\frac{u^- + u^+}{2}\right)Q = \frac{g}{2} [(\eta^+)^2 - (\eta^-)^2] + [(u^-)^2\eta^- - (u^+)^2\eta^+] \quad \text{(intake)} \]

and

\[ 0 = \frac{g}{2} [(\eta^+)^2 - (\eta^-)^2] + [(u^-)^2\eta^- - (u^+)^2\eta^+] \quad \text{(outflow)} \]

The equations from the intake and outflow regions will be referred to as the \textit{jump conditions}. After nondimensionalizing the jump conditions in the intake region,

\begin{align*}
(4.2) & \quad 0 = u^- \eta^- - u^+ \eta^+ - \tilde{Q} \\
(4.3) & \quad 0 = \frac{1}{2} [(\eta^+)^2 - (\eta^-)^2] + [(u^-)^2\eta^- - (u^+)^2\eta^+] - \frac{1}{2} (u^- + u^+)\tilde{Q}
\end{align*}

and in the outflow region,

\begin{align*}
(4.4) & \quad 0 = u^- \eta^- - u^+ \eta^+ + \tilde{Q} \\
(4.5) & \quad 0 = \frac{1}{2} [(\eta^+)^2 - (\eta^-)^2] + [(u^-)^2\eta^- - (u^+)^2\eta^+]
\end{align*}

where

\[ \tilde{Q} = \frac{Q}{H\sqrt{gH}} \approx 2.5 \times 10^{-3} \]

The nondimensionalized boundary conditions at the beginning of the canal for the steady state problem will be

\begin{align*}
\eta & = 1 \\
u & = \frac{7.5 \times 10^{-2}}{\sqrt{gH}} \approx 7.5 \times 10^{-3} =: \beta
\end{align*}

where \(7.5 \times 10^{-2}\) is the assumed original velocity of the water.

Taking \(\tilde{Q}\) small, perturbation theory can be used. In region I, \(u = \beta = 7.5 \times 10^{-3}\) and \(\eta = 1\). Thus in the intake region let \(u^- = \beta\) and let \(\eta^- = 1\). Since \(\beta = 7.5 \times 10^{-3}\) assume that \(\beta = a\tilde{Q}\) where \(a = 3\) since approximately 1/3 of the volume is taken out. Let

\begin{align*}
u^+ &= u_1 \tilde{Q} + u_2 \tilde{Q}^2 + O(\tilde{Q}^3) \\
\eta^+ &= 1 + \eta_1 \tilde{Q} + \eta_2 \tilde{Q}^2 + O(\tilde{Q}^3)
\end{align*}

where \(u_1, u_2, \eta_1,\) and \(\eta_2\) are constants.
Substitution of $u^-$, $\eta^-$, $u^+$, and $\eta^+$ into equations (4.2) and (4.3) and simplification yields

\[
0 = (a - u_1 - 1) - (u_1 \eta_1 + u_2)\tilde{Q} + O(\tilde{Q}^2)
\]
\[
0 = \eta_1 + (\eta_1^2/2 + a^2 - u_1^2 - a/2 - u_1/2 + \eta_2)\tilde{Q} + O(\tilde{Q}^2)
\]

Setting each coefficient equal to zero and doing some algebra results in $u_1 = a - 1$, $u_2 = 0$, $\eta_1 = 0$, and $\eta_2 = 1/2 - a$. Thus in region II

\[
u^+ = (a - 1)\tilde{Q} + O(\tilde{Q}^3) \approx 5 \times 10^{-3}
\]
\[
\eta^+ = 1 + (1/2 - a)\tilde{Q}^2 + O(\tilde{Q}^3) = 1 - O(10^{-6})
\]

In the outflow region $u^-$ and $\eta^-$ are the $u^+$ and $\eta^+$ in region II and

\[
u^+ = u_1 \tilde{Q} + u_2 \tilde{Q}^2 + O(\tilde{Q}^3)
\]
\[
\eta^+ = 1 + \eta_1 \tilde{Q} + \eta_2 \tilde{Q}^2 + O(\tilde{Q}^3)
\]

Substitution into equations (4.4) and (4.5) and simplification yields

\[
0 = (a - u_1) - (u_1 \eta_1 + u_2)\tilde{Q} + O(\tilde{Q}^2)
\]
\[
0 = \eta_1 + (\eta_2 + \eta_1^2/2 - 1/2 + a + (a - 1)^2 - u_1^2)\tilde{Q} + O(\tilde{Q}^2)
\]

Thus $u_1 = a$, $u_2 = 0$, $\eta_1 = 0$, and $\eta_2 = a - 1/2$ and in region III

\[
u^+ = a\tilde{Q} + O(\tilde{Q}^3) \approx 7.5 \times 10^{-3}
\]
\[
\eta^+ = 1 + (a - 1/2)\tilde{Q}^2 + O(\tilde{Q}^3) = 1 + O(10^{-6})
\]

In conclusion of this section, the velocity, $u$, changes from $7.5 \times 10^{-3}$ to $5 \times 10^{-3}$ when the water is taken out of the canal and the velocity returns to $7.5 \times 10^{-3}$ when the water is returned to the canal later downstream. Since the height, $\eta$, changes from 1 to $1 - O(10^{-6})$ to 1 + $O(10^{-6})$ it is assumed that the height is a constant.

5 Temperature Profile Analysis

To determine the steady-state temperature profile of the river with power plant operation, we must analyze the energy balance equations in each of our three regions.

For our assumption of incompressible flow ($\rho = constant$), inviscid flow, and constant $k$, and $C_p$, the differential form of the energy balance is given by

\[
\frac{\partial \theta}{\partial t} + u \cdot \nabla \theta = \alpha \nabla^2 \theta.
\]
The three terms of this equation, from left to right, represent rate of change, advection, and thermal diffusion. The integral form of the energy balance is

\[
\frac{\partial}{\partial t} \int_{\Omega} \rho C_p \theta dV = - \int_{\partial \Omega} \rho C_p \theta u \cdot n dS - \int_{\partial \Omega} q \cdot n dS
\]

with the three terms representing rate of change of total heat, advective heat transfer, and heat transfer through surface. By Fourier's law, \( q = -k \nabla \theta \).

To study the outflow regions, use the integral form of the energy balance with control volume

\[
\Omega = [x_{out} - \varepsilon, x_{out} + \varepsilon] \times [y, y + dy] \times \text{width}.
\]

Now, assuming our outflow water is added evenly across the cross-sectional surface at \( x = x_{out} \), the rate of change of total heat in our control volume is

\[
\left[ \frac{dy}{H} \right] \cdot [\rho C_p (QW) \theta_{out}].
\]

Assuming continuity of \( \theta \) across the singular point \( x = x_{out} \), for \( dy \) sufficiently small the mean value theorem allows us to assume \( \rho \) and \( \theta \) are constant in our control volume. Then, since our fluid flow is in the \( x \)-direction only,

\[
- \int_{\partial \Omega} \rho C_p \theta u \cdot n dS = \rho C_p \theta [u^+ W dy - u^- W dy]
\]

Next, by collapsing our width \( 2\varepsilon \rightarrow 0 \) and again using the mean value theorem we obtain

\[
\int_{\partial \Omega} k \nabla \theta \cdot n dS = -k \frac{\partial \theta^-}{\partial x} W dy + k \frac{\partial \theta^+}{\partial x} W dy.
\]

Thus,

\[
\rho C_p W Q \theta_{out} \frac{dy}{H} = \rho C_p W \theta [u^- - u^+] dy - W k \left[ \frac{\partial \theta^-}{\partial x} - \frac{\partial \theta^+}{\partial x} \right] dy \quad \forall \ y \in [0, H].
\]

Simplifying,

\[
\frac{Q}{H} \theta_{out} = \theta [u^- - u^+] - \alpha \left[ \frac{\partial \theta^-}{\partial x} - \frac{\partial \theta^+}{\partial x} \right],
\]

where

\[
\alpha = \frac{K}{C_p \rho}
\]

Since \( u^- - u^+ = \frac{Q}{H} \) from our fluid analysis, we obtain, finally

\[
\frac{\partial \theta^- (y)}{\partial x} - \frac{\partial \theta^+ (y)}{\partial x} = \frac{Q}{H \alpha} (\theta_{out} (y) - \theta (x_0, y))
\]

for all \( 0 < y \leq H \).

Proceeding similarly for the intake region, we obtain

\[
-\frac{Q}{H} \theta_{in} = -\frac{Q}{H} \theta_{in} - \alpha \left[ \frac{\partial \theta^-}{\partial x} - \frac{\partial \theta^+}{\partial x} \right],
\]
and so
\[ \frac{\partial \theta^-}{\partial x} = \frac{\partial \theta^+}{\partial x} \]
at the intake.

To study regions I, II, and III, we use the differential energy balance equation.

Since we are seeking a steady-state solution for our problem, \( \frac{\partial \theta}{\partial t} = 0 \). From our previous flow analysis, \( v = w = 0 \), and \( u \) may be assumed constant in each region with known values. And finally, since we assume the temperature distribution across the river is uniform,

\[ \frac{\partial^2 \theta}{\partial x^2} = 0. \]

Thus, our equation for energy balance in each region reduces to

\[ u \frac{\partial \theta}{\partial x} = \alpha \left( \frac{\partial^2 \theta}{\partial z^2} + \frac{\partial^2 \theta}{\partial y^2} \right), \]

an elliptic partial differential equation with constant coefficients within each region.

Thus, boundary conditions on the entire boundary of each region must be determined to enable solutions of this equation.

Let the boundaries be designated as shown below:

On \( l_1 \) we can assign our upstream temperature \( \theta^* \), and likewise on \( l_3 \) we assume the river eventually returns to its original temperature \( \theta^* \).

On \( l_2 \) we assume that conductive heat transfer with the earth is negligible compared to heat loss to vaporization, so

\[ \frac{\partial \theta}{\partial y} = 0. \]

On \( l_5 \) we determined that no jump occurs in either \( \theta = \theta_m \) or \( \frac{\partial \theta}{\partial x} \). And on \( l_6 \) we know \( \theta^- = \theta^+ \) and

\[ \frac{\partial \theta^-}{\partial x} - \frac{\partial \theta^+}{\partial x} = \frac{Q}{H \alpha} (\theta_{out} - \theta). \]

On \( l_4 \), the heat loss due to evaporation is accounted for through the equation

\[ k \frac{\partial \theta}{\partial y} = -\Phi_{ev} (\theta - \theta_{air}). \]
where $\Phi_{ev}$ is the heat loss per square meter per °C per second for the river and $k = \alpha \rho C_p$ is the effective thermal conductivity of the river. For most lakes and rivers, $\Phi_{ev} = \frac{30W}{m^2 \circ C}$, and for turbulent river flow $\alpha$ is taken to be $10m^2/\text{sec}$. Thus,

$$\frac{\partial \theta}{\partial y} = -\frac{1}{\alpha \rho C_p} \Phi_{ev}(\theta - \theta_{air})$$
on $l_4$.

Notice that in our model, if we assume no power plant, then the water temperature is in equilibrium with the air and $\theta^* = \theta_{air}$ where $\theta_{air}$ is a modified "temperature" including such factors as humidity.

And, finally, to relate $\theta_{out}$ and $\theta_{in}$, we assume that the power plant is producing 1000MW of heat (i.e. efficiency is constant at 50%). Since this heat equals $WQ(\rho C_p) (\theta_{out} - \theta_{in})$, we find that $\theta_{out} - \theta_{in} = 9.52^\circ C$.

So, our system is now well-defined with velocities $u$ defined for each region.

To analyze this system further we need to non-dimensionalize the system. Using

$$u = \begin{cases} 7.5 \times 10^{-2}m/s & \text{in I and III} \\ 5.0 \times 10^{-2}m/s & \text{in II} \end{cases}$$

$$x = L \bar{x}$$

$$y = H \bar{y}$$

$$\theta = \theta^* + (10^6C) \bar{\theta}.$$ 

So, after simplification, the governing system becomes (with bars removed),

$$\frac{H^2}{\alpha L} u \frac{\partial \theta}{\partial x} = \left( \frac{H}{L} \right)^2 \frac{\partial^2 \theta}{\partial x^2} + \frac{\partial^2 \theta}{\partial y^2}$$

$$l_1 : \quad \theta = 0$$

$$l_2 : \quad \frac{\partial \theta}{\partial y} = 0$$

$$l_3 : \quad \theta = 0$$

$$l_4 : \quad \frac{\partial \theta}{\partial y} = -\frac{H}{\alpha \rho C_p} \Phi_{ev} \bar{\theta}$$

$$l_5 : \quad \theta^- = \theta^+ , \quad \frac{\partial \theta^-}{\partial x} = -\frac{\partial \theta^+}{\partial x} = 0$$

$$l_6 : \quad \theta^- = \theta^+ , \quad \frac{\partial \theta^-}{\partial x} - \frac{\partial \theta^+}{\partial x} = \frac{LQ}{H \alpha} [1 + \theta_{in} - \theta_{out}]$$

The values of the parameters in these equations are

$$\frac{H^2}{L^2} = 10^{-6}$$
\[ \frac{H^2}{\alpha L} u = \begin{cases} \ 7.5 \times 10^{-5} & \text{in I and III} \\ \ 5.0 \times 10^{-5} & \text{in II} \end{cases} \]
\[ \frac{H}{\alpha \rho C_p} \Phi_{ev} = 7.5 \times 10^{-6} \]
\[ \frac{LQ}{\alpha \alpha} = 0.04 \]

Four of these parameters are of the order \( 10^{-5} \sim 10^{-6} \). So we will attempt to analyze these equations using a perturbation analysis expanding \( \theta \) in terms of a small parameter \( \epsilon \). To do this we write

\[ \frac{H^2}{L^2} = a \epsilon \]
\[ \frac{H^2}{\alpha L} u = \begin{cases} \ b \epsilon & \text{in I and III} \\ \ c \epsilon & \text{in II} \end{cases} \]
\[ \frac{H}{\alpha \rho C_p} \Phi_{ev} = d \epsilon \]

For convenience we also write \( \epsilon = \frac{LQ}{\alpha \alpha} \). Now the system can be written as

\[ a \epsilon \frac{\partial^2 \theta}{\partial x^2} + \frac{\partial^2 \theta}{\partial y^2} = b \epsilon \frac{\partial \theta}{\partial x} \quad \text{in I and III} \]
\[ a \epsilon \frac{\partial^2 \theta}{\partial x^2} + \frac{\partial^2 \theta}{\partial y^2} = c \epsilon \frac{\partial \theta}{\partial x} \quad \text{in II} \]

All boundary conditions and jump conditions remain as is except the boundary condition on the top surface which we write as

\[ \frac{\partial \theta}{\partial y}(x, \eta(x)) = -d \epsilon \theta(x, \eta(x)) \]

We write

\[ \theta(x, y) = G(x, y) + \epsilon \tilde{G}(x, y) \]

The differential equations (up to \( O(\epsilon^2) \)) become

\[ a \frac{\partial^2 G}{\partial x^2} + \frac{\partial^2 G}{\partial y^2} + \epsilon \frac{\partial^2 \tilde{G}}{\partial y^2} = b \epsilon \frac{\partial G}{\partial x} \quad \text{in I and III} \]
\[ a \frac{\partial^2 G}{\partial x^2} + \frac{\partial^2 G}{\partial y^2} + \epsilon \frac{\partial^2 \tilde{G}}{\partial y^2} = c \epsilon \frac{\partial G}{\partial x} \quad \text{in II} \]

Comparing coefficients we find

\[ \begin{cases} 
\frac{\partial^2 G}{\partial y^2} = 0 \\
\frac{\partial^2 G}{\partial x^2} + \frac{\partial^2 \tilde{G}}{\partial y^2} = b \frac{\partial G}{\partial x} \\
\frac{\partial^2 G}{\partial x^2} + \frac{\partial^2 \tilde{G}}{\partial y^2} = c \frac{\partial G}{\partial x}
\end{cases} \quad \text{as well as} \quad \begin{cases} 
\frac{\partial^2 G}{\partial y^2} = 0 \\
\frac{\partial^2 G}{\partial x^2} + \frac{\partial^2 \tilde{G}}{\partial y^2} = c \frac{\partial G}{\partial x}
\end{cases} \quad \text{in II} \]
Taking $l_1$ and $l_3$ to be infinitely far away, the boundary conditions become

\[
G(-\infty, y) = \tilde{G}(-\infty, y) = 0 \\
G(\infty, y) = \tilde{G}(\infty, y) = 0 \\
\frac{\partial G}{\partial y}(x, 0) = \frac{\partial \tilde{G}}{\partial y}(x, 0) = 0 \\
\frac{\partial G}{\partial y}(x, \eta(x)) = 0 \\
\frac{\partial \tilde{G}}{\partial y}(x, \eta(x)) = -dG(x, \eta(x)).
\]

And the jump conditions become

\[\begin{align*}
G^- = G^+ & \quad \tilde{G}^- = \tilde{G}^+ \\
\frac{\partial G^-}{\partial x} = \frac{\partial G^+}{\partial x} & \quad \frac{\partial \tilde{G}^-}{\partial x} = \frac{\partial \tilde{G}^+}{\partial x}
\end{align*}\]

(intake)

\[\begin{align*}
G^- = G^+ & \quad \tilde{G}^- = \tilde{G}^+ \\
1 = G(x_{out}, y) - G(0, y) - e \left( \frac{\partial G^+}{\partial x} - \frac{\partial G^-}{\partial x} \right) \\
0 = \tilde{G}(x_{out}, y) - \tilde{G}(0, y) - e \left( \frac{\partial \tilde{G}^+}{\partial x} - \frac{\partial \tilde{G}^-}{\partial x} \right)
\end{align*}\]

(outflow)

Here we have chosen our coordinate system such that the origin is located at the intake, i.e. $x_{in} = 0$. Now the equation $\frac{\partial^2 G}{\partial y^2} = 0$ holds in all three regions, so by the above boundary condition we get

\[
\frac{\partial G}{\partial y}(x, y) = \frac{\partial G}{\partial y}(x, 0) = 0
\]

and this leads to

\[G(x, y) = G(x, 0)\]

that is, $G$ is independent of $y$. From now on $G$ will be expressed as a function of $x$ alone and we will use primes to denote its derivative with respect to $x$. Therefore, we can now write the second differential equation as

\[aG'' + \frac{\partial^2 \tilde{G}}{\partial y^2} = bG' \quad \text{in I and III} \]

\[\Rightarrow \quad \frac{\partial^2 \tilde{G}}{\partial y^2} = -aG'' + bG' \quad \Rightarrow \quad \frac{\partial \tilde{G}}{\partial y}(x, y) - \frac{\partial \tilde{G}}{\partial y}(x, 0) = y(-aG'' + bG')
\]

But the third boundary condition is $\frac{\partial \tilde{G}}{\partial y}(x, 0) = 0$, so after integrating

\[
\frac{\partial \tilde{G}}{\partial y}(x, y) = y(-aG'' + bG')
\]
We can use the fourth boundary condition to get

\[-dG(x) = \eta(x)(-aG''(x) + bG'(x))\]

Using \(\eta(x) \approx 1\) we get a second order constant coefficient ODE for \(G(x)\), namely

\[aG''(x) - bG'(x) - dG(x) = 0 \quad \text{in I and III}\]

Similarly we find

\[aG''(x) - cG'(x) - dG(x) = 0 \quad \text{in II}\]

We have boundary conditions and jump conditions for \(G\) as follows

\[
\begin{align*}
G(-\infty) &= G(\infty) = 0 \\
G^- &= G^+ \\
G''^- &= G'^+ \\
1 &= G(x_{\text{out}}) - G(0) - e(G'^+ - G''^-) \\
\end{align*}
\]

(intake)

(outflow)

The system can be solved in the usual way

\[
G(x) = \begin{cases} 
A_1 \exp(r_1 x) + A_2 \exp(r_2 x) & \text{in I} \\
B_1 \exp(\tilde{r}_1 x) + B_2 \exp(\tilde{r}_2 x) & \text{in II} \\
C_1 \exp(r_1 x) + C_2 \exp(r_2 x) & \text{in III} 
\end{cases}
\]

where

\[
\begin{align*}
 r_1 &= \frac{b + \sqrt{b^2 + 4ad}}{2a} \\
 r_2 &= \frac{b - \sqrt{b^2 + 4ad}}{2a} \\
 \tilde{r}_1 &= \frac{c + \sqrt{c^2 + 4ad}}{2a} \\
 \tilde{r}_2 &= \frac{c - \sqrt{c^2 + 4ad}}{2a}
\end{align*}
\]

The conditions at \(\pm \infty\) now give

\[A_2 = 0, \quad C_1 = 0\]

The jump conditions at the intake give

\[
\begin{align*}
A_1 &= B_1 + B_2 \\
A_1 r_1 &= B_1 \tilde{r}_1 + B_2 \tilde{r}_2
\end{align*}
\]

the ones at the outflow give

\[
B_1 \exp(\tilde{r}_1 x_{\text{out}}) + B_2 \exp(\tilde{r}_2 x_{\text{out}}) = C_2 \exp(r_2 x_{\text{out}})
\]

\[
C_2 \exp(r_2 x_{\text{out}}) - A_1 - e(C_2 r_2 \exp(r_2 x_{\text{out}}) - B_1 \tilde{r}_1 \exp(\tilde{r}_1 x_{\text{out}}) - B_2 \tilde{r}_2 \exp(\tilde{r}_2 x_{\text{out}})) = 1
\]

This is a linear system of 4 equations in 4 unknowns

\[
\begin{align*}
0 &= -A_1 + B_1 + B_2 \\
0 &= -r_1 A_1 + B_1 \tilde{r}_1 + B_2 \tilde{r}_2 \\
0 &= B_1 \exp(\tilde{r}_1 x_{\text{out}}) + B_2 \exp(\tilde{r}_2 x_{\text{out}}) - C_2 \exp(r_2 x_{\text{out}}) \\
1 &= -A_1 + e\tilde{r}_1 B_1 \exp(\tilde{r}_1 x_{\text{out}}) + e\tilde{r}_2 B_2 \exp(\tilde{r}_2 x_{\text{out}}) + (1 - er_2)C_2 \exp(r_2 x_{\text{out}})
\end{align*}
\]
By solving this system and plugging in the expressions for $r_1, r_2, r_1, \text{ and } r_2$ and subsequently those for $a, b, c, d,$ and $e,$ the steady-state temperature profile of the river with power plant operation can be determined in terms of our original parameters $H, L, \alpha, \rho C_p,$ and $\Phi_v.$

6 Graphs

So, now we can determine an approximate temperature profile given our parameters, merely by solving a linear system of four equations. A careful tracing of these parameters will thus allow us to get a sense of the dependence of the temperature on the parameters. In the graphs below, the $x$-axis represents the distance that the outfall pipe is from the intake pipe. Thus, the intake pipe is located at $x = 0.$ In the first graph, we are assuming the outfall pipe is $1 km$ away from the intake pipe. Then the temperature decreases very slowly downstream (only about $0.5^\circ C$ in $20 km$). In the second graph, we see that the temperature returns to approximately its initial value after about $200 km$ downstream from the intake pipe. The third graph shows that if the outfall pipe is placed $1 km$ from the intake pipe, then the heat added at the outfall should not interfere with the intake pipe water temperature. But, notice that at shorter distances (such as $0.2 km$), the heat from the outfall raises the water temperature around the intake pipe by about $0.75^\circ C.$ Finally, the fourth graph summarizes the increase in temperature around the intake pipe for various distances between the intake and outfall pipes.
Temperature Gain at Intake for $0 \text{km} \leq x_{\text{out}} \leq 1 \text{km}$

Temperature Profiles for $x_{\text{out}} = 1 \text{km}, 0.5 \text{km},$ and $0.3 \text{km}$
7 Conclusion

We have constructed a two-dimensional model of the shallow water problem in our ideal channel with constant density. In the model, there were two singular points, which modeled a power plant with intake \( x_{in} \) from the river and outflow \( x_{out} \) back to the river respectively. By studying this model, we tried to provide a suggestion for the position of outflow of the power plant.

We employed the perturbation method near the steady-state and obtained the flow velocity and temperature distribution in the channel. We found that the temperature at the intake point decays exponentially as the distance between \( x_{out} \) and \( x_{in} \) increases. Therefore, we recommend that a distance of 1 km between water intake and outflow be employed with a result of negligible heat gain at the inlet and thus maintaining efficiency.

Our model also gave us an approximation that the heat from outflow would affect the downstream for a very long distance.

There are some possible future works to further our present study. In our model, we assume the outflow water does not affect the horizontal momentum of the flow. We may consider a more detailed mechanism at the intake and outflow and even more obvious, the time-dependent problem should be looked at.

One open problem, which still needs to be considered is a river with tidal flow. For example, what effects will tides have on the flow and temperature distributions in the Hudson River if a power plant is built there?
Students' Report

# 3

Subgroup 1
A Wrinkling Criteria
Equation for Web Spans

IMA Summer Program for Graduate Students

Mathematical Modeling

Week 1, Group 3
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Introduction

Any material which is thin compared to its length and width is termed a web. From an engineering standpoint, a web is any material which has a low stiffness in the out-of-plane direction. Wrinkling can be created by a number of processing factors such as misaligned rollers, eccentric rollers, uneven tension profile, active steering and guiding and other factors which will induce shear strain into the web. Preventing wrinkles in web is important because they may cause permanent defects or tearing in the web. A wrinkling criteria equation has been established in the following discussions.

Nomenclature

\( b \) — web span width
\( L \) — web span length
\( V \) — deformation of the web normal to the web plane \((x, y)\)
\( T_x, T_y \) — Tension in the \( x- \) and \( y- \) direction respectively
\( T_{xy} \) — shear force per unit length
\( \rho \) — surface density of the web

Assumptions

(1) Bending Stiffness is small and can be neglected;
(2) The two edges \( y = 0 \) and \( y = b \) are free boundaries

The Model
\[ \rho dx dy \frac{\partial^2 V}{\partial t^2} = (T_{x+dx} \frac{\partial V}{\partial x})_{x+dx} - T_x \frac{\partial V}{\partial x} dy + (T_{y+dy} \frac{\partial V}{\partial y})_{y+dy} - T_y \frac{\partial V}{\partial y} dx + \]

\[ (T_{x+dx,y} \frac{\partial V}{\partial y})_{x+dx} - T_{xy} \frac{\partial V}{\partial x} dy + (T_{x,y+dy} \frac{\partial V}{\partial x})_{y+dy} - T_{xy} \frac{\partial V}{\partial y} dx \]

and

\[ (T_{x+dx} - T_x) dy + (T_{x,y+dy} - T_{x,y}) dx = 0 \]

\[ (T_{x+dx,y} - T_{xy}) dy + (T_{y+dy} - T_y) dx = 0 \]

So, we have

\[ \rho \frac{\partial^2 V}{\partial t^2} = \frac{\partial}{\partial x} (T_x \frac{\partial V}{\partial x}) + \frac{\partial}{\partial y} (T_y \frac{\partial V}{\partial y}) + \frac{\partial}{\partial x} (T_{xy} \frac{\partial V}{\partial y}) + \frac{\partial}{\partial y} (T_{xy} \frac{\partial V}{\partial x}) \] \tag{1}

\[ \frac{\partial T_x}{\partial x} + \frac{\partial T_{xy}}{\partial y} = 0 \] \tag{2}

\[ \frac{\partial T_{xy}}{\partial x} + \frac{\partial T_y}{\partial y} = 0 \] \tag{3}

Equation (1) can be simplified as follows using (2) and (3):

\[ \frac{\partial^2 V}{\partial t^2} = T_x \frac{\partial^2 V}{\partial x^2} + 2T_{xy} \frac{\partial^2 V}{\partial x \partial y} + T_y \frac{\partial^2 V}{\partial y^2} \] \tag{4}

We will consider the equation (4) locally where we may regard the forces as constants. Let

\[ V = e^{i(\omega t - kx - ly)} \]

then

\[ \rho \omega^2 = T_x k^2 + 2T_{xy} kl + T_y l^2 \]

If a complex solution for \( \omega \) exists, we see that \( V \to \infty \) as \( t \to \infty \) where the wrinkle occurs. In other words, wrinkle occurs if

\[ T_{xy}^2 - T_x T_y > 0 \] \tag{5}

In such a case, the shear force has the dominant effect. The inequality allows us to define a wrinkle criteria equation:

\[ T_{xy}^2 - T_x T_y = 0 \] \tag{6}

In order to solve the equation, we introduce the "stress function" \( \phi \) such that

\[ T_x = \frac{\partial^2 \phi}{\partial y^2}, T_y = \frac{\partial^2 \phi}{\partial x^2}, T_{xy} = \frac{\partial^2 \phi}{\partial x \partial y} \]
which solves (2)-(3). Hence the wrinkling criteria equation has the form:

\[
\left( \frac{\partial^2 \phi}{\partial x \partial y} \right)^2 = \frac{\partial^2 \phi}{\partial x^2} \frac{\partial^2 \phi}{\partial y^2} \tag{7}
\]

with the free boundary conditions: \( T_y, T_{xy} = 0 \) at \( y = 0, b \), i.e.,

\[
\frac{\partial^2 \phi}{\partial x^2} = 0 \text{ at } y = 0, b \tag{8}
\]

since it implies the second boundary condition through equation (7).

It is unfortunately difficult to find the general solution of (7)-(8). But we may observe a particular solution is that \( \phi \) is independent of \( x \). Let’s pick one particular solution

\[
\phi = -\sin \frac{\pi y}{b}, 0 \leq y \leq b
\]

then we have

\[
T_z = (\frac{\pi}{b})^2 \sin \frac{\pi y}{b}, T_y = 0, T_{xy} = 0
\]

and the equation (1) is reduced to

\[
\rho \frac{\partial^2 V}{\partial t^2} = (\frac{\pi}{b})^2 \sin \frac{\pi y}{b} \frac{\partial^2 V}{\partial x^2}
\]

Let

\[
a(y) = \frac{\pi}{b \sqrt{\rho}} \sin \frac{\pi y}{b}
\]

we have

\[
\frac{\partial^2 V}{\partial t^2} = a(y)^2 \frac{\partial^2 \phi}{\partial x^2}
\]

Together with the boundary conditions \( V = 0 \) at \( x = 0, L \), we have the solution

\[
V = \sum_{n=1}^{\infty} \left( A_n \cos n \pi a(y) t + B_n \sin n \pi a(y) t \right) \sin \frac{n \pi}{L} x
\]

A part of the first mode is

\[
V = \sin \left( \frac{\pi^2 y t}{b \sqrt{\rho}} \right) \sin \frac{\pi}{L} x
\]

To see the profile of the first mode, we select that \( b = \pi, L = 4\pi \) and \( \rho = \frac{1}{4} \). The picture on the next paper shows the profile.
First_Mode_with_Time_Step_=_1
A Physical Description of the Criteria Equation

For given local tensions $T_x, T_y$ and $T_{xy}$, we consider a wedge element with angle $0 < \theta < \pi/2$. Balances of forces give

$$T_n = -(T_x - T_y) \cos 2\theta + T_x + T_{xy} \sin 2\theta$$

$$T_s = -\frac{1}{2}(T_x - T_y) \sin 2\theta - T_{xy} \cos 2\theta$$

Accordingly, we have

$$\max T_n = \frac{T_x + T_y}{2} + \sqrt{\left(\frac{T_x - T_y}{2}\right)^2 + T_{xy}^2}$$

$$\min T_n = \frac{T_x + T_y}{2} - \sqrt{\left(\frac{T_x - T_y}{2}\right)^2 + T_{xy}^2}$$

which are the two in-plane principal stresses. The absolute maximum shear stress is given by

$$T_a = \frac{1}{2}(\max T_n - \min T_n) = \frac{1}{2} \sqrt{(T_x - T_y)^2 + T_{xy}^2}$$
We can see that the criteria equation is equivalent to \( \min T_n = 0 \).

**Further Research**

There are many area that could be further studied either mathematically or physically. The following are some of them:

1. looking for the stress function in a general situation;
2. removing the assumption that the bending stiffness can be neglected;
3. finding a necessary condition under which wrinkle occurs;
4. working the problem numerically.

**References**

Students' Report
#3

Subgroup 2
A Model of Tension and Velocity in Web Handling Machinery

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1 Introduction

We will try to describe a model for calculating the tensions and velocities of a thin sheet of material called the web at various points in a device containing various rollers over which the web moves. An application of this model is to the newspaper printing process. We will consider the interaction between the web and two configurations of rollers. The first is the capstan roller which is typically used to change the direction of the web. The web will wrap partially around the the capstan roller. The other type of roller is the nipping roller which consists of a pair of rollers between which the web runs. Nipping rollers may use friction to grip the web and drive it through the machinery. See Figure 1.

Separate models for the static case in which tension and velocity of the web are constant in time and the dynamic case in which tension and velocity of the web vary with time, will be presented.

2 Notation

The following notation will be used to describe quantities in the models.

$T$ tension
$v$ velocity
$\epsilon$ elongation rate
$a$ width of web
$\rho$ density of web
$h$ thickness of web
Figure 1: A simplified section of web handling machinery. Rollers labeled A, B, and C are capstan rollers. The pair D1 and D2 are nipping rollers.

$L$ geometric distance between rollers

$\mu$ coefficient of friction

$r$ radius of roller

3 Assumptions

Throughout this paper we will assume the web is linearly elastic, i.e. the amount of elongation of the web is a linear function of the tension applied. The distance between adjacent pairs of rollers is fixed. This implies we will not discuss sections of machinery which contain movable rollers. Real examples of such are sometimes called dancing rollers or compensators. We will assume as the web is stretched along its length the width $a$ does not change.

4 Continuity Equation

We begin by considering a reference element of unstretched web. See Figure 2. The mass of this element is $\text{mass}_0 = L_0 h_0 \rho_0 a$. When this element is
subjected to tension, $T$, the length, density, and thickness of the web change but the mass must be conserved,

$$\text{mass}_T = L_T h_T \rho_T a = L_0 h_0 \rho_0 a = \text{mass}_0$$

By assumption the new length of the web is $L_T = L_0(1 + T \varepsilon)$. Substituting this in the equation above yields an equation of state for the web.

$$h_T \rho_T = \frac{h_0 \rho_0}{1 + T \varepsilon} \quad (1)$$

As the web runs from span $i$ to span $i + 1$ we can write a conservation of mass equation for span $i + 1$. The time rate of change in mass in span $i + 1$ is equal to the difference between mass entering span $i + 1$ and mass leaving span $i + 1$. Using our notation we see

$$\rho_i h_i v_i a - \rho_{i+1} h_{i+1} v_{i+1} a = \frac{d}{dt}(\rho_{i+1} h_{i+1} a L)$$

where $L$ is the length of span $i + 1$. Using equation (1) and canceling common factors yields the continuity equation.

$$\frac{v_i}{1 + T_i \varepsilon} - \frac{v_{i+1}}{1 + T_{i+1} \varepsilon} = \frac{d}{dt} \left( \frac{L}{1 + T_{i+1} \varepsilon} \right) \quad (2)$$

In the steady state case the right-hand side of the continuity equation is 0 and we derive an equation relating the tensions and velocities in spans $i$ and $i + 1$.

$$\frac{v_i}{1 + T_i \varepsilon} = \frac{v_{i+1}}{1 + T_{i+1} \varepsilon} \quad (3)$$
Typically there exists a span in the machinery where the tension is zero. In a newspaper press this may be last stage in the printing process where the papers are cut and folded. Hence if we assume $T_{i+1} = 0$ then we have

$$v_i = (1 + T_i \epsilon) v_{i+1}.$$  \hspace{1cm} (4)

Using equations (3) and (4) we can derive an equation relating tension and velocity in an arbitrary span of the machinery in terms of the velocity of the reference span with no tension. For arbitrary span $j$

$$v_j = (1 + T_j \epsilon) v_{i+1}$$  \hspace{1cm} (5)

provided span $i + 1$ is the reference span.

5 Capstan Equation

![Figure 3: Free body diagram for a differential element of the web and capstan.](image)

We next consider the Capstan roller case. Figure 3 shows the free body diagram for the differential element of the capstan and web. For this diagram, we can write the conservation of mass equation and the force balance equation to describe the relation between the tension and the velocity of the web as it passes around the capstan.
5.1 Conservation of Mass Equation

(time rate change in mass) = (incoming mass flow) - (outgoing mass flow)

Let

\[ Q = a \rho h v, \quad (Q + \frac{\partial Q}{\partial \theta} d\theta) \]

denote the incoming mass flow and outgoing mass flow respectively. We have the conservation of mass equation

\[ \frac{\partial}{\partial t} (a \rho h (r d \theta)) = Q - (Q + \frac{\partial Q}{\partial \theta} d\theta) \]

Using the equation of state for the web (1) and canceling common factors, we have the following equation

\[ \left( \frac{1 + \epsilon T}{c r} \right) \frac{\partial v}{\partial \theta} = \frac{\partial T}{\partial t} + \left( \frac{v}{r} \right) \frac{\partial T}{\partial \theta} \]  

(6)

5.2 Force Balance Equation

(time rate change in momentum) = (incoming momentum flow) - (outgoing momentum flow) + (forces applied to the element)

Let

\[ Qv = a \rho h v^2, \quad Qv + \frac{\partial (Qv)}{\partial \theta} d\theta \]

denote the incoming and outgoing momentum flows respectively. We have

\[ \frac{\partial}{\partial t} (a \rho h (r d \theta) v) = -T + (T + \frac{\partial T}{\partial \theta} d\theta) + Qv - (Qv + \frac{\partial (Qv)}{\partial \theta} d\theta) - \mu (T d\theta - \frac{1}{2} a \rho h (r d \theta) \frac{v^2}{r}) \]

By canceling the common factor \( d\theta \) and substituting

\[ \frac{\partial (Qv)}{\partial \theta} = v \frac{\partial Q}{\partial \theta} + Q \frac{\partial v}{\partial \theta} \]

we have the equation

\[ a \rho \frac{\partial}{\partial t} (\rho h v) = \frac{\partial T}{\partial \theta} - v \frac{\partial Q}{\partial \theta} - Q \frac{\partial v}{\partial \theta} + \mu (T - \frac{a \rho h v^2}{2}) \]  

(7)

Using equations (1),(6) yields

\[ \left( \frac{a \rho h_0}{1 + \epsilon T} \right) \frac{\partial v}{\partial t} + \frac{a \rho h_0 v}{(1 + \epsilon T)r} \frac{\partial v}{\partial \theta} = \frac{1}{r} \frac{\partial T}{\partial \theta} + \frac{\mu}{r} (T - \frac{a \rho h_0 v^2}{2(1 + \epsilon T)}) \]  

(8)
6 Nipping Roller

Nipping rollers are typically used to drive the web through the machinery. They do this through the friction on the web produced by a normal force exerted on the web by the rollers. See Figure 4.

![Diagram of nipping roller](image)

Figure 4: Free body diagram for a differential element of the web and nipping roller.

In the static case in which tension and velocity of the web are independent of time we may use the static version of the continuity equation, (3). Since this involves both tension and velocity we need another equation, namely a mass flow balance equation,

\[ T_{i+1} - T_i - f_n = Q_{i+1}v_{i+1} - Q_i v_i, \]  

where \( Q_i \) and \( Q_{i+1} \) are mass flow for which we have

\[ Q_j = \rho_j h_j a v_j = \frac{\rho_o h_o a v_j}{1 + T_j \epsilon}. \]

Equation (9) describes the balance of forces on the volume element shown in Figure 4. The system of equations (3) and (9) can be solved provided we know the tension and velocity in either span \( i \) or span \( i + 1 \). In this way we could find all the tensions and velocities in the machinery by solving these coupled systems.

For the dynamic case where tension and velocity do change with time we can use the time dependent version of the continuity equation, (2). Coupling this equation with the differential equation gotten from differentiating equation (9) with respect to \( t \) gives us a system of two differential equations in the unknown functions \( T(t) \) and \( v(t) \). Again by knowing functions describing the tension
and velocity in one span we can solve the differential equations for tension and velocity in adjoining spans.

7 Summary

We can set up a system of algebraic or differential equations which can be used to solve for the tension and velocity of the web in each span. Starting with a span in which the tension and velocity are known we solve for tension and velocity in adjoining spans until all tensions and velocities are known.

8 References


Students' Report
#3

Subgroup 3
Flutter and Resonance of a Moving Paper

IMA Summer Program for Graduate Students
Mathematical Modeling

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1 Introduction

In the designing of a printing machine, one important thing is to avoid the resonance and tearing of the paper. To avoid resonance of the paper, one has to know the natural frequency of the paper. By the existed experimental results, we know that the natural frequency of a printing system is affected by the speed $U_0$ of the moving paper and the density of the air (see Figure 1). By analyzing the mathematical model of the printing system, we get the natural frequency of the system with moving paper and coupled with air; therefore, we can see the effects of the air and the effect of the speed of the paper quantitatively.

To simplify the printing machine system, we make the following assumptions:

$H_1$: $\partial^2/\partial z = 0$ (2-D problem);

$H_2$: paper is linearly elastic 2-D body;

$H_3$: the air is ideal fluid;

$H_4$: dimensionless vertical displacement $v << 1$;

$H_5$: $U = U_0/c_0 < 1$, where $c_0 = \sqrt{T_0/\rho_0}$ is the wave speed in the paper.

Notations:

$x, y, z$: dimensionless coordinates;

$\rho$: density of the air;

$\rho_0$: density of the paper;

$T_0$: tension of the paper in the equilibrium state;

$v$: dimensionless vertical displacement.

2 Analysis of the Models

Case 1: Static without air
To understand the printing system, we study the simplest case first, i.e., the case where $U = 0$ and $\rho = 0$. By the assumption $v << 1$, the mathematical model is

$$\frac{\partial^2 v}{\partial t^2} = \frac{\partial^2 v}{\partial x^2}, \quad 0 < x < 1$$

$$v|_{x=0,1} = 0$$
We get the modes of the problem

\[ v_n = \sin(n\pi x)e^{i\omega_n t}, \quad \omega_n = n\pi \]

Then we study the resonance of the paper. We add a load term on the R. H. S. of the equation to get

\[ \partial^2 v/\partial t^2 = \partial^2 v/\partial x^2 + F(x,t) \]
\[ v|x=0,1 = 0 \]

Consider one frequency load

\[ F(x,t) = e^{i\omega t}f(x) = e^{i\omega t}\sum f_n\sin(n\pi x) \]

To solve the above boundary value problem, we try

\[ v(x,t) = V(x)e^{i\omega t} = e^{i\omega t}\sum v_n\sin(n\pi x) \]

and get

\[ v_n = \frac{f_n}{\omega^2 - \omega_n^2}, \quad \text{where} \quad \omega_n = n\pi \]

\[ v(x,t) = e^{i\omega t}\sum_{n=1}^{\infty} \frac{f_n}{\omega^2 - \omega_n^2} \]

Therefore, the resonance will happen when \( \omega = \omega_n \) for some \( n \), i.e., the resonance frequency is

\[ \omega = n\pi \]

**Case 2: Moving without air**

After studying the above case, we consider the case where the paper is moving. This problem is described by the following equations

\[ (1 - U^2)\partial^2 v/\partial x^2 - 2U\partial v/\partial x \partial t - \partial^2 v/\partial t^2 = 0, \quad 0 < x < 1 \]
\[ v|x=0,1 = 0 \]
Trying \( v(x,t) = e^{i\omega t}V(x) \) we get the equations for \( V(x) \)

\[
(1 - U^2)V'' - 2U\omega iV' + \omega^2 V = 0
\]

\[
V|_{x=0,1} = 0
\]

Making the exponential transformation \( V = e^{\alpha x}W, \alpha = \frac{\omega i}{1 - U^2} \) to cancel the first order term we get

\[
W'' + \frac{\omega^2}{(1 - U^2)^2} W = 0
\]

\[
W|_{x=0,1} = 0
\]

The eigenvalues of the problem are \( \omega_n = (1 - U^2)n\pi \).

The next step is to consider resonance. Adding a forcing term \( F(x,t) = e^{i\omega t}f(x) \) to the original equation we have

\[
(1 - U^2)\frac{\partial^2 v}{\partial x^2} - 2U\frac{\partial^2 v}{\partial x \partial t} - \frac{\partial^2}{\partial t^2} = e^{i\omega t}f(x), \quad 0 < x < 1
\]

\[
v|_{x=0,1} = 0
\]

Trying \( v(x,t) = e^{i\omega t}V(x) \) we get

\[
(1 - U^2)V'' - 2U\omega iV' + \omega^2 V = f(x)
\]

\[
V|_{x=0,1} = 0
\]

Let \( V(x) = e^{\alpha x}W(x) \) with \( \alpha = \frac{\omega i}{1 - U^2} \) we get

\[
(1 - U^2)W'' + \frac{\omega^2}{1 - U^2} W = e^{\frac{-i\omega x}{1 - U^2}}f(x)
\]

\[
W|_{x=0,1} = 0
\]

Eigen-expansion for \( W(x) \) is \( W(x) = \sum \omega_n \sin(n\pi x) \). Let

\[
e^{\frac{-i\omega x}{1 - U^2}}f(x) = \sum f_n \sin(n\pi x)
\]

Then

\[
\omega_n = \frac{(1 - U^2)f_n}{\omega^2 - (1 - U^2)^2(n\pi)^2}
\]
Therefore, the resonance frequency is
\[ \omega = (1 - U^2) n\pi \]

**Case 3:** Static with air
By assumption, ideal fluid \( \mu = 0 \) (viscosity coefficient)
\[ \frac{\partial^2 \phi}{\partial x^2} + \frac{\partial^2 \phi}{\partial y^2} = 0, \quad \text{(Air)} \]
\[ \frac{\partial^2 v}{\partial t^2} - \frac{\partial^2 v}{\partial x^2} = 2\nu \frac{\partial \phi}{\partial t} = 0, \quad \text{(Paper)} \]
\[ \frac{\partial v(x, t)}{\partial t} = \frac{\partial \phi(x, 0, t)}{\partial y}, \quad \text{(Coupled B. C.)} \]
\[ v|_{x=0,1} = 0, \quad \phi|_{x=0,1} = 0 \]

where \( \nu = \rho l/\rho_0 \), and \( l \) is the length of the paper; \( \phi \) is the potential: \( q_x = \frac{\partial \phi}{\partial x}, q_y = \frac{\partial \phi}{\partial y} \).

From the equation and boundary conditions of \( \phi \) we know that
\[ \phi(x, y, t) = a_n(t) e^{-n\pi y} \sin(n\pi x) \]

Trying \( v(x, t) = b_n(t) \sin(n\pi x) \) and using the equation for \( v \), and the coupled
B.C. we get
\[ b''_n + (n\pi)^2 b_n = 2\nu a'_n(t) \]
\[ b'_n = -n\pi a_n \]

Therefore
\[ (1 + \frac{\nu}{n\pi}) b'' + (n\pi)^2 b_n = 0 \]

Trying \( b_n(t) = e^{\omega_n t} \) we get
\[ \omega_n = \frac{n\pi}{\sqrt{1 + 2\nu/n\pi}} \]

So the resonance frequency for this case becomes
\[ \omega = \frac{n\pi}{\sqrt{1 + 2\nu/n\pi}} \]
Since \( \rho = 1.3 \times 10^{-3} \text{g/cm}^3, \rho_0 = 5.4 \times 10^{-3} \text{g/cm}^3 \), so for \( l = 100 \text{cm}, \nu = \rho l / \rho_0 \approx 1/3 \)

**Case 4: Moving with air**

The equations describing this problem are

\[
\begin{align*}
\partial^2 \phi / \partial x^2 + \partial^2 \phi / \partial y^2 &= 0, \quad \text{(Air)} \\
\partial^2 v / \partial t^2 + 2U \partial^2 v / \partial x \partial t - (1 - U^2) \partial^2 v / \partial x^2 &= 2v \partial \phi / \partial t |_{y=0}, \quad \text{(Paper)} \\
\partial v(x,t) / \partial t &= \partial \phi(x,0,t) / \partial y, \quad \text{(Coupled B. C.)} \\
v|_{x=0.1} = 0, \quad \phi|_{x=0.1} = 0
\end{align*}
\]

Trying \( \phi_n = b_ne^{i\omega_n t}e^{-n\pi y \sin(n\pi x)}, \ v_n(x,t) = e^{i\omega_n t}e^{\alpha x}W(x) \) with \( \alpha = \frac{i\omega}{1-U^2} \) we get

\[
W'' + \frac{\omega_n^2}{(1-U^2)^2} W = -\frac{e^{-\alpha x}}{1-U^2} 2\nu i\omega_n b_n \sin(n\pi x)
\]

\[
i\omega_n W = -n\pi b_n \sin(n\pi x)e^{-\alpha x}
\]

\[
W(0) = W(1) = 0
\]

By the second equation we have \( b_n = -\frac{i\omega_n e^{\alpha x} W}{n\pi \sin(n\pi x)} \), plug into the first equation we get

\[
W'' + \frac{\omega_n^2}{(1-U^2)^2} W = -\frac{2\nu \omega_n^2}{(1-U^2)n\pi} W
\]

Try one mode \( W = \sin(n\pi x) \) we have

\[
-(n\pi)^2 + \frac{\omega_n^2}{(1-U^2)^2} = -\frac{2\nu \omega_n^2}{(1-U^2)n\pi}
\]

Therefore the resonance frequency in this case is

\[
\omega = \omega_n \approx \frac{n\pi (1-U^2)}{\sqrt{1 + \frac{2\nu(1-U^2)}{n\pi}}}
\]
3 Summary

According to the above analysis, the air and the speed of the paper all affect the natural frequency of the paper, and therefore the resonance frequency. In order to avoid resonance, one has to take air and speed effect into consideration in the design of the system.

4 Further Directions

We basically studied the case \( U < 1 (U_0 < c_0) \), which is called subsonic case (here sound speed is the one in elastic body). It's easy to see that the problem is ill-posed when \( U > 1 \) by considering the characteristic curves of the model equation

\[
\frac{\partial^2 v}{\partial t^2} + 2U \frac{\partial^2 v}{\partial t \partial x} - (1 - U^2) \frac{\partial^2 v}{\partial x^2} = 0
\]

which are \( x = -(1 + U)t \), \( x = (1 - U)t \). Therefore for \( U > 1 \), the nonlinear effect should be taken into account. Because there is a similarity between our problem and aerodynamic problem, we may expect there will be some shocks when \( U > 1 \) (supersonic case).

![Diagram](image_url)

**Fig 1**
Risk Assessment for Propane
Gas Leakage in Valleys

IMA Summer Program for Graduate Students
Mathematical Modeling

Week 2, Group 1
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Section I: Introduction and Assumptions

Introduction

We want to analyze the risk of explosion resulting from the leakage of propane gas into a valley. Liquefied propane gas has escaped from a pipeline. Since propane is more dense than air the propane has collected in a valley. In the valley the propane has mixed with air to form a combustible mixture. A wind with constant velocity blows across the top of the valley and carries away some of the air/propane mixture.

The combustion proceeds according to this greatly simplified chemical reaction equation:

\[ \text{C}_3\text{H}_8 + 5\text{O}_2 \rightarrow 3\text{CO}_2 + 4\text{H}_2\text{O}. \]  

Hence, since air is approximately one-fifth oxygen, we see that to totally burn all our reactants, we need 25 moles of air for every mole of propane. The risk of explosion is controlled by two factors: (1) the amount of heat that could be produced by the combustion, and (2) the probability of ignition. We have defined the risk of explosion as

\[ \tilde{R} = \int_0^\infty \tilde{Q}(\tilde{t}) p(\tilde{t}) \, d\tilde{t}, \]  

where \( \tilde{Q}(\tilde{t}) \) is the amount of heat released by combustion at time \( \tilde{t} \) and \( p(\tilde{t}) \) is the probability of ignition at time \( \tilde{t} \). Also of interest to us is the sensitivity of the risk of explosions to changes in the wind speed and changes in the initial concentration of propane in the air/propane mixture.

Assumptions

1. The valley has rectangular cross section and is infinitely long (so end effects can be ignored). The valley has uniform depth \( Z \) and uniform width \( X \).
2. Temperature and pressure are constant throughout the valley and surrounding area.
3. The air/propane mixture obeys the ideal gas law. Since the volume of the valley is constant then we know the number of moles of air/propane mixture is constant.
4. At initial time \( \tilde{t} = 0 \) the valley is filled with the air/propane mixture, which has mixed thoroughly. The initial average concentration of propane is \( \tilde{C}_0 \).
5. Wind of constant speed \( U \) blows across the top of the valley.
Section II: Nomenclature

In the notation used below, the subscript $i$ is either 1 (for propane) or 2 (for air).

$A_n$: (used in spatially dependent model) Fourier cosine series coefficient.
$\tilde{A}(\tilde{t})$: (used in rising plume model), area of gas cloud between the limits of the walls of the valley extended into space (units m$^2$), defined by

$$\tilde{A}(\tilde{t}) = X \left[ Z + \tilde{h}(\tilde{t}) \right]$$

(2.1)

$C_l$: minimum volume fraction at which combustion can occur, value 0.022.
$C_m$: stoichiometric limit for combustion, value 1/26.
$C_u$: maximum volume fraction at which combustion can occur, value 0.095.
$\tilde{C}$: concentration of both species, units mol/m.
$\tilde{C}_0$: initial average concentration (units mol/m)
$\tilde{C}_i(\tilde{z}, \tilde{t})$: concentration of species $i$, units mol/m. To be calculated from equations.
$D$: mixing diffusivity of propane and air, units m$^2$/sec.
$\tilde{h}(\tilde{t})$: height of eddy currents in air, units m.
$p$: proportionality constant for probability density, units sec$^{-1}$.
$\tilde{p}(\tilde{t})$: probability of ignition at time $\tilde{t}$, units sec$^{-1}$.
$q$: heat released per mole of substance, units J.
$\tilde{Q}(\tilde{t})$: heat released by an ignition at time $\tilde{t}$, units J.
$\tilde{R}$: heat risk of explosion (units J), defined by

$$\tilde{R} = \int_0^\infty \tilde{Q}(\tilde{t})\tilde{p}(\tilde{t}) d\tilde{t}.$$  

(2.2)

$R_i$: (used in rising plume model) Richardson number.
$\tilde{S}_c$: sensitivity of heat risk to input concentration $\tilde{C}_0$ (units m/mol), defined by

$$\tilde{S}_c = \frac{1}{\tilde{R}} \frac{\partial \tilde{R}}{\partial \tilde{C}_0}.$$  

(2.3)

$\tilde{S}_u$: sensitivity of heat risk to wind speed $U$ (units sec/m), defined by

$$\tilde{S}_u = \frac{1}{\tilde{R}} \frac{\partial \tilde{R}}{\partial U}.$$  

$s$: Laplace transform variable.
$\tilde{t}$: time, units sec.
$\tilde{t}_1$: (used in spatially independent model) time at which $C_1 = C_u$, units sec.
\( \tilde{t}_2 \): (used in spatially independent model) time at which \( C_1 = C_m \) (stoichiometric limit), units sec.
\( \tilde{t}_3 \): (used in spatially independent model) time at which \( C_1 = C_l \), units sec.
\( \tilde{t}_4 \): (used in spatially dependent model) time at which \( \tilde{z}_1 = Z \), units sec.
\( \tilde{t}_5 \): (used in spatially dependent model) time at which \( \tilde{z}_1 = 0 \), units sec.
\( \tilde{t}_6 \): (used in spatially dependent model) time at which \( \tilde{z}_2 = Z \), units sec.
\( \tilde{t}_7 \): (used in spatially dependent model) time at which \( \tilde{z}_2 = 0 \), units sec.
\( \tilde{t}_8 \): (used in spatially dependent model) time at which \( \tilde{z}_3 = Z \), units sec.
\( \tilde{t}_9 \): (used in spatially dependent model) time at which \( \tilde{z}_3 = 0 \), units sec.
\( \tilde{u}_1 \): entrainment velocity, units m/sec.
\( U \): wind velocity, units m/sec.
\( V_e \): amount of air involved in the entrainment process, units m\(^2\).
\( \tilde{x} \): horizontal distance along channel, units m.
\( X \): width of channel, units m.
\( \tilde{z} \): vertical distance along channel, units m.
\( \tilde{z}_1 \): (used in spatially dependent model) height at which \( C_1(z) = C_u \), units m.
\( \tilde{z}_2 \): (used in spatially dependent model) height at which \( C_1(z) = C_m \), units m.
\( \tilde{z}_3 \): (used in spatially dependent model) height at which \( C_1(z) = C_l \), units m.
\( Z \): height of channel, units m.
\( \tilde{Z}_{e1}(\tilde{t}) \): explosion zone (zone where gas will explode if ignited in the flammability zone at time \( \tilde{t} \)) where \( C_1(z) < C_m \), units m.
\( \tilde{Z}_{e2}(\tilde{t}) \): explosion zone (zone where gas will explode if ignited in the flammability zone at time \( \tilde{t} \)) where \( C_1(z) > C_m \), units m.
\( \tilde{Z}_f(\tilde{t}) \): flammability zone (zone where gas can be ignited at time \( \tilde{t} \)), units m.
\( \phi \): the empty set.

Nondimensionalized variables will have no tildes. Laplace transformed quantities have hats.
Section III: Spatially Independent Model

It is assumed the wind blowing across the valley forms a turbulent layer of thickness on the order the height of the ground-based obstructions in its path. This wind layer will carry off propane gas from the valley. Since molecular diffusion of the propane takes place at a much slower rate, the wind is assumed to be the dominant mechanism by which propane is depleted from the valley. We also assume that mixing within the valley occurs at such a rapid rate that concentration differences are instantaneously distributed evenly throughout the valley. Mathematically, we say that $\dot{C}$ is independent of $\ddot{z}$ and is a function of $\dot{t}$ only.

If the turbulent layer has dimension $\ddot{h}$ (measured in meters, which in this model we assume to be a constant), then propane leaves the valley at the rate given by the product of the wind speed, the thickness of the turbulent layer, and the current concentration of propane in the valley. In our nomenclature

$$\frac{d(\dot{C}_1 Z X)}{dt} = -U \ddot{h} \dot{C}_1. \quad (3.1)$$

To nondimensionalize (3.1) we will normalize $\dot{C}_1$ by $C$, all distances by $Z$, and time by the transit time of the wind across the valley, $X/U$. Summarizing, we have the following:

$$C_1 = \frac{\dot{C}_1}{C}, \quad t = \frac{\dot{t} U}{X}, \quad h = \frac{\ddot{h}}{Z}. \quad (3.2)$$

Substituting (3.2) into (3.1) we arrive at the following dimensionless differential equation:

$$\frac{dC_1}{dt} = -h C_1. \quad (3.3)$$

Using the initial condition $C_1(0) = C_0$, this differential equation has solution

$$C_1(t) = C_0 e^{-ht}. \quad (3.4)$$

Whether the propane will ignite and how much will burn (and thus the amount of heat produced) depend on the concentration of propane in the air. If $C_1(t) < C_l = 0.022$ or $C_1(t) > C_u = 0.095$ the air/propane mixture will not ignite. Since five moles of oxygen are required to support the combustion of one mole of propane and since air is approximately one fifth oxygen, if $C_u \geq C_1(t) > C_m = 1/26$ then only $(1 - C_1)Z X/25$ moles of propane will burn before all the oxygen is consumed. If $C_l \leq C_1(t) \leq C_m$ then $C_1 Z X$ moles of propane will burn and there will be oxygen left over. Thus the times at which $C_1$ reaches
these crucial values are of interest. The time at which the propane concentration reaches the upper limit of flammability is

$$t_1 = \max \left\{ 0, -\frac{1}{h} \ln \frac{C_u}{C_0} \right\}. \quad (3.5)$$

The time at which the concentration reaches the point at which all the propane will burn is

$$t_2 = \max \left\{ 0, -\frac{1}{h} \ln \frac{C_m}{C_0} \right\}. \quad (3.6)$$

The air/propane mixture reaches the lower limit of flammability at time

$$t_3 = \max \left\{ 0, -\frac{1}{h} \ln \frac{C_l}{C_0} \right\}. \quad (3.7)$$

If we now consider the equation describing the risk of explosion, we have

$$\tilde{R} = \int_{i_1}^{i_2} \tilde{Q}_1(t) \tilde{p}(t) \, dt + \int_{i_2}^{i_3} \tilde{Q}_2(t) \tilde{p}(t) \, dt. \quad (3.8)$$

The integral involving \( \tilde{Q}_1 \) represents the dimensional form of the heat produced from the burning propane from the time at which the concentration is low enough for ignition to occur until the time at which the concentration of propane is equal to the stoichiometric limit. The second integral is the heat produced from the time at which the concentration of propane is equal to the stoichiometric limit until the time at which the concentration of propane has been lowered to the point at which the air/propane mixture will not burn.

We assume in this case that the probability density is uniform in any time period during which ignition can occur. Hence, we let \( \tilde{p}(t) = p \), where \( p \) is chosen so that the integral of the probability density is 1. Thus equation (3.8) becomes

$$\tilde{R} = pqXZC \left[ \int_{i_1}^{i_2} \frac{1 - C_1(t)}{25} \, dt + \int_{i_2}^{i_3} C_1(t) \, dt \right].$$

Then if we make the substitution \( t = \frac{iU}{X} \) we get

$$\tilde{R} = \frac{pqX^2ZC}{U} \left[ \int_{i_1}^{i_2} \frac{1 - C_1(t)}{25} \, dt + \int_{i_2}^{i_3} C_1(t) \, dt \right]. \quad (3.9)$$

which we can evaluate using equations (3.4)-(3.7) as

$$\tilde{R} = \begin{cases} 
\frac{pqX^2ZC}{hU} \left( \frac{1}{25} \ln \frac{C_u}{C_m} + \frac{C_m - C_u}{25} + C_m - C_l \right) & \text{if } C_u \leq C_0 \\
\frac{pqX^2ZC}{hU} \left( \frac{1}{25} \ln \frac{C_0}{C_m} + \frac{C_m - C_0}{25} + C_m - C_l \right) & \text{if } C_m \leq C_0 < C_u \\
\frac{pqX^2ZC}{hU} (C_0 - C_l) & \text{if } C_l < C_0 < C_m \\
0 & \text{if } C_0 \leq C_l.
\end{cases} \quad (3.10)$$
Thus the sensitivity to changes in wind speed becomes

\[ \tilde{S}_u = \frac{1}{R} \frac{d\tilde{R}}{dU} = \begin{cases} -\frac{1}{U} & \text{if } C_l < C_0 \\ 0 & \text{if } C_0 \leq C_l \end{cases} \]  

(3.11)

The sensitivity to changes in the initial concentration of propane is

\[ \tilde{S}_c = \frac{1}{R} \frac{d\tilde{R}}{dC_0} = \begin{cases} 0 & \text{if } C_u \leq C_0 \\ \frac{1}{25} \ln \frac{C_o}{C_m} + \frac{C_m - C_0}{25} + C_m - C_l & \text{if } C_m \leq C_0 < C_u \\ \frac{1}{C_0 - C_l} & \text{if } C_l < C_0 < C_m \\ 0 & \text{if } C_0 \leq C_l \end{cases} \]  

(3.12)
Risk versus Concentration
Spatially Independent Model

Risk

\[ 0.05 \]
\[ 0.04 \]
\[ 0.03 \]
\[ 0.02 \]
\[ 0.01 \]

\[ C_1 \]
\[ C_m \]
\[ C_u \]
Sensitivity versus Initial Concentration for Spatially Independent Model
Section IV: Spatially Dependent Model

Now we wish to complicate our model somewhat. We assume that the mixing inside the valley is only great enough to guarantee a striated concentrated distribution, rather than a uniform one; i.e., we assume that the concentration profile varies as a function of \( \tilde{z} \) according to a standard Fickian diffusion law:

\[
\frac{\partial \tilde{C}_1}{\partial \tilde{t}} = D \frac{\partial^2 \tilde{C}_1}{\partial \tilde{z}^2}.
\]  
(4.1)

For boundary conditions, we assume that no flux is coming in from the bottom:

\[
\frac{\partial \tilde{C}_1}{\partial \tilde{z}}(0, \tilde{t}) = 0.
\]  
(4.2)

For our boundary condition at \( \tilde{z} = Z \), we look at the following \textit{global} mass balance principle:

\[
X \frac{\partial}{\partial \tilde{t}} \left[ \int_0^{Z+\tilde{h}} \tilde{C}_1(\tilde{z}, \tilde{t}) d\tilde{z} \right] = -U \tilde{h} \dot{C}_1(Z + \tilde{h}, \tilde{t}).
\]  
(4.3)

Equation (4.3) simply states that the change in the amount of propane in the entire system is given by the mixing rate. However, we may simplify equation (4.3) using equation (4.1) to obtain the following:

\[
\left[ D \frac{\partial \tilde{C}_1}{\partial \tilde{z}}(\tilde{z}, \tilde{t}) \right]_0^{Z+\tilde{h}} + \frac{U \tilde{h}}{X} \dot{C}_1(Z + \tilde{h}, \tilde{t}) = 0.
\]

However, since \( \tilde{h} \ll Z \), we may approximate our function values by those at \( Z \). Using equation (4.2), we have

\[
\frac{\partial \tilde{C}_1}{\partial \tilde{z}}(Z, \tilde{t}) + \frac{U \tilde{h}}{DX} \dot{C}_1(Z, \tilde{t}) = 0.
\]  
(4.4)

Now we proceed to nondimensionalize our equations. We normalize \( \tilde{z} \) by \( Z \), our height. Since we are modeling a diffusion process, we normalize \( \tilde{t} \) by the diffusion time scale, \( Z^2/D \). We normalize our \( \tilde{C}_1 \) by \( C \) to get mole fractions. Summarizing, we have the following:

\[
z = \frac{\tilde{z}}{Z}, \quad \tilde{t} = \frac{D \tilde{t}}{Z^2}, \quad C_1 = \frac{\tilde{C}_1}{C}.
\]  
(4.5)

Substituting into equations (4.1), (4.2), and (4.4), we have the following system:

\[
\frac{\partial C_1}{\partial \tilde{t}} = \frac{\partial^2 C_1}{\partial \tilde{z}^2}
\]  
(4.6)
\[
\frac{\partial C_1}{\partial z}(0, t) = 0 \tag{4.7}
\]
\[
\frac{\partial C_1}{\partial z}(1, t) + \frac{Z U h}{D_X} C_1(1, t) = 0 \tag{4.8}
\]
\[
C_1(z, 0) = C_0. \tag{4.9}
\]

Now equation (4.8) tells us that a natural diffusion coefficient for this problem is given by \(Z U h/X\). This is the coefficient we choose. Doing so, equation (4.8) becomes
\[
\frac{\partial C_1}{\partial z}(1, t) + C_1(1, t) = 0. \tag{4.10}
\]

Now we wish to solve our system of equations [(4.6), (4.7), (4.9), and (4.10)] to give us \(C_1\). Unfortunately, exact solutions are always messy and seldom useful. However, we may glean asymptotic information from them to yield results to within the order of accuracy of our assumptions. We begin by postulating a Fourier cosine series expansion:
\[
C_1(z, t) = \sum_{n=1}^{\infty} A_n \exp(-\lambda_n^2 t) \cos(\lambda_n z). \tag{4.11}
\]

The eigenfunctions are guaranteed to be orthogonal in this problem.

This series automatically satisfies equations (4.6) and (4.7). To satisfy equation (4.10), we take one eigenfunction and plug in:
\[
-\lambda_n \sin(\lambda_n) + \cos(\lambda_n) = 0
\]
\[
\lambda_n \tan(\lambda_n) = 1. \tag{4.12}
\]

To solve our initial condition, we see that since the eigenfunctions are orthogonal, we have
\[
A_n = 2 \int_0^1 C_1(z, 0) \cos(\lambda_n z) \, dz
\]
\[
= 2C_0 \int_0^1 \cos(\lambda_n z) \, dz
\]
\[
= \frac{2C_0 \sin(\lambda_n)}{\lambda_n}. \tag{4.13}
\]

Now, since all of our eigenvalues are decaying, we see from equation (4.11) that the eigenvalue corresponding to \(n = 1\) will determine the leading order behavior of our solution for long time. Hence we have
\[
C_1(z, t) \sim \frac{2C_0 e^{-\lambda_1^2 t} \sin(\lambda_1)}{\lambda_1} \cos(\lambda_1 z). \tag{4.14}
\]

This is now our long-time approximation. For reference, \(\lambda_1 = 0.86\).
However, we must be careful when we use the words "long-time". We stated in section I that when \( \tilde{t} = 0 \), the gas had mixed thoroughly. If this is true, we may assume that at our \( \tilde{t} = 0 \) (dawn), the gas has already diffused into the leading order solution. Hence, we may adapt our initial condition to be of the following form:

\[
C_1(z, 0) = A_1 \cos(\lambda_1 z). \tag{4.15}
\]

Since \( C_0 \) is our average initial condition, we have

\[
\int_0^1 C_1(z, 0) \, dz = C_0.
\]

Substituting equation (4.15) into the above and solving for \( A_1 \) gives us the following expression:

\[
A_1 = \frac{C_0 \lambda_1}{\sin \lambda_1}. \tag{4.16}
\]

Now since our initial condition consists of only one eigenfunction, our exact solution becomes

\[
C_1(z, t) = \frac{C_0 \lambda_1 e^{-\lambda_1^2 t}}{\sin \lambda_1} \cos(\lambda_1 z). \tag{4.17}
\]

Now that we have an expression for \( C_1 \), we may construct an expression for our risk. We know that the dimensional risk is the following:

\[
\tilde{R} = \int_0^\infty \tilde{Q}(\tilde{t}) \tilde{p}(\tilde{t}) \, d\tilde{t}. \tag{4.18}
\]

Hence we need to know \( \tilde{Q} \) and \( \tilde{p} \). We first postulate that the probability of explosion at any time \( \tilde{t} \) is proportional to the volume of gas in the flammability zone, hence we assume \( \tilde{p} = p|\tilde{Z}_f(\tilde{t})| \).

For \( \tilde{Q}(\tilde{t}) \), we make the following argument: if gas in the flammability zone explodes above gas that is not in the flammability zone, then the pressure from the explosion will force the gas below the explosion into a new flammability zone caused by the fact that increased pressure changes our flammability limits. Hence, any explosion automatically uses up all gas from \( \tilde{Z} = 0 \) to the top of the flammability zone. We call this extended region the explosion zone. However, the converse is not true. If gas explodes below gas not in the flammability zone, the pressure wave will disperse the gas and not explode it.

The heat \( \tilde{Q} \) is going to depend only on the concentration of the rate-controlling reactant at any point and time. The discussion of how to determine this was given in section II. Hence we may represent the risk symbolically by the following:

\[
\tilde{R} = \int_{\tilde{t}_4}^{\tilde{t}_0} \text{p}|\tilde{Z}_f(\tilde{t})| \left\{ \int_{\tilde{Z}_{c1}(\tilde{t})}^{\tilde{Z}_{c2}(\tilde{t})} qX \tilde{C}_1(z, t) \, dz + \int_{\tilde{Z}_{c2}(\tilde{t})}^{\tilde{Z}_{c2}(\tilde{t})} qX \left[ \frac{1 - \tilde{C}_1(z, t)}{25} \right] \, dz \right\} \, d\tilde{t}.
\]
Nondimensionalizing the right-hand side, we have the following:

\[
\tilde{R} = \frac{pqX^2Z^2C}{\bar{h}U} \int_{t_4}^{t_9} p|Z_f(t)| \left\{ \int_{Z_{e1}(t)}^{Z_{e2}(t)} qXC_1(z,t) \, dz + \int_{Z_{e1}(t)}^{Z_{e2}(t)} qX \left[ \frac{1 - C_1(z,t)}{25} \right] \, dz \right\} \, dt.
\]  

(4.19)

From equation (4.19), it is clear that \( \tilde{R} \) is proportional to \( 1/U \). Hence, we have the following:

\[
\tilde{S}_u = \frac{1}{\tilde{R}} \frac{\partial \tilde{R}}{\partial U} = -\frac{1}{U}.
\]  

(4.20)

Note that equation (4.24) agrees with the results from model 1.

To calculate \( \tilde{S}_c \), we must be more careful. We have calculated that \( t_j < t_{j+1} \), \( j = 4, 5, \ldots \). However, \( |Z_f(t)| \) and \( Z_e(t) \) are different. Here is a brief summary of our regions for different time periods:

\[
\begin{align*}
t_4 < t < t_5 &: Z_f(t) = (z_1(t), 1); & Z_{e1}(t) = \phi; & Z_{e2}(t) = (0, 1) \\
t_5 < t < t_6 &: Z_f(t) = (0, 1); & Z_{e1}(t) = \phi; & Z_{e2}(t) = (0, 1) \\
t_6 < t < t_7 &: Z_f(t) = (0, 1); & Z_{e1}(t) = (z_2(t), 1); & Z_{e2}(t) = (0, z_2(t)) \\
t_7 < t < t_8 &: Z_f(t) = (0, 1); & Z_{e1}(t) = (0, 1); & Z_{e2}(t) = \phi \\
t_8 < t < t_9 &: Z_f(t) = (0, z_3(t)); & Z_{e1}(t) = (0, z_3(t)); & Z_{e2}(t) = \phi.
\end{align*}
\]  

(4.21)

The integral is quite complicated and was done numerically using a rectangular rule. Graphs of the risk versus the initial concentration \( C_0 \) and graphs of the sensitivity \( \tilde{S}_c \) versus the initial concentration \( C_0 \) follow.
Combustion Sequence

$t_4$ (too much propane)

$t_5$

$t_6$

$t_7$

$t_8$

$t_9$ (too little propane)
Risk versus Initial Concentration for Spatially Dependent Model
Sensitivity $S_c$ versus Initial Concentration for Spatially Dependent Model
Section V: Consideration of Entrainment

Introduction

In model I and II, we ignored the physical process of entrainment. It is the process by which air is mixed into the gas cloud (propane-air mixture) due to turbulence from shear flow of pure air passing the cloud. This process will effectively increase the height \( H \) of the cloud above the valley, thus resulting in a faster dissipation.

Because the gas is at constant temperature and pressure and we have assumed an ideal gas, the volume balance gives us:

\[
\frac{\partial (LA)}{\partial t} = \frac{\partial V_e}{\partial t} - ULH
\]

where \( L \) is a standard length of the valley, and \( A \) is the cross-sectional area of the cloud. Thus, the volume of gas changes as a result of the entrained air minus the volume of gas blown beyond the valley. Assuming \( V_e \) as a volume per length, the equation becomes

\[
\frac{\partial A}{\partial t} = \frac{\partial V_e}{\partial t} - UH \tag{5.1}
\]

The other governing equation comes from model I, with the well-mixed cloud assumption, namely, the propane balance equation:

\[
\frac{\partial (C_1 A)}{\partial t} = -UC_1 H \tag{5.2}
\]

Using the "box model" for entrainment, we assume that the shape of the cloud, after slumping, maintains a rectangular cross-section, and thus \( A = X(Z + H) \). Also for this model

\[
\frac{\partial V_e}{\partial t} = \frac{\alpha^3 \rho_a XU^3}{(\rho - \rho_a)gH} \tag{5.3}
\]

where \( \alpha \) is the ratio of entrainment velocity to wind velocity. We assume from other similar experiments, that \( \alpha = 0.0532 \). Since the molecular weight of \( C_3H_8 \) is 44 and the average molecular weight of air is 29, and the air and the gas have the same concentration because of the constant temperature and pressure, we have

\[
\rho = 44C_1 + 29C_2 = 44C_1 + 29(C - C_1) = 15C_1 + 29C = 15C_1 + \rho_a
\]

thus

\[
\rho - \rho_a = 15C_1.
\]
Therefore (3) can be written as

$$\frac{\partial V_s}{\partial t} = \frac{\alpha^3 \rho_u X U^3}{15C_1 g H}.$$ (5.4)

Substituting this result in (1) and introducing the following dimensionless variables

$$t = \frac{U}{X} \tilde{t}, \quad x_1 = \frac{C_1(Z + H)}{CZ}, \quad x_2 = \frac{H}{Z}$$

we can transform governing equations (1) and (2) to the following dimensionless form

$$\frac{dx_1}{dt} = -\frac{x_1 x_2}{1 + x_2}$$

$$\frac{dx_2}{dt} = a \frac{1 + x_2}{x_1 x_2} - x_2$$

where

$$a = \frac{\alpha^3 \rho_u U^2 X}{15g Z^2 C}.$$ 

**Phase Plane Analysis**

The equations for $x_1, x_2$ are nonlinear autonomous ODEs. We can perform a phase plane analysis to reveal some features of a solution of the system of ODEs. From the above equations we have

$$\frac{dx_2}{dx_1} = \frac{(1 + x_2)[x_1 x_2^2 - a(1 + x_2)]}{x_1^2 x_2^2}$$

The trajectories of $(x_1, x_2)$ are shown on the following phase plane diagram. On the phase plane, we see that for various starting concentrations, there is an initial large increase in $x_2$ (the cloud height) followed by a drop in concentration with a slower height increase.

**Numerical Analysis**

Since we could not get a closed-form solution of the nonlinear system, we performed numerical calculations.

The Runge–Kutta method of order 4 has been used to solve the system with time step size 0.001 for the given values of $C_0$ and $U$. We then used the numerical solution to determine the risk, $R$, using a trapezoid rule integrating scheme, based on the two-integral formula from model I. The forward difference formula was used to approximate the sensitivities $S_U = \frac{1}{R} \frac{\partial R}{\partial U}$ and $S_{C_0} = \frac{1}{R} \frac{\partial R}{\partial C_0}$ for this model.
Height of Propane Plume
versus Time, Entrainment
Model
Value of Concentration versus Time for Entrainment Model
Risk versus Initial Concentration $C_0$ for Entrainment Model
Sensitivity $S_c$ versus Initial Concentration $C_0$ for Entrainment Model
Risk versus Wind Speed U
for Entrainment Model
Sensitivity $S_u$ versus 
Wind Speed $U$ for Entrainment Model
Velocity Field Superimposed on Graph of Height of Plume versus Concentration
Section VI: Conclusions and Future Research

Conclusions

Throughout each of our three models, we found a clear dependence of risk on the important physical parameters of wind velocity $U$ and initial average concentration of propane in the valley $C_0$. In the first model, the dependence was found in closed form as the sensitivity $\hat{S}_u = -1/U$ and as $\hat{S}_c$, which is graphed in Figure 1. The second model, which incorporated diffusion, also resulted in the closed form solution $\hat{S}_u = -1/U$. The sensitivity $\hat{S}_c$, calculated numerically, appeared to qualitatively agree with the first model. The entrainment model also gave numerical solutions for $\hat{S}_u$ and $\hat{S}_c$ with $\hat{S}_c$ again qualitatively unchanged. However, the risk now appears to be proportional to $U^\alpha$ for some $\alpha \in (-4, -3)$ rather than $\alpha = -1$ as in the other models. Note that the sensitivity and the risk are related as: $\hat{S}_u = \alpha/U$ is equivalent to $R(C_0, U) = K(C_0)U^\alpha$.

Since each model with its own key assumptions produces physically reasonable results, further work needs to be performed to study, modify, and develop these models to determine the most accurate process representative.

Future Research

Future work on this project could be directed towards the following:

1. combining the diffusion and entrainment models.
2. working with more complicated geometric valley shapes, such as triangular and semicircular valleys. We could also vary the aspect ratio of our valleys.
3. modeling the explosion process in the valley and the effects of ignition location.
4. modeling continuous propane leaks.
5. checking our results against any data available.

These efforts would hopefully then lead to a clearer understanding of the relationship between risk and $U$ and $C_0$ as measured by the calculated sensitivities.
Students' Report
#5
IMA Summer Program for Graduate Students

Mathematical Modeling

Model of Radionuclide Contaminants in an Aquifer

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1 Introduction

In the past, thousands of canisters containing radioactive waste were buried in the ground. Unfortunately, some of the containers end up acting as sieves, and the radioactive waste is subject to leaching. An offset fault, which results in ground water coming in contact with a portion of the canisters, constitutes a leach incident. In one particular example, 62,500 canisters of C-14, each with a volume of $2.22 \times 10^5 \text{cm}^3$ are buried. Of these canisters, 250 are subject to leaching at a time.  

The primary concern of this report is to get some understanding of the amount of material released as a function of time at a fixed distance away from the site. We will not be concerned with how the radioactive waste gets into the aquifer.

2 Nomenclature

\[
\begin{align*}
 b &= \text{non-dimensional coefficient in convection term of governing equation} \\
 k &= \text{non-dimensional coefficient in radioactive decay term} \\
 k_1 &= \text{constant in Darcy's law } [L^3 T M^{-1}] \\
 n &= \text{porosity of porous medium } = \text{volume of void } / \text{total volume} \\
 p(x, t) &= \text{pressure } [MT^{-2} L^{-1}] \\
 t &= \text{time } [T] \\
 v(x, t) &= \text{velocity of the fluid } [LT^{-1}] \\
 x &= \text{the direction of fluid flow } [L] \\
 C(x, t) &= \text{concentration of radioactive material } [ML^{-3}] \\
 C_0 &= \text{input concentration at a fixed time} \\
 D(v, n) &= \text{diffusivity & dispersion constant (Fick's law) } [L^2 T^{-1}] \\
 E(v, n) &= \text{convection constant } [LT^{-1}], \text{in this report we assume } E = v. \\
 J(x, t) &= \text{flux density of radioactive material } [ML^{-2} T^{-1}] \\
 Q(\bar{x}, T) &= \text{total amount of radionuclide to flow past the downflow location } \bar{x} \text{ from time zero to } T \\
 L &= 500 \text{ meters } \approx \text{distance between point of contamination and point of concentration measurement} \\
 T &= 800 \text{ years } = \text{approximate time of interest} \\
 \lambda &= \text{radioactive decay constant } [T^{-1}]
\end{align*}
\]

3 Governing Equations

In our model, we would like to include, diffusion (the spreading of material due to molecular movement), convection (the movement of the material due to the velocity of the aquifer), radioactive decay, and possibly adsorption (the loss of material due to its reaction with the surrounding porous medium, i.e. lodging, chemical reaction, etc.).

To model diffusion, we will assume that Fick’s Law is applicable:

\[ J = -D \frac{\partial C}{\partial x}. \]

Here we assume that all forms of diffusion, including molecular diffusion and mechanical dispersion, can be expressed in the above form. In general, \( D \) will be non-constant, depending on the velocity of the aquifer and the position and time. For this report, we will assume \( D \) is constant. To include the radioactive decay we use:

\[ \frac{\partial C}{\partial t} = -\lambda C. \]

And for adsorption we have

\[ \frac{\partial C}{\partial t} = f(C). \]

For our problem, the total flux density will be due to diffusion and convection, e.g.

\[ J = -D \frac{\partial C}{\partial x} + EC. \]

In general, \( E \) may depend on the velocity and porosity, but here we will assume that \( E = v \).

Using the conservation of mass yields the equation of motion

\[ \frac{\partial C}{\partial t} = -\frac{\partial J}{\partial x} - \lambda C - f(C). \]

Finally, substituting the equation for the total flux density into the above equation yields

\[ \frac{\partial C}{\partial t} = D \frac{\partial^2 C}{\partial x^2} - v \frac{\partial C}{\partial x} - \lambda C - f(C). \]

We now would like to non-dimensionalize our governing equation. To simplify the problem further, we shall assume that \( v \) and \( \rho \) are constant with respect to \( x \). Let

\[ \hat{x} = x/L \quad \hat{t} = t/T \quad \hat{v} = v/L \quad \hat{C} = C/C_0 \]

so that the governing equation becomes

\[ \frac{\partial \hat{C}}{\partial \hat{t}} = \frac{DT}{L^2} \frac{\partial^2 \hat{C}}{\partial \hat{x}^2} - \hat{v} \frac{\partial \hat{C}}{\partial \hat{x}} - \lambda T \hat{C} \]

where \( \frac{DT}{L^2} = \frac{3}{250}, \frac{vT}{L} = 2, \lambda T = 0.6, \) and \( \lambda T = 6 \times 10^{-3} \).

By examining these parameters, \( \frac{DT}{L^2} \) will be taken to be \( \varepsilon \). Note that \( 6 \times 10^{-3} \) is of the same order as \( \varepsilon \); however, since the radioactive decay is an important element, this will remain in our model. For the remainder of the paper we will use the governing equation in the following form:

\[ u_t = \varepsilon u_{xx} - b(t)u_x - ku. \]
4 Perturbation Analysis

4.1 Zeroth Order Approximation

The equation we are considering is

\[ u_t = \varepsilon u_{xx} - b(t)u_x - ku. \]

Initially, we are considering \( \varepsilon = 0 \) and \( b(t) = \text{constant} \). Thus, we are solving

\[ u_t = -bu_x - ku \]

which is a first order, linear, partial differential equation. The domain is

\[ (x, t) \in (0, \infty) \times (0, \infty), \]

with the conditions that \( u(x, 0) = 0 \) and \( u(0, t) = f(t) \). This equation can be solved exactly by the method of characteristics. The equation can be rewritten as

\[ (b, 1) \cdot \nabla u = -ku \]

The characteristics are given by

\[ \frac{dx}{ds} = b \quad \text{and} \quad \frac{dt}{ds} = 1. \]

Hence,

\[ x = bs + x_0 \quad \text{and} \quad t = s + t_0 \]

Along the characteristics, we get

\[ \frac{du}{ds} = -ku. \]

Thus the solution is

\[ u = \alpha \exp(-ks). \]

Consider the piecewise smooth curve given by the positive \( x \)- and \( t \)-axes. Parametrize this curve by \( \tau \) such that on the positive \( t \)-axis, \( \tau = t \), and on the positive \( x \)-axis, \( \tau = -x \). The initial condition for \( u \) is given on this curve. For \( \tau > 0 \), we have \( u(0) = f(\tau) \), \( t_0 = \tau \) and \( x_0 = 0 \). Thus in this region,

\[ x = bs \]
\[ t = s + \tau \]

\[ \Rightarrow \quad s = \frac{\tau}{b} \quad \text{and} \quad \tau = t - \frac{x}{b} \]

Hence,

\[ u(x, t) = f(t - \frac{x}{b}) \exp \left( -k \frac{x}{b} \right). \]

If \( \tau < 0 \), then \( u(0) = 0 \), \( x_0 = -\tau \) and \( t_0 = 0 \). So in this region,

\[ x = bs - \tau \]
\[ t = s \]

\[ \Rightarrow \quad s = t \quad \text{and} \quad \tau = bt - x \]

and the solution is \( u \equiv 0 \).
First Order Approximation with \( f(t) = \frac{1}{1+\log(1+t)} \)

We are also interested in the case \( b = b(t) \). The equations for the characteristics become

\[
\begin{align*}
t &= s + t_0 \\
x &= x_0 + \int_0^t b(\sigma + t_0) \, d\sigma.
\end{align*}
\]

There will be a distinguished characteristic through the origin below which \( u \equiv 0 \), i.e. if \( x < \int_0^t b(\sigma) \, d\sigma \). Above this characteristic, i.e. \( x > \int_0^t b(\sigma) \, d\sigma \), we must solve for \( s \) and \( \tau \) from the equations

\[
\begin{align*}
t &= s + \tau \\
x &= \int_0^\tau b(\sigma + \tau) \, d\sigma.
\end{align*}
\]

### 4.2 Regular Perturbation

We will now try to find out more about what is actually going on by considering the equation we started out with and writing:

\[ u(x, t) = u_0(x, t) + \varepsilon u_1(x, t) + O(\varepsilon^2) . \]

Above we found \( u_0 \) to be

\[
u_0(x, t) = \begin{cases} 
 f(t - \frac{x}{\varepsilon}) \exp \left( -k\frac{x}{\varepsilon} \right) & \text{for } x < bt \\
0 & \text{for } x > bt
\end{cases}
\]
which, in terms of our coordinates along the characteristics, is

\[ u_0(x, t) = \begin{cases} \frac{f(\tau)}{\tau} \exp(-ks) & \text{for } \tau > 0 \\ 0 & \text{for } \tau < 0 \end{cases} \]

If we put \( u \) into our differential equation and neglect terms of order \( \varepsilon^2 \) and higher, we find

\[ u_{0,t} + \varepsilon u_{1,t} = \varepsilon(u_{0,xx} + \varepsilon u_{1,xx}) - b(t)(u_{0,x} + \varepsilon u_{1,x}) - k(u_0 + \varepsilon u_1) \]
\[ = -b(t)u_{0,x} - ku_0 + \varepsilon(u_{0,xx} - b(t)u_{1,x} - ku_1) \]

Since the boundary conditions are

\[ u(0, t) = f(t) \quad \text{and} \quad u(x, 0) = 0 \]

these translate as follows for our new set of equations which we get on comparing coefficients in the PDE above:

\[ u_0(0, t) = f(t) \quad \text{and} \quad u_0(x, 0) = 0 \]
\[ u_1(0, t) = 0 \quad \text{and} \quad u_1(x, 0) = 0 \]

We have already done the calculations for \( u_0 \) and for \( u_1 \) we end up with the following PDE

\[ u_{1,t} = u_{0,xx} - b(t)u_{1,x} - ku_1 \]

along with the homogeneous boundary conditions

\[ u_1(0, t) = 0 \quad \text{and} \quad u(x, 0) = 0 . \]

Therefore we need to compute

\[ u_{0,xx} = \frac{1}{b^2} \left[ f''(t - \frac{x}{b}) + 2k f'(t - \frac{x}{b}) + k^2 f(t - \frac{x}{b}) \right] \exp(-k \frac{x}{b}) . \]

This is valid only for \( x < bt \) and obviously

\[ u_{0,xx} = 0 \]

for \( x > bt \).

Since we will again employ the method of characteristics in order to solve our PDE, we will have to express \( u_{0,xx} \) in terms of \( s \) and \( \tau \). We find

\[ u_{0,xx} = \begin{cases} g(\tau) \exp(-ks) & \text{for } \tau > 0 \\ 0 & \text{for } \tau < 0 \end{cases} \]

where

\[ g(\tau) = \frac{1}{b^2} \left[ f''(\tau) + 2k f'(\tau) + k^2 f(\tau) \right] . \]

Therefore, we need to solve

\[ u_{1,s} = \begin{cases} -ku_1 + g(\tau) \exp(-ks) & \text{for } \tau > 0 \\ -ku_1 & \text{for } \tau < 0 \end{cases} \]

subject to

\[ u_1(0) = 0 \]

(both boundary conditions, of which just one is applicable for either of the two cases \( \tau > 0 \) or \( \tau < 0 \) translate to the same initial conditions !).
4 PERTURBATION ANALYSIS

The general solution to homogeneous form of the above ODE is

\[ u_1 = h(\tau)\exp(-ks) \]

so that for \( \tau < 0 \), where the homogeneous equation is all we have to look at, we find by exploiting the initial condition:

\[ u_1 \equiv 0. \]

However, for \( \tau > 0 \) we need to compute a special solution of the nonhomogeneous ODE we are concerned with, which will be of the form

\[ u_1(s, \tau) = (A(\tau) + B(\tau)s)\exp(-ks). \]

Our ODE then tells us

\[ u_1,\tau = -ku_1 + B(\tau)\exp(-ks) \]

Therefore we find

\[ B(\tau) = g(\tau) \]

and the initial condition at \( s = 0 \) then reveals

\[ A(\tau) = 0. \]

Therefore

\[ u_1(s, \tau) = \begin{cases} g(\tau)s\exp(-ks) & \text{for } \tau > 0 \\ 0 & \text{for } \tau < 0 \end{cases} \]

Our first order approximation using regular perturbation thus turns out to be

\[ u(s, \tau) = \begin{cases} u_0(s, \tau) + \varepsilon g(\tau)s\exp(-ks) & \text{for } \tau > 0 \\ 0 & \text{for } \tau < 0 \end{cases} \]

or, in terms of \( x \) and \( t \),

\[ u(x, t) = \begin{cases} u_0(x, t) + \varepsilon g(t - \frac{x}{b})\exp(-k\frac{x}{b}) & \text{for } x < bt \\ 0 & \text{for } x > bt \end{cases} \]

Thus, we did not find what we had expected to find at first, namely that a perturbation analysis of the kind we just performed would give insight as to what is happening in the boundary layer that exists around the line \( x = bt \). On the contrary, our first order regular approximation preserves this line and just makes the formulas we think will govern the solution outside said boundary layer a little more accurate in the regions where they apply. To find out more about the boundary layer we will therefore have to perform a singular perturbation analysis, which we will do in the next subsection.

4.3 Solution by the singular perturbation method:

We assume that \( b(t) = b \) is constant in time. The equation we want to solve is

\[ \frac{\partial u}{\partial t} = \varepsilon \frac{\partial^2 u}{\partial x^2} - b \frac{\partial u}{\partial x} - ku \]

with the following initial and boundary conditions:

\[ u(x, 0) = 0 \text{ and } u(0, t) = f(t) \]
First we set $\varepsilon$ to zero and compute the solution $u$ without diffusion by the method of characteristics:

$$u(x, t) = \begin{cases} f(t - \frac{x}{b}) \exp\left(-k\frac{x}{b}\right) & 0 < x < bt \\ 0 & x > bt \end{cases}$$

Since the equation is parabolic, we know that our solution must be smooth. But the solution $u$ has a jump along the characteristic $x = bt$ which results from neglecting the diffusion term in the original equation. This is because we have very large gradients in a neighborhood of the moving wave front and therefore the term $u_{xx}$ is important. In perturbation theory this region is referred to as the 
boundary layer.

We now magnify the boundary layer by introducing the new variables $\tilde{x}$ and $w$:

$$\tilde{x} = \frac{x - bt}{\varepsilon^\alpha}, \quad w(\tilde{x}, t) = u(x, t)$$

$u$ is called the outer solution and $w$ is called the inner solution.

The equation then becomes:

$$\frac{\partial w}{\partial t} = \varepsilon^{1-2\alpha} \frac{\partial^2 w}{\partial \tilde{x}^2} - kw$$

Therefore we must choose $\alpha = 1/2$ to balance the terms in the equation. This yields:

$$\frac{\partial w}{\partial t} = \frac{\partial^2 w}{\partial \tilde{x}^2} - kw$$

To obtain the boundary conditions for $w$ we write both the inner and the outer solutions in terms of an intermediate variable

$$x_\eta = \frac{(x - bt)}{\eta(\varepsilon)}, \quad \text{where } \varepsilon^{1/2} < \eta(\varepsilon) < 1.$$ 

Then,

$$\tilde{x} = x_\eta \frac{\eta}{\varepsilon^{1/2}}$$

As $\varepsilon \to 0$, for fixed $x_\eta$,

$$\tilde{x} \to \infty, \quad x > bt$$

$$\tilde{x} \to -\infty, \quad x < bt$$

Imposing now that $u$ and $w$ coincide at $x_\eta$ as $\varepsilon \to 0$, we obtain the following boundary conditions for $w$:

$$w \to 0 \quad \text{as } \tilde{x} \to \infty$$

$$w \to f(0) \exp(-kt) \quad \text{as } \tilde{x} \to -\infty$$

and the initial condition

$$w(\tilde{x}, 0) = \begin{cases} 0 & \tilde{x} \geq 0 \\ f(0) & \tilde{x} < 0 \end{cases}$$

Now we define $v$ by

$$w(\tilde{x}, t) = \exp(-kt)v(\tilde{x}, t).$$
5 Extensions of the Model

5.1 Change of velocity

5.1.1 Introduction

Due to changes in the medium and environment in which an aquifer is located, there will occasionally be deviation from the normal rate of flow. Typically, as in the case of a surface water increase to the 100 year flood levels or due seismic events, the flow rate of the aquifer could jump by a factor of five for a very short period.

For this type of occurrence we model the increase in amount of radionuclide that will pass a location in the downflow direction. We will denote the total amount of radionuclide to flow past the downflow location, \( z^* \), from time zero to time \( t = T \) as \( Q(z^*; T) \).
5 EXTENSIONS OF THE MODEL

5.1.2 Error Bounds

As an initial estimate of $Q(x^*;T)$, we present upper and lower bounds. The equations we have, considering $b = b(t); \tau > 0$, are

$$\frac{du}{ds} = -ku \quad u(s = 0, \tau) = f(\tau)$$
$$\frac{dx}{ds} = b(t) \quad x(s = 0, \tau) = 0$$
$$\frac{dt}{ds} = 1 \quad t(s = 0, \tau) = \tau.$$

Thus

$$t = s + \tau$$
$$x = \int_0^s b(\sigma + \tau)d\sigma$$
$$u(s, \tau) = f(\tau)\exp(-ks)$$

Now we have

$$x^* = \int_0^{s=t-\tau} b(\sigma + \tau)d\sigma \quad \tau \in (0, t_m), \quad t \in (t_n, T)$$

with

$t_n$ = the first time at which the concentration $u(x^*, t)$ is not zero
$t_m$ = the time at which the radionuclide seen at $(x^*, \text{time} = T)$ was released at $x = 0$.

With $b_1$ and $b_2$ as the lower and upper bounds for the flow rate,

$$b_1 \leq b(t) \leq b_2 \quad t \in (0, T)$$
$$b_1s \leq x^* \leq b_2s$$
$$b_1(t - \tau) \leq x^* \leq b_2(t - \tau)$$

To get an estimate for $t_n$, let $\tau = 0$. Then

$$b_1t_n \leq x^* \leq b_2t_n$$
$$\frac{x^*}{b_2} \leq t_n \leq \frac{x^*}{b_1}.$$

To estimate $t_m$, let $t = T$. Then

$$b_1(T - t_m) \leq x^* \leq b_2(T - t_m)$$
$$T - \frac{x^*}{b_1} \leq t_m \leq T - \frac{x^*}{b_2}.$$

Therefore,

$$Q(x^*; T) = 0 \quad \text{if} \quad T < t_n$$

If $T > t_n$

$$Q(x^*; T) = \int_{t_n}^{T} u(x, t)dt = \int_0^{t_m} u(s, \tau)d\tau = \int_0^{t_m} f(\tau)\exp(-ks)d\tau.$$
Since \( \frac{\epsilon^*}{b_2} \leq s \leq \frac{\epsilon^*}{b_1} \),

\[
\exp \left( -k \frac{x^*}{b_1} \right) \int_0^{T - \frac{x^*}{b_1}} f(\tau) d\tau \leq Q(x^*; T) \leq \exp \left( -k \frac{x^*}{b_2} \right) \int_0^{T - \frac{x^*}{b_2}} f(\tau) d\tau
\]

5.1.3 Expected Value

The error bounds for \( Q(x; t) \) given above can be a poor approximation. This occurs if \( b_1 = \min b(t) \) and \( b_2 = \max b(t) \) are very far apart or if the average value of \( b(t) \) is closer to either \( b_1 \) or \( b_2 \). To give a better estimate of what should be expected values of \( Q(x; t) \) it is reasonable to consider

\[
b^*(t) = \frac{\int_0^t b(\sigma) d\sigma}{t};
\]

the average of the flow rate from time 0 to \( t \).

So consider

\[
Q(x; t) = \exp \left( -k \frac{x}{b^*(t)} \right) \int_0^{T - \frac{x}{b^*(t)}} f(\tau) d\tau.
\]

This estimate for \( Q(x; t) \) can be shown to be the least-square error approximation.

To consider the specific example where the flow velocity is increased by a factor of 5

\[
b(t) = \begin{cases} 
2 & 0 \leq t \leq 5 \\
10 & 5 \leq t \leq 6 \\
2 & t > 6
\end{cases}
\]

Then the characteristics can be seen in the figure below:
Recall that the dimensional values for position are evaluated by a factor of $\frac{1}{2}$ kilometer:

\[ x^* = 22 \Rightarrow x^* = 11 \text{ km}. \]

Also, for time a factor of 10 years is used. Thus, the flow increase from time $5 \leq t \leq 6$ corresponds to an actual increase over the ten year period from years 50 to 60. In an actual analysis for flow increase to be realistic, the increase should be taken over a one year period. Given that, we have the following exact solution:

\[
Q(x^* = 22; t) = \begin{cases} 
0 & 0 \leq t \leq 7 \\
\int_0^{1-7} \exp(-7k) f(\tau) d\tau & 7 \leq t \leq 12 \\
Q(22; 12) + \int_5^{12} \exp(-(4\tau - 13)k) f(\tau) d\tau & 12 \leq t \leq 17 \\
Q(22; 17) + \int_6^{11} \exp(-11k) f(\tau) d\tau & t > 17 
\end{cases}
\]

Notice that the lower bound is equivalent to the solution, where $b(t)$ is a constant value of 2. The effect of the increase in the flow for a period of time makes a dramatic change in the total amount of radionuclide that passes the downflow location. This increase is due to the flow actually reaching the location sooner and, while traveling faster, having less time to decay.

### 5.2 Adsorption

In the problem contaminated water is flowing through a porous medium. The contaminating species can form physico-chemical bonds to the surface of the medium. This phenomenon is called adsorption. Let
5 EXTENSIONS OF THE MODEL

R = free contaminant (e.g. radionuclide)
S = free adsorption site
RS = contaminant-site complex.

The situation can be modeled by a chemical reaction

\[ R + S \xrightarrow{k_1} RS \]
\[ RS \xrightarrow{k_2} R + S \]

\(k_1\) and \(k_2\) are rate constants for the reactions. Now let

\[ u = \text{concentration of } R \]
\[ v = \text{concentration of } RS \]
\[ A = \text{total concentration of adsorption site, bound and free, a constant.} \]

Note that \(k_1, k_2, \text{and } A\) are empirical constants. The concentration of \(S\) is then \(A - v\).

If the above reaction was occurring in a beaker the equations would be

\[ \frac{du}{dt} = k_2 v - k_1 u(A - v) \]
\[ \frac{dv}{dt} = -\frac{du}{dt} \]

but here extra terms and an extra equation are added to the model:

\[ \frac{\partial u}{\partial t} = \varepsilon u_{xx} - bu_x - ku + k_2 v - k_1 u(A - v) \]
\[ \frac{\partial v}{\partial t} = k_1 u(A - v) - k_2 v - kv \]

which is a reaction-diffusion system. (The \(kv\) term represents decay of \(R\) in the \(RS\) complex). Actually the system is more complicated than this. The reaction

\[ R \xrightarrow{k} R^* \]

represents the radioactive decay of \(R\) to some other species \(R^*\) (which is the source of the \(ku\) term). To fully model adsorption in this way requires consideration of the following reactions,

\[ R + S \xrightarrow{k_1} RS \]
\[ RS \xrightarrow{k_2} R + S \]
\[ RS \xrightarrow{k} R^* S \]
\[ R^* S \xrightarrow{k_3} R^* + S \]
\[ R^* + S \xrightarrow{k_4} R^* S \]

which would lead to a still larger system of equations.
Rather than pursuing this, an adsorption model in analogy with population dynamics has the form
\[ \alpha u(u - \beta), \]
where \( \beta \) represents a "carrying capacity." \( \beta \) is not a true carrying capacity since in principle \( u \) can exceed \( \beta \). However, if \( u \) is normalized so that the maximum expected value of \( u \) is less than \( \beta \), this gives an approximate adsorption model.

If this is added to the zeroth order model, the equation along the characteristics becomes
\[
\begin{align*}
\frac{du}{ds} &= -ku + \alpha u(u - \beta) \\
&= -(k + \alpha \beta)u + \alpha u^2.
\end{align*}
\]

This equation can be integrated by elementary means:
\[ u(s, \tau) = \frac{c(\tau) \exp(-(k + \alpha)s)}{c(\tau) \gamma \exp(-(k + \alpha)s) - 1} \]
where \( \gamma = \frac{\alpha}{k+\alpha\beta} \) and \( c(\tau) \) is related to the initial condition \( f(\tau) \) specified earlier by
\[ c(\tau) = \frac{-f(\tau)}{1 - f(\tau)\gamma}. \]

In terms of \( (x, t) \) the exact form of \( u \) will depend on \( b(t) \). For \( b(t) \equiv b \) a constant
\[ u(x, t) = \frac{c(t - \frac{x}{b}) \exp(-(k + \alpha\frac{x}{b}))}{c(t - \frac{x}{b}) \gamma \exp(-(k + \alpha\frac{x}{b}) - 1}. \]

6 Conclusion

In this report, we have attempted to provide a qualitative understanding of the various phenomena that occur when radioactive waste leaks into an aquifer. Typically, the radioactive waste is composed of several different species. We have constructed a mathematical model that describes the concentration profile of one such species in the aquifer, taking into account the effects of convection, diffusion, and radioactive decay. We have also considered the inclusion of nonlinear adsorption effects.

As a first approximation, we neglected diffusive effects and assumed that the aquifer flows at a constant rate. This resulted in an exponentially decaying concentration profile with a jump at the moving "wave front." Using
the method of singular perturbation, we then analyzed the effect of diffusion in the region of the wave front, and obtained a smooth solution. Having done this, we calculated the change in concentration at some fixed point \( x_0 \) in the aquifer, from the time the leakage occurred to some specified time later. We then wanted to find out whether this result would change if for some relatively short duration after the occurrence of the leakage, the flow rate deviated from, and returned to, its constant value. This could result from various geological activities, such as the sudden movement of tectonic plates. We concluded that the result would not change, but that the concentration front would reach the point \( x_0 \) either sooner or later, depending on whether the flow rate decreased or increased.

In this analysis, the phenomenon of diffusion was modeled assuming constant diffusivity; however, this assumption is not realistic. One of the directions of future research could be to incorporate a velocity-dependent diffusivity. This would result in a strongly non-linear diffusion term in our equation.

7 Additional Graphs

The graphs in this section were obtained using a numerical scheme *fully implicit* in time.

![Graph of radioactive waste in an aquifer](image)

**Figure 1:** Comparison of the numerical solution with the analytical solution correct up to order \( \sqrt{\epsilon} = \sqrt{3/250} \) for \( f = b \equiv 1 \).
Figure 2: Effect of a seasonal change in the flow upon the concentration in the aquifer.
Students' Report
# 6
High-Temperature Corrosion

IMA Summer Program for Graduate Students
Mathematical Modeling

Week 2, Group 3
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1 Introduction

At high temperatures, corrosion can take place in seconds and lead to millions of dollars of damage in the industrial setting. Oxidation is the most prevalent high temperature corrosion reaction since oxygen is so common in the environment. Hence, we shall consider the oxidation of alloy metals at high temperatures in this report.

There are three different physical mechanisms involved in the corrosion process: reaction, diffusion, and advection. Initially, there is a reaction between metal and oxygen atoms on the surface resulting in the formation of a metal oxide. A protective layer is formed if the metal oxide completely coats the surface of the alloy. This process is called external oxidation. The diffusion of oxygen is effectively stopped so that corrosion inside the alloy takes place at a much slower rate. Internal oxidation occurs when a protective layer is not formed. Oxygen atoms diffuse through the oxidized region until they encounter and react with metal atoms at the new alloy surface. Oxygen atoms do not diffuse through the metal oxide blocks in the region, and percolation theory is used to study the effect of the amount of oxide on the diffusivity of oxygen. Simultaneously, metal atoms are also diffusing through the alloy toward the oxidized region. In addition, the oxide molecules occupy significantly more volume than the metal and oxygen atoms alone. This increase in volume pushes the unoxidized region forward at a certain velocity. As a result, advection occurs and contributes to the movement of the metal atoms in the unoxidized region. Figure 1 illustrates the processes of reaction, diffusion, and advection where Region I is the oxidized region and Region II is the unoxidized region. The interface between the two regions is given by $w(t)$.

![Diagram](image)

Figure 1: Typical configuration of an oxidized alloy if a protective layer has not been formed.

Our model will try to represent these behaviors in an $AB$ alloy, where $A$ is a noble metal and $B$ reacts with oxygen to form an oxide. From this representation we will determine a percentage of $B$ which is sufficient to ensure the formation of a protective oxide layer.
2 Nomenclature and Assumptions

We introduce the following symbols and functions in the formulation of our model:

- $P_{O_2}$: Amount of oxygen in the environment
- $C_o$: Concentration of oxygen at the surface
- $q$: Number of oxygen atoms required to form one molecule of the oxide, $BO_q$
- $t$: Time
- $T$: Temperature
- $\sigma$: Ratio of the volume of an oxide molecule to the volume of a $B$ atom
- $U_e$: Ratio of lattice points in the alloy to unit volume
- $w(t)$: Width of oxidized region
- $v(t)$: Velocity of the interface due to expansion
- $A(x,t)$: Noble metal concentration
- $B(x,t)$: Reactive metal concentration
- $Z(x,t)$: Oxide volume fraction
- $O(x,t)$: Oxygen concentration
- $D_o(T,x,t)$: Diffusivity of oxygen through $A$
- $D_m(T,x,t)$: Mutual diffusivity of $A$ and $B$
- $\beta(Z)$: Monotonically decreasing function such that $\beta(0) = 1$ and $\beta(1) = 0$ used to account for the effects of percolation on the diffusivity of oxygen

We use the following assumptions to build our model:

- We assume the temperature to be fixed at some high temperature between 300 °C and 3300 °C.
- We assume $C_o = k\sqrt{P_{O_2}}$ where $k$ is a coefficient which depends on the noble metal $A$.
- To simplify the model, we consider movement of the oxidized region in one direction only.
- We assume the chemical reaction forming the metal oxide is the only chemical reaction taking place.
- Since reactions take place so quickly, we assume they occur instantaneously on the environmental alloy surface which maintains concentrations and equilibrium and at the interface which establishes boundary conditions.

The concentration profiles of $A$, $B$, $O$, and $Z$ are illustrated in Figure 2. The interface between the oxidized and unoxidized regions is indicated by $w(t)$. In Region I, we see that the concentration of $O$ decreases to zero at the interface. The concentration of $A$ remains constant in Region I and we note that $A + Z = 1$ in this region. In Region II, the concentration of $B$ atoms is zero at the interface and increases asymptotically to $B_0$ with depth. The concentration of $A$ asymptotically decreases and $A + B = 1$ in this region. Finally, note that $B = 0$ in Region I and $Z = 0$ in Region II.
3 Governing Equations

Region I

Oxygen is diffusing through Region I at a rate which depends on the amount of oxide present in the region. This diffusion is represented by the following equation

\[
\frac{\partial O}{\partial t} = D_o \frac{\partial}{\partial x} \left( \beta(Z) \frac{\partial O}{\partial x} \right),
\]

(1)

where \( \beta(Z) \) is experimentally determined to be the linear function given by \( 1 - \alpha Z \). The constant \( \alpha \) depends on the structure of the oxidation formations: if the formations are spherical \( \alpha = \frac{3}{2} \), if the formations are horizontal needles \( \alpha = 1 \), and if the formations are vertical needles \( \alpha = 2 \). The initial and boundary conditions for (1) are given by

I.C. \( O(x, 0) = 0 \)

B.C. \( O(0, t) = C_o \)
\( O(w(t), t) = 0 \).

In addition, once the oxidized material is formed, the volume fraction remains constant in time so that

\[
\frac{\partial Z}{\partial t} = 0.
\]

(2)

Region II

In Region II, the concentration of the metal \( B \) in time and space is a function of the diffusivity of \( B \) and the velocity of the interface. In any control volume in Region II, we have

\[
\int_{x_o - \Delta x}^{x_o + \Delta x} (B(x, t_o + \Delta t) - B(x, t_o)) \, dx = \\
+ \int_{t_o}^{t_o + \Delta t} D_m \left( \frac{\partial B(x_o + \Delta x, t)}{\partial x} - \frac{\partial B(x_o - \Delta x, t)}{\partial x} \right) \, dt
\]
\[
\int_{t_o}^{t_o+\Delta t} v(t)(B(x_o + \Delta x, t) - B(x_o - \Delta x, t))dt.
\]

We divide both sides by \(2\Delta x\Delta t\) and take the limit as \(\Delta t \to 0\) and \(\Delta x \to 0\) to obtain

\[
\frac{\partial B}{\partial t}(x, t) = \frac{\partial}{\partial x} \left( D_m \frac{\partial B}{\partial x}(x, t) - v(t)B(x, t) \right)
\]

I.C. \(B(x, 0) = B_o\)

B.C. \(B(w(t), t) = 0\)

\(B(\infty, t) = B_o\).

The velocity function \(v(t)\) is determined by the net increase in volume caused by the formation of the \(Z\) oxide at the interface for some time period \(\Delta t\), or

\[
v(t) = (1 - \frac{1}{\sigma})Z \frac{dw}{dt}
\]

Interface

Since the interface, \(x = w(t)\), and hence the boundary conditions there, are moving in time, we require an additional condition to solve equations (1) and (3). We assume an equilibrium condition exists at the interface, so that the flux of \(O\) atoms is \(q\) times the flux of \(B\) atoms which gives

\[
qD_m \frac{\partial B}{\partial x} = -D_o \beta(Z) \frac{\partial O}{\partial x} \text{ at } x = w(t).
\]

We may determine the location of the interface by using a conservation condition for the \(B\) atoms. The amount of \(Z\) formed must be in equilibrium with the influx of \(B\) atoms:

\[
Z(x, t_o)[(w(t_o + \Delta t) - w(t_o)) = \sigma D_m \frac{\partial B(x, t_o)}{\partial x} \Delta t
\]

so that

\[
Z \frac{dw}{dt} = \sigma D_m \frac{\partial B(x, t)}{\partial x}.
\]

The System of Equations

\[
\frac{\partial O}{\partial t} = D_o \frac{\partial}{\partial x} \left( \beta(Z) \frac{\partial O}{\partial x} \right) \text{ in Region I}
\]

\[
\frac{\partial B}{\partial t}(x, t) = \frac{\partial}{\partial x} \left( D_m \frac{\partial B}{\partial x}(x, t) - v(t)B(x, t) \right) \text{ in Region II}
\]

I.C. \(0 = O(x, 0)\) \(\quad B_o = B(x, 0)\)

B.C. \(0 = O(w(t), t)\) \(\quad 0 = B(w(t), t)\)

\(C_o = O(0, t)\) \(\quad B_o = B(\infty, t)\).

\(v(t) = (1 - \frac{1}{\sigma})Z \frac{dw}{dt}\) at the interface

\(qD_m \frac{\partial B}{\partial x} = -D_o \beta(Z) \frac{\partial O}{\partial x}\) at the interface

\(Z \frac{dw}{dt} = \sigma D_m \frac{\partial B(x, t)}{\partial x}\) at the interface
4 Nondimensionalization and Analytical Solution

The independent variables for our problem are \( t \) and \( x \), and the parameters of the problem are \( A_0, B_0, C_0, D_m, D_o, \sigma, \) and \( q \). Recall that \( U_c \) is the ratio of the number of lattice points to a unit of volume. We normalize the concentrations of \( A, B \), and \( O \) atoms by forming the ratio of atom concentration to \( U_c \). The parameters \( A_0, B_0, C_0, \sigma, \) and \( q \) are nondimensional. Recall that the units for diffusivity are \( \text{length}^2 / \text{time} \), and since there are no natural lengths or time scales associated with this problem, we introduce the nondimensional quantities \( \eta \) and \( \tilde{D} \) to be

\[
\eta = \frac{x}{(D_m t)\frac{1}{2}} \quad \tilde{D} = \frac{D_o}{D_m}.
\]

Our solution now depends only on \( \eta \) and the partial differential equations are reduced to a system of ordinary differential equations which we may solve under the assumption of a similarity solution. In this case, the position of the interface in the new coordinate system is a constant given by

\[
\eta_o = \frac{v(t)}{(D_m t)^{\frac{1}{2}}}.
\]  

(7)  

In terms of our new variable \( \eta \), we have

\[
\frac{\partial O}{\partial t} = -\frac{1}{2} \frac{x}{D_m t} \frac{dO}{d\eta} \quad \text{and} \quad \frac{\partial^2 O}{\partial x^2} = \frac{1}{D_m t} \frac{d^2 O}{d\eta^2}.
\]

(8)

Since \( \frac{\partial Z}{\partial t} = 0 \) in Region I, we have that \( \frac{\partial Z}{\partial \eta} = 0 \) in this Region so that \( Z \) is constant. Hence, \( \beta(Z) \) is constant in Region I and Equation (1) for oxygen diffusion becomes

\[
\gamma \frac{d^2 O}{d\eta^2} = -\frac{1}{2} \frac{dO}{d\eta},
\]

where \( \gamma = \tilde{D}\beta(Z) \). The boundary conditions are

\[
O(\eta = 0) = C_o \quad \text{and} \quad O(\eta = \eta_o) = 0.
\]

For Equation (3), we use expressions analogous to those in Equation (8) for \( \frac{\partial B}{\partial t} \) and \( \frac{\partial B^2}{\partial x} \).

Substituting (4) for \( v(t) \) in the advection term in Equation (3) gives

\[
\frac{\partial}{\partial x}(v(t)B) = \frac{\partial}{\partial x} \left( (1 - \frac{1}{\sigma})Z \frac{d\eta}{dt} B \right).
\]

(9)

We now substitute the time derivative of Equation (7) into (9) and take the spatial derivative so that advection in terms of \( \eta \) is given by

\[
\frac{1}{2} (1 - \frac{1}{\sigma}) \eta_o t^{-1} Z \frac{dB}{d\eta}.
\]

(10)

The diffusion equation for \( B \) is then

\[
\eta \frac{dB}{d\eta} = -\frac{1}{2} \frac{d^2 B}{d\eta^2} + \delta \frac{dB}{d\eta},
\]

where \( \delta = (1 - \frac{1}{\gamma})Z \eta_o \) and

\[
B(\eta = \eta_0) = 0 \quad \text{and} \quad B(\eta = \infty) = B_o.
\]
Solving for \( O(\eta) \) yields

\[
O(\eta) = c_1 \int_{\eta}^{\eta_0} e^{-\frac{1}{4}s^2} \, ds + c_2
\]

where\( c_1 = \frac{C_0}{\int_{\eta}^{\eta_0} e^{-\frac{1}{4}s^2} \, ds} \) and \( c_2 = 0 \).

Solving for \( B(\eta) \) yields

\[
B(\eta) = c_3 \int_{\eta_0}^{\eta} e^{-\frac{1}{4}s^2 + \frac{\xi}{8} s} \, ds + c_4
\]

where\( c_3 = \frac{B_0}{\int_{\eta_0}^{\eta} e^{-\frac{1}{4}s^2 + \frac{\xi}{8} s} \, ds} \) and \( c_4 = 0 \).

At the interface, condition (5) becomes

\[
\gamma c_1 e^{-\frac{1}{4}\eta_0^2} = q c_3 e^{-\frac{1}{4}\eta_0^2 + \frac{\xi}{8}\eta_0}.
\]

Substituting for \( c_1 \) and \( c_3 \) and collecting known input parameters yields

\[
\frac{q B_0}{\gamma C_0} = \frac{\int_{\eta_0}^{\eta} e^{-\frac{1}{4}s^2 + \frac{\xi}{8} s} \, ds}{\int_{\eta}^{\eta_0} e^{-\frac{1}{4}s^2} \, ds} e^{\frac{1}{4}\eta_0^2 (1 - \frac{\xi}{4}) - \frac{\xi}{8}\eta_0}.
\]

The second interface condition given by (6) becomes

\[
\frac{Z \eta_0}{2\sigma} = \frac{B_0 e^{-\frac{1}{4}\eta_0^2 + \frac{\xi}{8}\eta_0}}{\int_{\eta_0}^{\eta} e^{-\frac{1}{4}s^2 + \frac{\xi}{8} s} \, ds}.
\]

We now use Equations (13) and (14) to solve for \( \eta_0 \) and \( Z \).
5 Numerical Results

From a numerical standpoint Equations (13) and (14) are more easily managed if a value of $Z$ is supplied. Solving (13) and (14) for $B_0$, we are reduced to one equation which we can use to solve for $\eta_o$:

$$\frac{2C_0\beta(Z)D_o\sigma}{D_m\eta Z} = \eta_o e^{\frac{\text{a}^2}{\text{b}^2\gamma^2}} \int_0^{\text{a}^2} e^{-\frac{s^2}{\text{b}^2\gamma^2}} ds. \quad (15)$$

With $\eta_o$ and $Z$, we may now solve for $B_0$ using Equation (14). The following quantities in Equation (15) have been experimentally determined:

- $\frac{D_m\sigma}{D_e\text{c}_o}$ ranges between 0.1 and 10
- $\sigma = 2$
- $\frac{D_o}{D_m}$ ranges between $10^3$ and $10^4$

To solve (15) for $\eta_o$, we will first consider an asymptotic argument. Equation (15) can be rewritten as

$$\frac{2C_0\sigma}{qZ} = \eta_o e^{\frac{\text{a}^2}{\text{b}^2\gamma^2}} \int_0^{\text{a}^2} e^{-\frac{s^2}{\text{b}^2\gamma^2}} ds \quad (16)$$

Using the change of variable $s = t\sqrt{\gamma}$ this becomes

$$\frac{2C_0\sigma}{qZ} = \eta_o e^{\frac{\text{a}^2}{\text{b}^2\gamma^2}} \int_0^{3\text{b}^2\gamma} e^{-\frac{t^2}{\gamma^2}} dt, \quad (17)$$

so now $\eta_o$ and $\gamma$ appear only in the combination $\frac{\eta_o}{\sqrt{\gamma}}$. When this is small, we can expand the right side of (17)

$$\frac{2C_0\sigma}{qZ} = \eta_o \left(1 + O \left( \frac{\eta_o^2}{\gamma} \right) \right) \left( \eta_o \sqrt{\gamma} + O \left( \eta_o^3 \right) \right)$$

$$\approx \frac{\eta_o^2}{\gamma}$$

We use this approximation to generate a starting value for Newton's method.

The following plots were generated using Matlab.

In Fig 3, the oxygen verses depth graph was run for several time steps. The left side corresponds to the boundary of the metal at the environment ($x = 0$), and the point at which the oxygen concentration drops identically to zero is the interface ($x = w(t)$). The consecutive lines thus correspond to a moving interface. The formula for $O$ verses $\eta$ is given above in Section 4. We then convert this to a function in terms of $x$ with fixed $t$ via the similarity transformation.

The equation

$$\int_0^b e^{-ax^2} dx = \frac{1}{2} \sqrt{\frac{\pi}{a}} erf(b\sqrt{a}) \quad (18)$$

is used to convert Equation (11) to a form usable by Matlab.

In Fig 4, the B alloy concentration verses space graph was also run for several time steps. At time $t = 0$, the concentration of B at the interface is $B_0$; at all other times the concentration there is zero. As time progresses, the initial slope of B near the interface can be seen to be flatter.

In Fig 5, the oxide concentration, $Z$, verses B alloy concentration was computed in a number of steps. $Z$ was taken as a given. Equation (17) was then solved using Matlab's equation solver with an initial guess $\eta_o = \sqrt{\frac{2C_0\sigma}{qZ}}$. $B_0$ was then solved using equation (12) in Section 4. The
right most point (turning point) of the graph is precisely the $B_o$ concentration for which external oxidation will take place. As shown, the graph viewed with $B_o$ as the independent variable becomes a multi-valued function. By bifurcation analysis, the lower branch of each graph is a stable solution and the upper branch is an unstable one. The lower branch is corresponding to the internal oxidation process that as the initial concentration $B_o$ is increasing, the concentration of the oxide formed in oxidized region is also increasing. When $B_o$ is increased to a value larger than the turning point, the oxide concentration is almost one hundred percent ($Z = 1$ line in the figure); the external oxidation then takes place.

6 Conclusion

The model appears to give a reasonable estimate for the percentage of $B$ needed to form a protective layer in an $AB$ alloy. Although no specific metals were considered in this paper, the overall theory appears sound. Binary alloy experiments may be performed in the laboratory so that we may verify that our model does indeed capture the mechanisms the corrosion. In industrial settings, however, more complicated corrosion patterns need to be addressed. Of particular interest are corrosion patterns involving the commonly used alloy steel.
Figure 4: Profile of Metal B Concentration Versus Depth in Alloy.

Figure 5: Profile of Oxide Concentration Versus $B_e$ for $\gamma = 10^3$. 
7 Future Research

In our problem, we chose to consider a binary alloy in which only one of the atoms was reactive. More complicated alloys exist in which several metal atoms react with oxygen forming several oxidized regions rather than a single oxidized region. These layers will make diffusivity more complicated to predict and add various advection terms to the partial differential equations given in Section 3. In addition, experiments could be performed using specific alloys to see if a protective layer is formed as predicted by the model.

There are other corrosion processes, such as carburization, that occur at the same time as oxidation. In this case, competition for reactive metal atoms occurs. We give a brief description for the following two cases:

1. Simultaneous oxidation

2. Competitive corrosive reactions.

Simultaneous oxidation occurs when more than one element of the alloy reacts with oxygen. In the simplest case, consider an $AB$ alloy where $B$ forms an oxide which could be a protective layer and $A$ forms an oxide which could not. There will now be two oxidized regions, one containing both oxides and the other containing only one oxide. Each region gives rise to an advection term. The partial differential equations describing this system are similar to those presented in this paper so that the solution techniques should also be similar and similarity solutions are likely to be employed. The different oxidized regions formed in this case are illustrated in Figure 6.

![Figure 6: Typical corrosion pattern for simultaneous oxidation in a binary alloy.](image)

Competitive corrosive reactions refer to corrosion processes other than oxidation. A possible situation consists of looking at carburization as well as oxidation. This is more realistic than the problem considered here since the environment contains carbon dioxide. Unfortunately, most metal atoms, $M$, combine with carbon to give a variety of carbides depending upon the concentration of carbon present. The most common of these carbides are: $M_2C_7$, $M_2C_3$, and $MC$. This, combined with oxidation, will form various reaction layers. Again, multiple advection terms are introduced and there is the additional consideration of whether a metal atom will bond
with an oxygen or a carbon atom. The diffusivity of carbon and oxygen will be hard to calculate for so many layers, and the solution itself will be considerably more difficult for this case than for the previous case.
Students' Report

#7
Flame Propagation
Through Combustible Gases
in a Cylinder

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1 Introduction

We have considered the situation of a planar flame front propagating through a cylinder of unit cross sectional area. The flame front travels along the axis of the cylinder. Initially the cylinder is filled with a gas containing chemical species A which is converted by the passing flame to chemical species B. Gases A and B have the same molecular weight. This very simple reaction can be described as

\[ A \rightarrow B. \]

Both the reactant and product gases will be assumed to obey the ideal gas law. At time \( t = 0 \) the planar flame front is introduced at one end of the cylinder. As the flame front moves through the cylinder, it is useful to think of the cylinder as being divided into three regions, (1) the burnt region of gas, (2) the unburnt region of gas, and (3) the thin region consisting of the flame.

2 Nomenclature

- \( u(x,t) \) particle velocity, units m/s
- \( \rho(x,t) \) density, units kg/m\(^3\)
- \( p(x,t) \) pressure, units kg/(m s\(^2\))
- \( T(x,t) \) temperature, units K
- \( y(x,t) \) mass fraction of species A, nondimensional
- \( e(x,t) \) internal energy, units J/kg
- \( r(T,y) \) rate of reaction, units kg/(m\(^3\) s)
- \( \mu(x,t) \) viscosity, units kg/(m s)
- \( K \) thermal conductivity, units J/(K m s)
- \( \gamma = \frac{\epsilon_s}{\epsilon_v} \) ratio of specific heats, nondimensional
- \( R = c_p - c_v \) gas constant, units J/(K kg)
- \( Q \) heat of reaction, units J/kg
- \( \lambda \) diffusivity, units kg/(m s)
- \( \tau \) stress, units kg/(m s\(^2\))
3 Governing Equations

We are considering a one-dimensional tube of length \( L \) with length coordinate \( z \). The flame will be given as an initial condition at \( t = 0 \) with position at \( z = 0 \). Our governing equations are derived from conservation laws. First consider conservation of mass. The rate of change in mass contained in the interval between \( x_o \) and \( x_1 \) is given by

\[
0 = \frac{d}{dt} \int_{x_o}^{x_1} \rho(x,t) \, dx
= \int_{x_o}^{x_1} \frac{\partial \rho}{\partial t}(x,t) \, dx + \rho(x_1,t)u(x_1,t) - \rho(x_o,t)u(x_o,t)
= \int_{x_o}^{x_1} \frac{\partial \rho}{\partial t}(x,t) + \frac{\partial}{\partial x}(\rho u) \, dx
\]

\( x_o \) and \( x_1 \) are moving with the slice of mass under consideration. Since \( x_o \) and \( x_1 \) are arbitrary this produces

\[
\frac{\partial \rho}{\partial t} + \frac{\partial}{\partial x}(\rho u) = 0. \tag{1}
\]

This equation simply relates change in density, \( \rho \), at a point with the mass flux, \( \rho u \), at that point.

Next consider conservation of momentum. In the interval between \( x_o \) and \( x_1 \) the change in momentum is given by

\[
\frac{d}{dt} \int_{x_o}^{x_1} \rho(x,t)u(x,t) \, dx = -(\rho(x_1,t) - \rho(x_o,t)) + \mu \left( \frac{\partial u}{\partial x}(x_1,t) - \frac{\partial u}{\partial x}(x_0,t) \right)
\]

The pressure terms on the right represent the momentum imparted to the slice due to the pressure difference. The other terms represent a "viscous" effect, actually this is internal resistance to expansion and contraction. Carrying out the differentiation and using equation (1) gives us

\[
\rho \left[ \frac{\partial u}{\partial t} + u \frac{\partial u}{\partial x} \right] = -\frac{\partial p}{\partial x} + \frac{\partial}{\partial x}(\mu \frac{\partial u}{\partial x}). \tag{2}
\]

Now consider conservation of energy. In the interval between \( x_o \) and \( x_1 \) the change in energy, which is the sum of the internal energy, \( \rho e \), and the kinetic energy, \( \frac{1}{2} u^2 \), is given by

\[
\frac{d}{dt} \int_{x_o}^{x_1} e(x,t)\rho(x,t) + \frac{1}{2} \rho(x,t)u(x,t)^2 \, dx =
K\left( \frac{\partial T}{\partial x}(x_1,t) - \frac{\partial T}{\partial x}(x_0,t) \right) + \tau(u(x_1,t) - u(x_0,t)) + \lambda Q\left( \frac{\partial u}{\partial x}(x_1,t) - \frac{\partial u}{\partial x}(x_0,t) \right)
\]

The first term on the right is the change in energy due to thermal diffusion. The second term on the right is the mechanical work done. The third term on
the right is the change in energy due to molecular diffusion. Differentiating, we arrive at
\[
\rho \left[ \frac{\partial}{\partial t} \left( e + \frac{u^2}{2} \right) + \frac{\partial}{\partial x} \left( e + \frac{u^2}{2} \right) \right] = \frac{\partial}{\partial x} (K \frac{\partial T}{\partial x}) + \frac{\partial}{\partial x} (\tau u) + Q \frac{\partial}{\partial x} (\lambda \frac{\partial y}{\partial x})
\] (3)

Next consider conservation of species. The change in the mass of reactant is given by
\[
\frac{d}{dt} \int_{x_0}^{x_1} \rho(x,t)y(x,t) \, dx = - \int_{x_0}^{x_1} r(T,y) \, dx + \lambda \left( \frac{\partial y}{\partial x}(x_1,t) - \frac{\partial y}{\partial x}(x_0,t) \right)
\]

Similarly we get
\[
\rho \left[ \frac{\partial y}{\partial t} + u \frac{\partial y}{\partial x} \right] = -r + \frac{\partial}{\partial x} (\lambda \frac{\partial y}{\partial x}).
\] (4)

The ideal gas law is an equation of state.
\[
pv = nRT
\]

We rewrite this as
\[
p = \frac{n \text{molecular weight}}{v} \frac{\bar{R}}{(\text{molecular weight})} T \equiv \rho RT
\] (5)

The stress, \( \tau \), can be written as
\[
\tau = -p + \mu \frac{\partial u}{\partial x}
\] (6)

and the internal energy, \( e \), as
\[
e = \frac{p}{\rho (\gamma - 1)} + Qy
\] (7)

which is a sum of the thermal energy plus the reaction energy.

From equations (2)–(7) we get
\[
\rho c_v \left( \frac{\partial T}{\partial t} + u \frac{\partial T}{\partial x} \right) = rQ + \frac{\partial u}{\partial x} \left( -p + \mu \frac{\partial u}{\partial x} \right) + \frac{\partial}{\partial x} (K \frac{\partial T}{\partial x})
\] (8)

4 Nondimensionalization

\( L \) length scale, length of cylinder
\( V \) velocity scale, flame speed
\( t_o = L/V \) time scale
\( T_o \) initial temperature
\( \rho_0 \) initial density
\( p_0 \) initial pressure
\( \lambda \) mass diffusivity
\( \mu \) viscosity
\( K \) thermal conductivity

We replace \( z \) by \( L \hat{z} \), \( u \) by \( V \hat{u} \), \( t \) by \( t_0 \hat{t} \), \( T \) by \( T_0 \hat{T} \), \( \rho \) by \( \rho_0 \hat{\rho} \), \( p \) by \( p_0 \hat{p} \). The governing equations in nondimensional form, are:

\[
\frac{\partial \hat{\rho}}{\partial \hat{t}} + \frac{\partial (\hat{\rho} \hat{u})}{\partial \hat{z}} = 0
\]

\[
\gamma M_o^2 \hat{\rho} \left[ \frac{\partial \hat{u}}{\partial \hat{t}} + \hat{u} \frac{\partial \hat{u}}{\partial \hat{z}} \right] = -\frac{\partial \hat{p}}{\partial \hat{z}} + \gamma M_o^2 \frac{L_d Pr}{L} \frac{\partial}{\partial \hat{z}} \left( \frac{\partial \hat{u}}{\partial \hat{z}} \right)
\]

\[
\hat{\rho} \left[ \frac{\partial \hat{T}}{\partial \hat{t}} + \hat{u} \frac{\partial \hat{T}}{\partial \hat{z}} \right] = \hat{r} \alpha - (\gamma - 1) \hat{p} \frac{\partial \hat{u}}{\partial \hat{z}} + \frac{L_d Pr}{L} M_o^2 \gamma (\gamma - 1) \mu \left( \frac{\partial \hat{u}}{\partial \hat{z}} \right)^2 + \frac{L_d}{L} \frac{\partial}{\partial \hat{z}} \left( \hat{K} \frac{\partial \hat{T}}{\partial \hat{z}} \right)
\]

\[
\hat{\rho} \left[ \frac{\partial \hat{y}}{\partial \hat{t}} + \hat{u} \frac{\partial \hat{y}}{\partial \hat{z}} \right] = \hat{r} + \frac{L_d Le}{L} \frac{\partial}{\partial \hat{z}} \left( \frac{\partial \hat{y}}{\partial \hat{z}} \right)
\]

\[
\hat{p} = \hat{\rho} \hat{T}
\]

where
\( c_s^2 = \gamma p_0 / \rho_0 \) characteristic speed of pressure disturbances
\( M_o = V / c_0 \) Mach number
\( L_d \sim 10^{-4} \) characteristic diffusion length
\( Pr = \frac{c_s^2}{K} \) Prandtl number
\( Le = \frac{c_s^2}{K} \) Lewis number
\( \alpha = \frac{Q}{c_s L} \)
\( \hat{r} = \frac{Lr}{\rho_0 c_s V} \)
\( \hat{K} = \frac{K}{\rho_0 c_s V L} \)

Orders of magnitude:
\( M_o \sim 10^{-2}, \quad \frac{L_d}{L} \sim 10^{-4}, \quad \alpha \sim 1, \quad Pr \sim 1, \quad Le \sim 1 \)

We will henceforth drop tildes from quantities.
5 Outside the Flame

Considering equation (10) and the above orders of magnitude we see that outside the flame (where the spatial gradients are small) the equation reduces to

\[
\frac{\partial p}{\partial x} = 0
\]  
(14)

or \( p \equiv p(t) \). By a similar argument equations (11) and (12) away from the flame simplify to

\[
\rho \left( \frac{\partial T}{\partial t} + u \frac{\partial T}{\partial x} \right) = - (\gamma - 1) p \frac{\partial u}{\partial x}
\]  
(15)

and

\[
\frac{\partial y}{\partial t} + u \frac{\partial y}{\partial x} = 0
\]  
(16)

We now define a weighted mass coordinate, \( \psi \), by

\[
\psi(x, t) = \int_{0}^{x} \rho(\xi, t) \, d\xi
\]  
(17)

and perform a change of coordinates so that our independent variables are now \( \psi \) and \( t \). If \( F = F(\psi, t) \) then

\[
\frac{\partial F}{\partial t} \rightarrow \frac{\partial F}{\partial \psi} \frac{\partial \psi}{\partial t} + \frac{\partial F}{\partial \psi} (-\rho u) + \frac{\partial F}{\partial t}
\]

for constant \( x \) and

\[
\frac{\partial F}{\partial x} \rightarrow \frac{\partial F}{\partial \psi} \frac{\partial \psi}{\partial x} = \frac{\partial F}{\partial \psi} \rho
\]

for constant \( t \). Using this transformation our governing equations become

\[
\frac{\partial \rho}{\partial t} + \rho^2 \frac{\partial u}{\partial \psi} = 0,
\]

(18)

\[
\frac{\partial p}{\partial x} = 0,
\]

(19)

\[
\frac{\partial T}{\partial t} = - (\gamma - 1) T \rho \frac{\partial u}{\partial \psi},
\]

(20)

and

\[
\frac{\partial y}{\partial t} = 0.
\]

(21)

From the physical description of the problem we arrive at the following boundary conditions. Since the end walls of the cylinder are fixed,

\[
u(0, t) = u(1, t) = 0.
\]

(22)
Since the ends of the cylinder are insulated,
\[
\frac{\partial T}{\partial x}(0, t) = \frac{\partial T}{\partial x}(1, t) = 0.
\] (23)

Since there is no mass flux through the end walls of the cylinder,
\[
\frac{\partial y}{\partial x}(0, t) = \frac{\partial y}{\partial x}(1, t) = 0.
\] (24)

Multiplying equation (20) by \( \rho \) and using equation (18) we get the following differential equation.
\[
\frac{1}{T} \frac{\partial T}{\partial t} = \frac{\gamma - 1}{\rho} \frac{\partial \rho}{\partial t}
\] (25)
whose solution is
\[
T = (\phi(\psi))^{\gamma} \rho^{\gamma - 1}
\] (26)
where we have introduced \((\phi(\psi))^{\gamma}\) as a constant of integration. Using the equation of state \( p = \rho T \) we get
\[
\rho = \frac{p^{1}\gamma}{\phi(\psi)}
\] (27)

Equation (18) can be rewritten as
\[
\frac{\partial}{\partial \psi} \left( \frac{1}{\rho} \right) = \frac{\partial u}{\partial \psi}
\] (28)
which upon integration over the burnt region (from 0 to \( \psi \)) gives
\[
u(\psi, t) = \int_{0}^{\psi} \frac{\partial}{\partial t} \left( \frac{1}{\rho} \right) d\psi = -\frac{1}{\gamma} (p(t))^{-\frac{\gamma + 1}{\gamma}} p'(t) \int_{0}^{\psi} \phi(\psi) d\psi
\] (29)
and upon integration over the unburnt region (from \( \psi \) to 1) gives
\[
u(\psi, t) = \int_{\psi}^{1} \frac{\partial}{\partial t} \left( \frac{1}{\rho} \right) d\psi = \frac{1 - \psi}{\gamma} (p(t))^{-\frac{\gamma + 1}{\gamma}} p'(t)
\] (30)

At \( t = 0 \) we know \( \rho = 1 \) and \( T = 1 \) which implies \( \phi(\psi) \equiv 1 \) on the unburnt side.

<table>
<thead>
<tr>
<th>burnt</th>
<th>unburnt</th>
</tr>
</thead>
<tbody>
<tr>
<td>( T = \phi^{\gamma} \rho^{\gamma - 1} )</td>
<td>( T = \rho^{\gamma - 1} )</td>
</tr>
<tr>
<td>( p = (\phi \rho)^{\gamma} )</td>
<td>( p = (\rho)^{\gamma} )</td>
</tr>
<tr>
<td>( u = -\frac{1}{\gamma} (p(t))^{-\frac{\gamma + 1}{\gamma}} p'(t) \int_{0}^{\psi} \phi(\psi) d\psi )</td>
<td>( u = \frac{1 - \psi}{\gamma} (p(t))^{-\frac{\gamma + 1}{\gamma}} p'(t) )</td>
</tr>
</tbody>
</table>
The total energy density is the internal energy density plus the kinetic energy density, \( \rho e + \frac{1}{2} u^2 \). The total energy in the slice from \( x_f - \epsilon \) to \( x_f + \epsilon \) is

\[
\int_{x_f - \epsilon}^{x_f + \epsilon} \rho(e + \frac{1}{2} u^2) \, dx. \tag{31}
\]

The change in energy is the work done, \(-pu\big|_{x_f - \epsilon}^{x_f + \epsilon}\). Hence

\[
\frac{\partial}{\partial t} \int_{x_f - \epsilon}^{x_f + \epsilon} \rho(e + \frac{1}{2} u^2) \, dx = -pu\big|_{x_f - \epsilon}^{x_f + \epsilon}. \tag{32}
\]

\[
\int_{x_f - \epsilon}^{x_f + \epsilon} \frac{\partial}{\partial t} \rho(e + \frac{1}{2} u^2) \, dx + \rho(e + \frac{1}{2} u^2)u\big|_{x_f - \epsilon}^{x_f + \epsilon} + pu\big|_{x_f - \epsilon}^{x_f + \epsilon} = 0. \tag{33}
\]

We expect the \( t \) derivatives to be continuous so the integral above vanishes as \( \epsilon \) goes to 0. In the flame we expect the velocity \( u \) to be negligible compared to the internal energy \( e \). Therefore we are left with

\[
\rho u(e + \frac{P}{\rho})\big|_{x_f - \epsilon}^{x_f + \epsilon} = \int_{x_f - \epsilon}^{x_f + \epsilon} \frac{\partial}{\partial x} \rho u(e + \frac{P}{\rho}) \, dx = 0 \tag{34}
\]

Since \( x_f \) and \( \epsilon \) are arbitrary then we have

\[
\frac{\partial}{\partial x} \rho u(e + \frac{P}{\rho}) = 0 \tag{35}
\]

Thus \( \rho u(e + \frac{P}{\rho}) \) is conserved across the flame front. However \( \rho u \) is the mass flux which is also a conserved quantity at the point \( x_f \). Hence \( e + \frac{P}{\rho} \) is conserved across \( x_f \). Thus

\[
e^+ + \frac{P}{\rho^+} = e^- + \frac{P}{\rho^-} \tag{36}
\]

We will replace \( e \) by \( \frac{P}{\rho(\gamma - 1)} + Qy \) and \( \frac{P}{\rho} \) by \( RT \).

\[
\frac{\gamma}{\gamma - 1} RT^+ + Qy^+ = \frac{\gamma}{\gamma - 1} RT^- + Qy^- \tag{37}
\]

Since \( y^+ = 1 \) and \( y^- = 0 \) then

\[
\frac{\gamma}{\gamma - 1} RT^+ + Q = \frac{\gamma}{\gamma - 1} RT^- \tag{38}
\]

Using \( R = c_p - c_v \) and the definition of \( \gamma \) and \( \alpha \) this reduces to

\[
T^- = T^+ + \frac{\alpha}{\gamma} \tag{39}
\]
We define a quantity \( w \) which is the position of the flame front in the \( \psi \) coordinates by \( w = \psi(x_f(t), t) \). From equation (39) and our table we have

\[
T^-(w, t) = \phi(w)p^{\frac{x-1}{\gamma}} = p^{\frac{x-1}{\gamma}} + \frac{\alpha}{\gamma}
\]  

which implies

\[
\phi(w) = 1 + \frac{\alpha}{\gamma} p^{\frac{1-x}{\gamma}}.
\]

Using the fact that the total mass in the cylinder is 1, the expression for the density in terms of the pressure, and the fact that the pressure is independent of \( \psi \) gives

\[
1 = p^{-\frac{1}{\gamma}} \left( \int_0^w \phi(\psi) \, d\psi + \int_w^1 \, d\psi \right)
\]

which implies

\[
p^{\frac{1}{\gamma}} = \int_0^w \phi(\psi) \, d\psi + (1 - w)
\]

Differentiating with respect to \( t \) and using the expression for \( \phi(w) \) gives

\[
\dot{p} = \alpha \dot{w}
\]

Using the fact that at \( t = 0, \ w = 0 \) and \( p = 1 \) we have

\[
p = 1 + \alpha w.
\]

Then

\[
\phi(\psi) = 1 + \frac{\alpha}{\gamma} (1 + \alpha \psi)^{\frac{1-x}{\gamma}}.
\]

Now from the definition of \( w \) we have

\[
\dot{w} = \rho(x_f - u).
\]

The expression \( \dot{x}_f - u \) is the difference in the flame speed and the molecular speed at the flame front. If we had a function for this in terms of \( w, p, \) or \( \rho \) (which depend on \( w \) through equation (45)) then we would have a differential equation in \( w \). Thus we suppose a simple form for this expression, namely \( \dot{x}_f - u = 1 \) and see what this implies about \( w \). For this case the resulting differential equation is

\[
\dot{w} = \rho(x_f, t) = (1 + \alpha w)^{\frac{1}{\gamma}}
\]

where we have used expression from the unburnt side of the cylinder. Coupling equation (47) with the initial condition that at \( t = 0, \ w = 0 \) we get a solution of the form

\[
w(t) = \frac{1}{\alpha} \left[ \left( \frac{\alpha(\gamma - 1)t}{\gamma} + 1 \right)^{\frac{\gamma}{\gamma-1}} - 1 \right]
\]
Hence on the unburnt side of the cylinder we have the following expressions for $p$, $\rho$ and $T$.

\[ p(t) = \left( \frac{\alpha (\gamma - 1) t}{\gamma} + 1 \right)^{\frac{\gamma}{\gamma - 1}} \]  
(49)

\[ \rho(t) = \left( \frac{\alpha (\gamma - 1) t}{\gamma} + 1 \right)^{\frac{1}{\gamma - 1}} \]  
(50)

\[ T(t) = \left( \frac{\alpha (\gamma - 1) t}{\gamma} + 1 \right) \]  
(51)

6 Inside the Flame

The equations of balance are given as follows:

Balance of mass:

\[ \rho_t + (\rho u)_x = 0 \]  
(52)

Balance of momentum:

\[ \rho(u_t + uu_x) = -\frac{1}{\gamma M_0^2 p_x} + \frac{L_d P_0}{L} (\mu u_x)_x \]  
(53)

Balance of energy:

\[ \rho(T_t + u T_x) = \alpha r - (\gamma - 1)p u_x + \gamma (\gamma - 1)M_0^2 \frac{L_d P_0}{L} \mu (u_x)^2 + \frac{L_d}{L} (K T_x)_x \]  
(54)

Chemistry:

\[ \rho(y_t + u y_x) = -r + \frac{L_d L_e}{L} (\lambda y_x)_x \]  
(55)

Ideal gas:

\[ p = \rho T \]  
(56)

Experiments indicate that the flame thickness $\delta$ and Mach number $M_0$ are given as follows:

\[ \delta = \frac{L_d}{L} \sim 10^{-4}, \quad M_0 \sim 10^{-2} \]

To apply the perturbation, we set

\[ x = x_f(t) + \delta \xi, \quad t = t \]

Further, we denote

\[ \hat{u} = \hat{x}_f(t) - u \]

Then, the equations can be written in the following forms:

\[ \rho_t - \frac{\hat{u}}{\delta} \rho \xi = -\rho u \xi \frac{1}{\delta} \]  
(57)
\[
\rho(u_t - \frac{\partial}{\partial \xi} u \xi) = -\frac{1}{\gamma M_0^2} \rho \frac{1}{\delta} + \frac{\delta P_r}{\delta^2} (\mu u \xi) \xi \quad (58)
\]

\[
\rho(T_t - \frac{\partial}{\partial \xi} T \xi) = \alpha \frac{\partial}{\partial \xi} - (\gamma - 1) \rho u \xi \xi + \gamma(\gamma - 1) M_0^2 \frac{\delta P_r}{\delta^2} \rho u \xi^2 + \frac{\delta}{\delta^2} (K T \xi) \xi \quad (59)
\]

\[
\rho(\gamma_t - \frac{\partial}{\partial \xi} \gamma \xi) = -\frac{\partial}{\partial \xi} + \frac{\delta L_c}{\delta^2} (\gamma \xi) \xi \quad (60)
\]

Notice that \( u \xi = -\xi u \xi \) and that inside the flame the gradient in time is small. So, by neglecting the small terms in the equations, we obtain the following simplified equations:

\[
(\rho u \xi) \xi = 0 \quad (61)
\]

\[
p \xi = 0 \quad (62)
\]

\[
- \rho u T \xi = \alpha \xi + (\gamma - 1) \rho u T \xi + (K T \xi) \xi \quad (63)
\]

\[
- \rho u \xi = -\xi + L_c (\gamma \xi) \xi \quad (64)
\]

The momentum equation is therefore approximated to be \( p = p(t) \) and the mass equation \( p u = \dot{\psi}(t) \). Using also the ideal gas equation \( p(t) = \rho T \), the equation of energy and equation of chemistry are reduced as follows (assume that the original \( K \) and \( \lambda \) are constants, so the nondimensionalized values for \( K \) and \( \lambda \) are both equal to 1):

\[
\gamma \dot{\psi}(t) T \xi + T \xi = -\alpha \xi \quad (65)
\]

\[
\dot{\psi}(t) \xi + L_c \xi \xi = \xi \quad (66)
\]

\[
\begin{align*}
\xi & \to +\infty, \quad T \to T^+, \quad y \to 1 \\
\xi & \to -\infty, \quad T \to T^-, \quad y \to 0
\end{align*}
\]

**Outer solution:** outside the boundary layer, \( \xi \approx 0 \), so equations (14) and (15) become:

\[
\begin{align*}
\gamma \dot{\psi}(t) T \xi + T \xi & = 0 \\
\dot{\psi}(t) \xi + L_c \xi \xi & = 0
\end{align*}
\]

The solution of this system is

\[
\begin{align*}
\xi > 0, \quad T & = T^+ + (T^- - T^+) e^{-\gamma \psi(t) \xi}, \quad y = 1 - e^{-\frac{\psi(t) \xi}{L_c}} \\
\xi < 0, \quad T & = T^-
\end{align*}
\]

y = 0
**Inner solution:** suppose $E >> 1$, let $\xi = \epsilon \eta$, then the system becomes:

$$T_{\eta} = -\alpha \epsilon^2 \dot{r}$$

$$L_e y_{\eta} = \epsilon^2 \dot{r}$$

From the outer solution, we can write

$$T = T^- + \epsilon T_1 + \ldots, \quad y = 0 + \epsilon y_1 + \ldots$$

then

$$\dot{r} = Dc y_1 e^{-\frac{E}{\tau} + \frac{\epsilon E T_1}{(\tau^-)^2}}$$

$$T_{1\eta} = -\alpha \epsilon^2 D y_1 e^{-\frac{E}{\tau} + \frac{\epsilon E T_1}{(\tau^-)^2}}$$

$$L_e y_{1\eta} = \epsilon^2 D y_1 e^{-\frac{E}{\tau} + \frac{\epsilon E T_1}{(\tau^-)^2}}$$

Combining these equations we get

$$T_{1\eta} + \alpha L_e y_{1\eta} = 0$$

Integrating this equation twice and using the conditions $T_1, y_1 \rightarrow 0$ as $\eta \rightarrow -\infty$ we get

$$T_1 + \alpha L_e y_1 = 0$$

Thus

$$y_1 = -\frac{T_1}{\alpha L_e}$$

Plugging into (18) to get

$$T_{1\eta} = \epsilon^2 D \frac{T_1}{L_e} e^{-\frac{E}{\tau} + \frac{\epsilon E T_1}{(\tau^-)^2}}$$

let $\epsilon = 1/E$, then the equation becomes

$$T_{1\eta} = \epsilon^2 D \frac{T_1}{L_e} e^{-\frac{E}{\tau} + \frac{T_1}{(T^-)^2}}$$

Multiplying both sides by $T_{1\eta}$, then integrating the resulted equation we get

$$\frac{1}{2} T_{1\eta}^2 = \frac{\epsilon^2 D (T^-)^4}{L_e} e^{-\frac{E}{\tau}} \left( \frac{T_1}{(T^-)^2} - 1 \right) e^{\frac{T_1}{(T^-)^2}} + A$$

Since $T_1 \rightarrow 0$ as $\eta \rightarrow -\infty$, so $T_{1\eta} \rightarrow 0$ as $\eta \rightarrow -\infty$ and therefore

$$A = \frac{D (T^-)^4}{L_e E^2} e^{-\frac{E}{\tau}}$$
Since $T_1 \to -\infty, \frac{\partial T}{\partial \eta} \to -\gamma \dot{w}(t)(T^- - T^+)$ as $\eta \to +\infty$, so by (3) we have
\[ \frac{\gamma^2 \dot{w}(t)^2}{2}(T^- - T^+)^2 = A \]
Therefore
\[ \dot{w}(t) = \frac{(T^-)^2}{\gamma E(T^- - T^+)} \sqrt{\frac{2D}{L_e}} e^{-\frac{E}{2T^-}} \]
From the solution outside the flame, we know
\[ T^- - T^+ = \frac{\alpha}{\gamma} \]
\[ T^+ = (1 + \alpha w)^{\frac{2}{\gamma}} \]
and
\[ \dot{w}(t) = 1, \quad T^+ = 1 \quad \text{as} \quad t = 0 \]
Hence, we have
\[ D = \frac{L_e}{2} (\alpha E)^2 (1 + \frac{\alpha}{\gamma})^{-4} \exp\left(\frac{E}{1 + \frac{\alpha}{\gamma}}\right) \]
and the following initial problem:
\[ \dot{w}(t) = \frac{(T^-)^2}{(1 + \frac{\alpha}{\gamma})^2} \exp\left\{ \frac{E}{2} \left( \frac{1}{1 + \frac{\alpha}{\gamma}} - \frac{1}{T^-} \right) \right\} \]
\[ w(0) = 0 \]
The $w(t)$ can be therefore solved.

7 Moving Boundary

We now consider a moving boundary on the right side of the cylinder. Since much of the analysis is similar to the fixed boundary case, we shall describe the parts which differ from the previous one only.

Our new boundary conditions become:
\[ u(0, t) = 0, \quad u(L(t), t) = L'(t) \]
\[ \frac{\partial T}{\partial x}(0, t) = \frac{\partial T}{\partial x}(L(t), t) = 0 \]
where $L(t)$ is a given function which determines the position of the right boundary at time $t$.

Since $dx = \frac{d\psi}{\rho}$, we see from conservation of mass that
\[ \int_0^{L(t)} dx = \int_0^{w(t)} \frac{d\psi}{\rho} + \int_{w(t)}^1 \frac{d\psi}{\rho} \]
We use the expressions for \( \rho \) on the burnt and unburnt sides, and also the value of \( \phi(w(t)) \), and obtain

\[
\dot{p}(t) = -\frac{\gamma L}{L} p + \frac{\alpha}{L} \dot{w}(t)
\]

where \( \dot{w}(t) \) has been obtained from the singular perturbation analysis inside the flame. An alternative model for \( \dot{w}(t) \), motivated by the dependence of the flame speed on the pressure ahead of it, was also considered:

\[
\dot{w}(t) = p^{1/\gamma}[1 + (p - 1)/2]
\]

We may now solve the two o.d.e.'s for \( w(t) \) and \( p(t) \) numerically, and hence obtain \( \rho(\psi, t) \) and \( T(\psi, t) \) everywhere. The values of \( \phi(\psi) \) required in these calculations were obtained by matching the grid points in \( \psi \) with the values taken by \( w(t) \) at those points. Thus for \( \psi = w(t^*) \),

\[
\phi(\psi) = 1 + \frac{\alpha}{\gamma} p^{(1-\gamma)/\gamma}(t^*)
\]

Finally we need to revert to our original coordinate system \((x, t)\). For \( 0 \leq x \leq x_f \), we have

\[
\int_0^x dx' = \int_0^\psi \frac{d\psi'}{\rho(\psi', t)}
\]

For \( x_f \leq x \leq L(t) \), we have

\[
\int_x^{L(t)} dx' = \int_\psi^1 \frac{d\psi'}{\rho(\psi', t)}
\]

Since both expressions hold for \( x = x_f \), we get the following:

\[
\int_0^{w(t)} \phi(\psi') d\psi' = p(t)^{1/\gamma}L(t) - (1 - w(t))
\]

Thus, for \( 0 \leq x \leq x_f \):

\[
x = p(t)^{-1/\gamma} \left[ p(w^{-1}(\psi))^{1/\gamma}L(w^{-1}(\psi)) - (1 - \psi) \right]
\]

For \( x_f \leq x \leq L(t) \):

\[
x = L(t) - p^{-1/\gamma}(t)(1 - \psi)
\]
Students' Report
# 8
Fluid Flow in a Filtering Device

IMA Summer Program for Graduate Students Mathematical Modeling

Week 3, Group 2
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Section I: Introduction and Assumptions

Filters are commonly used, both within industry and in an average household. One filter of considerable importance is the oil filter of a car. This should be replaced at regular intervals to prevent damage to the engine from particles being carried in with the oil.

This model will simulate the flow of a liquid through a filter, and then introduce particles in the liquid to determine the amount of time until the flow through a filter is $1/e$ times its initial flow, at which time we conclude that the filter should be changed.

For simplification purposes, the following assumptions have been made:

- we consider one pleat of the filter and assume it is rectangular in shape
- we assume no flow through the walls $W_1$, $W_2$, and $W_3$ (see figure 1)
- there is symmetry about the $x$-axis
- the fluid used is incompressible
- the filter is stationary and will not tear
- fluid flows through the filter in the vertical direction only
- we assume symmetric flow about $y = 2$ and $y = -2$ (see figure 1).
Figure 1. Nondimensional schematic of two-dimensional filter.
Section II: Nomenclature

\[ A_j: \text{integration constants } (j = 1, 2, 3, 4, 5, 6). \]
\[ \tilde{C}(\tilde{x}, \tilde{t}): \text{concentration of particles in filter at position } \tilde{x} \text{ and time } \tilde{t}. \text{ Units mol/cm.} \]
\[ C_c: \text{concentration at which filter is completely clogged, units mol/cm.} \]
\[ \tilde{C}_f: \text{concentration of particles in fluid entering device, units mol/cm}^2. \]
\[ \tilde{C}_t: \text{concentration of fluid entering device, units mol/cm}^2. \]
\[ D: \text{nondimensional function used when solving equations.} \]
\[ h: \text{one-half the width of filter pleat. Units cm.} \]
\[ j: \text{indexing variable.} \]
\[ \tilde{k}(\tilde{C}): \text{proportionality function (units g/(cm}^2\text{-sec}) \text{used in permeability law, given} \]
\[ \text{in this model by} \]
\[ \tilde{k}(\tilde{C}) = \frac{\tilde{k}_0}{C_c - \tilde{C}(\tilde{x}, \tilde{t})}. \quad (2.1) \]
\[ \tilde{k}_0: \text{proportionality constant [units g-mol/(cm}^3\text{-sec}) \text{used in permeability law} \]
\[ L: \text{length of filter. Units cm.} \]
\[ n: \text{indexing variable.} \]
\[ N: \text{discretization parameter used in numerical scheme.} \]
\[ \tilde{P}_i: \text{pressure of fluid upon leaving filter device. Units g/(cm}^2\text{-sec)} \text{.} \]
\[ \tilde{P}_t(\tilde{x}, \tilde{y}, \tilde{t}): \text{pressure of fluid after passing through filter. Units g/(cm}^2\text{-sec)} \text{.} \]
\[ \tilde{P}_o: \text{given pressure of fluid upon entering filter device. Units g/(cm}^2\text{-sec)} \text{.} \]
\[ \tilde{P}_o(\tilde{x}, \tilde{y}, \tilde{t}): \text{pressure of fluid before passing through filter. Units g/(cm}^2\text{-sec)} \text{.} \]
\[ \tilde{q}(\tilde{t}): \text{flow density through filter [units g/(cm}^2\text{-sec)] \text{at time } \tilde{t}, \text{defined as} \]
\[ \tilde{q}(\tilde{t}) = \rho \int_0^L \tilde{v}_o(\tilde{x}, \tilde{h}^-, \tilde{t}) d\tilde{x}. \quad (2.2) \]
\[ \tilde{Q}: \text{total flow (units g/cm) through filter when we dispose of it, defined as} \]
\[ \tilde{Q} = \int_0^{\tilde{t}_c} \tilde{q}(\tilde{t}) d\tilde{t}. \quad (2.3) \]
\[ \tilde{t}: \text{time. Units sec.} \]
\[ \tilde{t}_c(\tilde{k}_0, \tilde{C}_f): \text{quantity defined as that time at which } \tilde{q}(\tilde{t}_c) = \tilde{q}(0)/e. \text{ At } \tilde{t}_c, \text{ we change} \]
\[ \text{the filter since the rate through it has decayed by the } 1/e \text{ factor. Units sec.} \]
\[ T: \text{fictional nondimensionalization parameter. Units sec.} \]
\[ U: \text{fictional nondimensionalization parameter. Units cm/sec.} \]
\[ \tilde{u}_i(\tilde{x}, \tilde{y}, \tilde{t}): \text{velocity in } \tilde{x} \text{ direction of fluid after passing through filter. Units cm/sec.} \]
$\tilde{u}_o(\tilde{x}, \tilde{y}, \tilde{t})$: velocity in $\tilde{x}$ direction of fluid before passing through filter. Units cm/sec.

$V$: fictional nondimensionalization parameter. Units cm/sec.

$\tilde{v}_i(\tilde{x}, \tilde{y}, \tilde{z}, \tilde{t})$: velocity in $\tilde{y}$ direction of fluid after passing through filter. Units cm/sec.

$\tilde{v}_o(\tilde{x}, \tilde{y}, \tilde{z}, \tilde{t})$: velocity in $\tilde{y}$ direction of fluid before passing through filter. Units cm/sec.

$\tilde{v}(\tilde{x}, \tilde{y}, \tilde{z})$: velocity vector of fluid. Units cm/sec.

$\tilde{w}_i(\tilde{x}, \tilde{y}, \tilde{z})$: velocity in $\tilde{z}$ direction of fluid after passing through filter. Units cm/sec.

$\tilde{w}_o(\tilde{x}, \tilde{y}, \tilde{z})$: velocity in $\tilde{z}$ direction of fluid before passing through filter. Units cm/sec.

$W_j$: $(j = 1, 2, 3)$ impermeable walls of filter.

$\tilde{x}$: length in direction along filter. Units cm.

$\tilde{y}$: length in direction across filter. Units cm.

$\tilde{z}$: length in height of filter. Units cm.

$Z$: height of filter. Units cm.

$\alpha$: nondimensional parameter used in equations:

$$\alpha = \frac{\rho h^4 (\tilde{P}_o - \tilde{P}_i)}{\mu^2 L^2}. \quad (2.4)$$

$\beta$: ratio of concentration of particles in pre-filtration area to the clogging concentration of the filter:

$$\beta = \frac{\tilde{C}_f h}{C_c}. \quad (2.5)$$

$\Delta t$: discretization parameter in $t$ used for numerical scheme.

$\Delta x$: discretization parameter in $t$ used for numerical scheme.

$\gamma$: nondimensional parameter used in equations.

$\mu$: dynamic viscosity of fluid, units g/(cm·sec).

$\nu$: kinematic viscosity of fluid, units cm²/sec.

$\rho$: density of fluid, value g/cm³.

$\zeta$: aspect ratio of three-dimensional filter device, given by $\zeta = Z/L$.

Nondimensionalized variables will have no tildes.
Section III: Two-Dimensional Governing Equations

We begin by assuming that the filter is a two-dimensional object with length $L$, width $2h$, and distance $2h$ between filters. We also assume that the concentration of the particles is so low that the density in both regions is the same. We then use the two-dimensional Navier-Stokes equations in rectangular coordinates:

$$\frac{\partial \hat{u}}{\partial \hat{x}} + \frac{\partial \hat{v}}{\partial \hat{y}} = 0$$  \hspace{1cm} (3.1)

$$\rho \left( \frac{\partial \hat{u}}{\partial \hat{t}} + \hat{u} \frac{\partial \hat{u}}{\partial \hat{x}} + \hat{v} \frac{\partial \hat{u}}{\partial \hat{y}} \right) = - \frac{\partial \hat{p}}{\partial \hat{x}} + \mu \left( \frac{\partial^2 \hat{u}}{\partial \hat{x}^2} + \frac{\partial^2 \hat{u}}{\partial \hat{y}^2} \right)$$  \hspace{1cm} (3.2)

$$\rho \left( \frac{\partial \hat{v}}{\partial \hat{t}} + \hat{u} \frac{\partial \hat{v}}{\partial \hat{x}} + \hat{v} \frac{\partial \hat{v}}{\partial \hat{y}} \right) = - \frac{\partial \hat{p}}{\partial \hat{y}} + \mu \left( \frac{\partial^2 \hat{v}}{\partial \hat{x}^2} + \frac{\partial^2 \hat{v}}{\partial \hat{y}^2} \right).$$  \hspace{1cm} (3.3)

These equations are general and hold for the fluid before and after it passes through the filter, though not in the filter itself.

At the filter, the change in concentration of particles on the filter is equal to the concentration of particles coming in:

$$\frac{\partial \tilde{C}}{\partial \tilde{t}} = \tilde{C}_f \tilde{v}_o(\tilde{x}, \tilde{h}).$$  \hspace{1cm} (3.4)

Next we proceed to nondimensionalize our equations. We nondimensionalize $\hat{x}$ by our filter length $L$ and $\hat{y}$ by half of our filter width, which is $h$. We nondimensionalize our velocities $\hat{u}$ and $\hat{v}$ by $U$ and $V$, respectively, which are at this time unknown. In addition, we nondimensionalize $\hat{t}$ by $T$, which is as of yet unknown. We nondimensionalize $\tilde{C}$ by our clogging concentration $C_c$. Our pressure values vary between $\tilde{P}_o$ and $\tilde{P}_i$, so we normalize to make them vary between 1 and 0. Summarizing, we have the following:

$$x = \frac{\tilde{x}}{L}, \hspace{1cm} y = \frac{\tilde{y}}{h}, \hspace{1cm} u = \frac{\tilde{u}}{U}, \hspace{1cm} v = \frac{\tilde{v}}{V}, \hspace{1cm} t = \frac{\tilde{t}}{T}, \hspace{1cm} C = \frac{\tilde{C}}{C_c}, \hspace{1cm} p = \frac{\tilde{p} - \tilde{P}_i}{\tilde{P}_o - \tilde{P}_i}.$$  \hspace{1cm} (3.5)

Once again, these nondimensionalizations apply to the fluid both before and after it passes through the filter.

Using equations (3.5) in (3.1), we have the following:

$$\frac{U}{L} \frac{\partial u}{\partial x} + \frac{V}{h} \frac{\partial v}{\partial y} = 0.$$
In order to simplify our equations, we let \( U/L = V/h \) to yield

\[
\frac{\partial u}{\partial x} + \frac{\partial v}{\partial y} = 0.
\]

(3.6)

Using equations (3.5) in (3.4), we have

\[
\frac{C_c}{T} \frac{\partial C}{\partial t} = \hat{C}_f V v_o(x, 1^-),
\]

and substituting \( Uh/L \) for \( V \) yields

\[
\frac{\partial C}{\partial t} = \frac{\hat{C}_f U h T}{L C_c} v_o(x, 1^-).
\]

(3.7)

Since we want \( O(1) \) changes in our concentration, we let

\[
T = \frac{L C_c}{\hat{C}_f U h}.
\]

(3.8)

Then equation (3.7) becomes

\[
\frac{\partial C}{\partial t} = v_o(x, 1^-).
\]

(3.9)

Now nondimensionalizing equation (3.2), we have

\[
\rho \left( \frac{\hat{C}_f U^2 h}{L C_c} \frac{\partial u}{\partial t} + \frac{UV}{h} \frac{\partial u}{\partial y} + \frac{U^2}{L} \frac{\partial u}{\partial x} \right) = -\frac{\hat{P}_o - \hat{P}_i}{L} \frac{\partial p}{\partial x} + \mu \left( \frac{U}{L^2} \frac{\partial^2 u}{\partial x^2} + \frac{U}{h^2} \frac{\partial^2 u}{\partial y^2} \right).
\]

Using \( U/L = V/h \), we may express everything in terms of \( U \):

\[
\frac{\rho U^2}{L} \left( \frac{\beta}{L} \frac{\partial u}{\partial t} + \frac{v}{h} \frac{\partial u}{\partial y} + \frac{u}{L} \frac{\partial u}{\partial x} \right) = -\frac{\hat{P}_o - \hat{P}_i}{L} \frac{\partial p}{\partial x} + \frac{\mu U L}{h^2} \left( \frac{h^2}{L^2} \frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2} \right).
\]

Now we want to set the coefficient of the pressure equal to unity so that we may examine the relative contributions from the other terms. Doing so, we have the following:

\[
\frac{\rho U^2}{\hat{P}_o - \hat{P}_i} \left( \frac{\beta}{L} \frac{\partial u}{\partial t} + \frac{v}{h} \frac{\partial u}{\partial y} + \frac{u}{L} \frac{\partial u}{\partial x} \right) = -\frac{\partial p}{\partial x} + \frac{\mu U L}{h^2} \left( \frac{h^2}{L^2} \frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2} \right).
\]

Since we will eventually wish to examine oil and other viscous fluids, we want the viscous diffusive terms to be dominant. Hence, we set the coefficient of the diffusive terms equal to unity to yield

\[
U = \frac{h^2 (\hat{P}_o - \hat{P}_i)}{\mu L}
\]

(3.10)
\[
\alpha \left( \beta \frac{\partial u}{\partial t} + v \frac{\partial u}{\partial y} + u \frac{\partial u}{\partial x} \right) = -\frac{\partial p}{\partial x} + \left( \frac{h^2}{L^2} \frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2} \right). 
\] (3.11)

Now, since \( h \ll L \), we see that both the first diffusive term and \( \alpha \) are negligible, so equation (3.11) reduces to
\[
\frac{\partial p}{\partial x} = \frac{\partial^2 u}{\partial y^2}. 
\] (3.12)

Now using equations (3.5) in equation (3.3), we have the following:
\[
\rho \left( \frac{\hat{C}_f UV h}{L C_c} \frac{\partial v}{\partial t} + \frac{UV}{L} u \frac{\partial v}{\partial x} + \frac{V^2}{h} v \frac{\partial v}{\partial y} \right) = -\frac{\hat{P}_o - \hat{P}_i}{h} \frac{\partial p}{\partial y} + \mu \left( \frac{V}{L^2} \frac{\partial^2 v}{\partial x^2} + \frac{V}{h^2} \frac{\partial^2 v}{\partial y^2} \right). 
\]

Using our relation between \( U \) and \( V \), we have the following:
\[
\frac{\rho U^2 h^2}{L^2 (\hat{P}_o - \hat{P}_i)} \left( \beta \frac{\partial v}{\partial t} + u \frac{\partial v}{\partial x} + v \frac{\partial v}{\partial y} \right) = -\frac{\partial p}{\partial y} + \frac{\mu U}{L (\hat{P}_o - \hat{P}_i)} \left( \frac{h^2}{L^2} \frac{\partial^2 v}{\partial x^2} + \frac{\partial^2 v}{\partial y^2} \right). 
\]

Using equation (3.10), we have
\[
\frac{\alpha h^2}{L^2} \left( \beta \frac{\partial v}{\partial t} + u \frac{\partial v}{\partial x} + v \frac{\partial v}{\partial y} \right) = -\frac{\partial p}{\partial y} + \frac{h^2}{L^2} \left( \frac{h^2}{L^2} \frac{\partial^2 v}{\partial x^2} + \frac{\partial^2 v}{\partial y^2} \right). 
\]

Now, since \( h \ll L \), we see that we may neglect all terms but the pressure term and our equation becomes the following:
\[
\frac{\partial p}{\partial y} = 0. 
\] (3.13)

Our system of equations (3.6), (3.12), and (3.13) are called the lubrication equations. Note that our time dependence has scaled out of all but equation (3.9).

Now we wish to postulate some boundary conditions. As shown in figure 1, we place our axes such that the problem becomes symmetric. We then only need consider the region \( 0 < x < 1, \ 0 < y < 2 \). Since our filter is along \( y = 1 \), we split the problem into two regions. We begin with the region before the fluid reaches the filter \((0 < x < 1, \ 0 < y < 1^-)\), which we call region \( o \). In this region, we have a pressure condition at the inflow which has scaled to become
\[
p_o(0, y, t) = 1. 
\] (3.14)

We assume that the boundary at \( x = 1 \) is a wall through which no fluid can pass, so
\[
u_o(1, y, t) = 0. 
\] (3.15)

Since \( y = 0 \) is a line of symmetry, we have
\[
u_o(x, 0, t) = 0 \quad \text{(3.16a)}
\]
\[
\frac{\partial u_o}{\partial y}(x, 0, t) = 0. \quad \text{(3.16b)}
\]
We assume that the filter is porous only in the vertical direction, hence

$$u_o(x, 1, t) = 0. \quad (3.17a)$$

Also, by doing a simple concentration balance, we see that

$$\tilde{C}_t \tilde{v}_i(\tilde{x}, h^+, \tilde{t}) \, d\tilde{t} \, d\tilde{x} = \tilde{C}_f \tilde{v}_o(\tilde{x}, h^-, \tilde{t}) \, d\tilde{t} \, d\tilde{x} - \tilde{C}_f \tilde{v}_o(\tilde{x}, h^-, \tilde{t}) \, d\tilde{t} \, d\tilde{x}.$$ 

We nondimensionalize our concentrations by $\tilde{C}_i$. Nondimensionalizing the rest of the equation, we have

$$v_i(x, 1^+, t) = (1 - C_f)v_o(x, 1^-, t). \quad (3.17b)$$

We assume that initially our concentration in the filter is 0, so

$$C(x, 0) = 0. \quad (3.18)$$

We now proceed to solve our equations in region $o$. From (3.13) we see immediately that $p_o$ is a function of $x$ and $t$ only. Solving equation (3.12) subject to our boundary conditions (3.16b) and (3.17a), we have

$$u_o(x, y, t) = \frac{y^2 - 1}{2} \frac{\partial p_o}{\partial x}. \quad (3.19)$$

The velocity $u_o$ can now satisfy equation (3.15) only if

$$\frac{\partial p_o}{\partial x} (1, t) = 0. \quad (3.20)$$

Using equation (3.19) in equation (3.6), we have the following:

$$\frac{\partial v_o}{\partial y} = -\frac{y^2 - 1}{2} \frac{\partial^2 p_o}{\partial x^2}.$$ 

Solving the above subject to boundary condition (3.16a), we have

$$v_o(x, y, t) = -\left(\frac{y^3}{6} - \frac{y}{2}\right) \frac{\partial^2 p_o}{\partial x^2}. \quad (3.21)$$

We now define our boundary conditions in region $i$, where the fluid has already passed through the filter. This is the region $0 < x < 1, 1^+ < y < 2$. In this case, the pressure boundary condition is specified at $x = 1$:

$$p_i(1, y, t) = 0. \quad (3.22)$$

Now the boundary at $x = 0$ is the wall, so

$$u_i(0, y, t) = 0. \quad (3.23)$$
Since \( y = 2 \) is also a line of symmetry, we have

\[
v_i(x, 2, t) = 0 \tag{3.24a}
\]

\[
\frac{\partial u_i}{\partial y}(x, 2, t) = 0. \tag{3.24b}
\]

We assume that the filter is porous only in the vertical direction, hence

\[
u_i(x, 1, t) = 0. \tag{3.25}
\]

Solving the equations in this region in a perfectly analogous manner to the way in which we solved the equations in region \( o \), we have

\[
u_i(x, y, t) = \frac{(2 - y)^2}{2} \frac{\partial p_i}{\partial x} \tag{3.26}
\]

\[
\frac{\partial p_i}{\partial x}(0, t) = 0 \tag{3.27}
\]

\[
v_i(x, y, t) = \left[ \frac{(2 - y)^3}{6} - \frac{(2 - y)}{2} \right] \frac{\partial^2 p_i}{\partial x^2}. \tag{3.28}
\]

In addition, we have the following permeability law:

\[
\tilde{p}_o(\tilde{x}, h^-, \tilde{t}) - \tilde{p}_i(\tilde{x}, h^+, \tilde{t}) = \tilde{k}(\tilde{C})\tilde{v}_o(\tilde{x}, h^-, \tilde{t}).
\]

Here we postulate the form of \( \tilde{k} \) given in section II. This then states that regardless of the pressure differential, no fluid will flow through the filter when \( \tilde{C} = C_c \), the clogging concentration. Nondimensionalizing, we have

\[
p_o(x, 1^-, t) - p_i(x, 1^+, t) = \frac{\tilde{k}_0 h^3}{\mu L^2 C_c [1 - C(x, t)]} v_o(x, 1^-, t) = \frac{\tilde{k}_0}{1 - C(x, t)} v_o(x, 1^-, t). \tag{3.29}
\]
Section IV: Steady Flow, No Particles

The first model we consider is that of steady flow with no particles in the fluid. Hence we have $C_f = 0$, and equation (3.4), together with boundary condition (3.18), implies that $C \equiv 0$ for all $t \geq 0$. Thus, there is no time dependence in the problem. Then equation (3.17b) becomes

$$v_i(x, 1^+) = v_o(x, 1^-) = v(x, 1)$$

and equation (3.29) becomes

$$p_o(x, 1^-) - p_i(x, 1^+) = k_0 v(x, 1).$$

Now we continue our solution of the problem. Since there is no time dependence in the problem, $p_o$ and $p_i$ are functions of $x$ only. Using equations (3.21) and (3.28) in (4.1), we have the following:

$$p_o''(x) = -p_i''(x)$$

$$p_o(x) + p_i(x) = A_1 x + A_2.$$  

(4.3)

Now using equations (3.21) and (3.28) in equation (4.2), we have

$$p_o(x) - p_i(x) = \frac{k_0}{3} p_o''(x).$$

(4.4)

Combining equations (4.3) and (4.4) and solving for $p_o(x)$, we have

$$2p_o(x) - \frac{k_0}{3} p_o''(x) = A_1 x + A_2.$$ 

$$p_o(x) = \frac{A_1 x + A_2}{2} + A_3 e^{-\gamma x} + A_4 e^{\gamma x},$$

(4.5a)

where $\gamma = \sqrt{6/k_0}$. Using equation (4.3), we immediately see that

$$p_i(x) = \frac{A_1 x + A_2}{2} - A_3 e^{-\gamma x} - A_4 e^{\gamma x}.$$  

(4.5b)

Using our boundary condition (3.14) in (4.5a), we have

$$\frac{A_2}{2} + A_3 + A_4 = 1,$$

(4.6)

while equation (3.20) gives us

$$\frac{A_1}{2} - \gamma A_3 e^{-\gamma} + \gamma A_4 e^{\gamma} = 0.$$  

(4.7)
For our \( p_i(x) \) conditions, we use (3.22):

\[
\frac{A_1 + A_2}{2} - A_3 e^{-\gamma} - A_4 e^{\gamma} = 0, \tag{4.8}
\]

and we use (3.27) to find

\[
\frac{A_1}{2} + \gamma A_3 - \gamma A_4 = 0. \tag{4.9}
\]

Equations (4.6)-(4.9) are a system of four equations in four unknowns which we may solve using Maple to find

\[
A_1 = -\frac{2\gamma(e^\gamma - 1)}{D}, \quad A_2 = 1 + \frac{\gamma(e^\gamma - 1)}{D}, \quad A_3 = \frac{e^\gamma}{D}, \quad A_4 = \frac{1}{D}, \tag{4.10a}
\]

\[
D = 2(e^\gamma + 1) + \gamma(e^\gamma - 1). \tag{4.10b}
\]

Using equations (4.10) in (4.5), we have

\[
p_o(x) = \frac{1}{2} + \frac{\gamma(1 - 2x)(e^\gamma - 1)}{2D} + \frac{e^{\gamma(1-x)} + e^{\gamma x}}{D}, \tag{4.11a}
\]

\[
p_i(x) = \frac{1}{2} + \frac{\gamma(1 - 2x)(e^\gamma - 1)}{2D} - \frac{e^{\gamma(1-x)} + e^{\gamma x}}{D}. \tag{4.11b}
\]

Now we have our flow completely determined. Summarizing, using (4.11a) in (3.19), we have

\[
u_o(x, y) = \left[ 1 - e^\gamma + e^{\gamma x} - e^{\gamma(1-x)} \right] \frac{\gamma(y^2 - 1)}{2D}. \tag{4.12}
\]

Using equation (4.11b) in equation (3.26), we have

\[
u_i(x, y) = \left[ 1 - e^\gamma - e^{\gamma x} + e^{\gamma(1-x)} \right] \frac{\gamma[(2 - y)^2 - 1]}{2D}. \tag{4.13}
\]

Using equation (4.11a) in equation (3.21), we have the following:

\[
v_o(x, y) = -\frac{\gamma^2}{D} \left[ e^{\gamma(1-x)} + e^{\gamma x} \right] \left( \frac{y^3}{6} - \frac{y}{2} \right). \tag{4.14}
\]

Using equation (4.11b) in equation (3.28), we have

\[
v_i(x, y) = -\frac{\gamma^2}{D} \left[ e^{\gamma(1-x)} + e^{\gamma x} \right] \left[ \frac{(2-y)^3}{6} - \frac{(2-y)}{2} \right]. \tag{4.15}
\]

As shown in figure 2, the lower velocity profile at the filter \( v_o(x, 1^-) \) is nearly parabolic in shape. This contradicted our first guess at the profile, since we originally thought the flow should be faster at the inlet and decay monotonically as \( x \) moved toward the outlet. However, further examination convinced us that our solutions were indeed correct. As will
be shown in section V, this implies that our filter will have a higher concentration at both ends, rather than a monotonic profile as we first thought.

Now we wish to plot streamlines. In region 0, the equations for the streamlines are given by

$$\frac{dy}{dx} = \frac{v_o}{u_o} = -\frac{1}{y^2 - 1} \left( \frac{\partial p_o}{\partial x} \right)^{-1} \left( \frac{\partial^2 p_o}{\partial x^2} \left( \frac{y^3}{3} - y \right) \right),$$

a differential equation which can be separated to yield

$$\log \left( \frac{y^3}{3} - y \right) = -\log \left( \frac{\partial p_o}{\partial x} \right) + A_5,$$

where $A_5$ is a constant of integration. Then using equation (4.11a) our solution is the following:

$$\frac{y^3}{3} - y = \frac{e^{A_5 D}}{\gamma} \left[ e^{\gamma x} - e^{\gamma(1-x)} + 1 - e^\gamma \right]^{-1}. \quad (4.16)$$

In region 1, the equations for the streamlines are given by

$$\frac{dy}{dx} = \frac{v_i}{u_i} = \frac{1}{(2 - y)^2 - 1} \left[ \frac{(2 - y)^3}{3} - (2 - y) \right] \left( \frac{\partial p_i}{\partial x} \right)^{-1} \left( \frac{\partial^2 p_i}{\partial x^2} \right),$$

a differential equation which can be separated to yield

$$\log \left[ \frac{(2 - y)^3}{3} - (2 - y) \right] = -\log \left( \frac{\partial p_i}{\partial x} \right) + A_6,$$

where $A_6$ is a constant of integration. Then using equation (4.11b) our solution is the following:

$$\frac{(2 - y)^3}{3} - (2 - y) = \frac{e^{A_6 D}}{\gamma} \left[ e^{\gamma(1-x)} - e^{\gamma x} + 1 - e^\gamma \right]^{-1}. \quad (4.17)$$

These streamlines are graphed in figure 3.
Figure 3.
Streamlines for Steady Flow Case
Section V: 2-Dimensional Flow with Particles

The next model we consider is that of flow with particles in the fluid. Hence we no longer have our simplification that \( C_f = 0 \), and the problem is time-dependent. However, we may simplify our equations. Using equation (3.21) in equation (3.9), we have the following at \( y = 1 \):

\[
\frac{\partial C}{\partial t} = \frac{1}{3} \frac{\partial^2 p_o}{\partial x^2}.
\]  

(5.1)

Using equations (3.21) and (3.28) in equation (3.17b), we have

\[
(1 - C_f) \frac{\partial^2 p_o}{\partial x^2} = -\frac{\partial^2 p_i}{\partial x^2}.
\]  

(5.2)

Using equation (3.21) in equation (3.29), we have the following:

\[
p_o(x, t) - p_i(x, t) = \frac{k_0}{3[1 - C(x, t)]} \frac{\partial^2 p_o}{\partial x^2}.
\]  

(5.3)

Our boundary conditions are given by equations (3.14), (3.18), (3.20), (3.22), and (3.27), which we rewrite for easy reference:

\[
p_o(0, t) = 1.
\]  

(5.4)

\[
\frac{\partial p_o}{\partial x}(1, t) = 0.
\]  

(5.5)

\[
p_i(1, t) = 0.
\]  

(5.6)

\[
\frac{\partial p_i}{\partial x}(0, t) = 0
\]  

(5.7)

\[
C(x, 0) = 0.
\]  

(5.8)

We wish to solve the system of equations numerically, hence we also need initial conditions for \( p_o \) and \( p_i \). We assume that the filter has no particles in it at time \( t = 0 \), so we use our results from section IV:

\[
p_o(x, 0) = \frac{1}{2} + \frac{\gamma(1 - 2x)(e^{\gamma} - 1)}{2D} + \frac{e^{\gamma(1-x)} + e^{\gamma x}}{D}
\]  

(5.9)

\[
p_i(x, 0) = \frac{1}{2} + \frac{\gamma(1 - 2x)(e^{\gamma} - 1)}{2D} - \frac{e^{\gamma(1-x)} + e^{\gamma x}}{D}, \text{ where}
\]  

(5.10)
\[ D = 2(e^\gamma + 1) + \gamma(e^\gamma - 1). \quad (5.11) \]

We discretize our \( x \) direction by \( \Delta x = 1/N \), and our \( t \) direction by \( \Delta t = (\Delta x)^2 \). We choose this \( \Delta t \) so that our scheme, which is first-order in \( t \) and second-order in \( x \), has the same size error in both directions. We then introduce a discretization notation by \( f(n, j) = f(n\Delta x, j\Delta t) \), where \( f \) is \( p_o \), \( p_i \), or \( C \). Our four unknowns, we let \( n = 1, \ldots, N \) for \( p_o \) [since we know \( p_o(0, t) \)], \( n = 0, \ldots, N - 1 \) for \( p_i \) [since we know \( p_i(1, t) \)] and \( n = 1, \ldots, N \) for \( C \) (for reasons which will be discussed later).

We break our scheme into two parts. First, we discretize equation (5.1) and perform an explicit Euler step in time to solve for the concentration at the next time step:

\[
C(n, j) = C(n, j - 1) + \frac{\Delta t}{3(\Delta x)^2} \left[ p_o(n - 1, j - 1) - 2p_o(n, j - 1) + p_o(n + 1, j - 1) \right], \\
1 \leq n \leq N. \quad (5.12)
\]

Note that for \( n = N \) we use the Neumann condition; that is, approximating (5.5) with respect to \( x \) by a central difference scheme, we see that

\[
p_o(N + 1, j) = p_o(N - 1, j). \quad (5.13)
\]

We use equation (5.13) in (5.12) when \( n = N \) and throughout the rest of the scheme. We also use its counterpart for \( p_i \), namely

\[
p_i(-1, j) = p_i(1, j). \quad (5.14)
\]

Next we solve for our new pressures implicitly by discretizing equations (5.2) and (5.3) and solving them together. At interior grid points, we approximate second derivatives using the standard second-order central difference scheme, so that (5.2) becomes

\[
(1 - C_f) \left[ p_o(n - 1, j) - 2p_o(n, j) + p_o(n + 1, j) \right] + p_i(n - 1, j) - 2p_i(n, j) + p_i(n + 1, j) = 0, \\
1 \leq n \leq N - 1. \quad (5.15)
\]

In equation (5.15), note that for \( n = 1 \) we use equation (5.4) so that the right-hand side to our equation is nonzero. We use equation (5.6) for \( n = N - 1 \), but the right-hand side remains the same. Discretizing (5.3), we have the following:

\[
p_i(n, j) - p_o(n, j) + \frac{k_0 \left[ p_o(n - 1, j - 1) - 2p_o(n, j - 1) + p_o(n + 1, j - 1) \right]}{3(\Delta x)^2[1 - C(n, j)]} = 0, \\
1 \leq n \leq N. \quad (5.16)
\]

In equation (5.16), we again use (5.4) for \( n = 1 \), and for \( n = N \) we use (5.6) and equation (5.13).

We now have \( 2N - 1 \) equations in \( 2N \) unknowns. To obtain the final equation, we construct the second-order forward-difference second-derivative scheme, since we do not know \( p_o(-1, j) \). Hence, we have the following expression:

\[
(1 - C_f) \left[ 2p_o(0, j) - 5p_o(1, j) + 4p_o(2, j) - p_o(3, j) \right] + p_i(-1, j) - 2p_i(0, j) + p_i(1, j) = 0. \quad (5.17)
\]
For equation (5.17), we use equation (5.14) and (5.4).

Examining equations (5.15)-(5.17), it becomes apparent why we did not calculate $C(0, t)$. Since $C(0, t)$ never appears in our expressions, it wouldn't be used to calculate new pressure conditions from which it in turn would be calculated at the next time step. Hence, if we tried to calculate it, we would get spurious results. However, since the concentration profile is nearly symmetric, we can make a reasonable approximation to $C(0, t)$ by examining $C(1, t)$.

Now that we have expressions for our pressure, we need to check our flow rate. Nondimensionalizing equation (2.2), we have

$$\tilde{q}(t) = \rho L V \int_0^1 u(x, 1, t) \, dx.$$ 

Using equations (3.10) and (3.21)

$$\frac{\tilde{q}(t) \mu L}{\rho h^3 (\bar{P}_o - \bar{P}_i)} = \frac{1}{3} \int_0^1 \frac{\partial^2 p_o}{\partial x^2} \, dx.$$ 

Integrating and using equation (5.5), we have

$$\frac{3\tilde{q}(t) \mu L}{\rho h^3 (\bar{P}_o - \bar{P}_i)} \equiv q(t) = -\frac{\partial p_o}{\partial x}(0, t). \tag{5.18}$$

Since we are taking ratios, we see that $t_c$ is that time at which $q(t_c)/q(0) = e^{-1}$.

We also nondimensionalize equation (2.3) to yield

$$\frac{3\dot{Q} \mu L}{\rho h^3 (\bar{P}_o - \bar{P}_i)} = \frac{L C_c}{C_f U h} \int_0^{t_c} q(t) \, dt$$

$$\frac{3\dot{Q} \tilde{C}_f}{\rho L C_c} \equiv Q = \int_0^{t_c} q(t) \, dt. \tag{5.19}$$

Using our code, we performed several tests, the results of which are graphed on the following pages. The first test we performed was to test the sensitivity of $t_c$ and $C$ to changes in $C_f$ as we varied it from 0 to 0.05. Figure 4 shows that we saw very little change in $t_c$ as $C_f$ varies. Note that we are varying $C_f$ over a small range, so we would expect a small variance. As far as $t_c$ is concerned, the graph shows us that for varying values of $C_f$ the number of nondimensional time units is not changing considerably. However, since our scaling in equation (5.8) depends explicitly on $C_f$, the dimensional $t_c$ does vary with respect to $C_f$.

Figure 5 shows the change in concentration at the outlet of the filtering device as a function of $t$ for varying $k_0$. Note that as $k_0$ increases, the concentration approaches its final value more slowly, and that the final value is smaller. This can also be seen in figure 6, which shows $C(x, t_c)$ as a function of $x$ for varying $k_0$. Note that, as discussed briefly in section IV, due to the shape of our velocity profile, the maximum values of $C$ are at
the ends of the filter. As indicated in figure 5, as \( k_0 \) increases, the maximum value of our profile decreases. In addition, our profile begins to flatten. This is reasonable, since as \( k_0 \to \infty \), equation (3.29) indicates that there would be no flow of particles and hence we would have a flat profile of \( C \equiv 0 \). Figure 7 shows the maximum concentration at \( t_c \) vs. \( k_0 \). Note that as you increase \( k_0 \), the filter must be thrown away at smaller concentrations.

Figure 8 shows the outer and inner pressures \( p_o \) and \( p_i \) at \( t_c \) as a function of \( x \) for various values of \( k_0 \). Note that for smaller \( k_0 \), a lower pressure gradient is needed to make the fluid flow through, as indicated by equation (3.29). As expected, the pressures are larger near the inlet than at the outlet.

Figure 9 is a graph of \( q(t) \) vs. \( t \) for varying \( k_0 \). Note that as \( k_0 \) increases, the flow starts off at a slower rate [as indicated by (3.29)], but takes longer to decay to \( 1/e \) times its initial value. This variance of \( t_c \) with \( k_0 \) is indicated explicitly in figure 10. Note that it is nearly linear for large values of \( k_0 \). However, figure 11 shows that even though the time that you use the filter is longer for larger values of \( k_0 \), the flow you force through the filter (which is indicated by \( Q \)) is smaller.

Hence, which value of \( k_0 \) one should use for an efficient filter depends on your definition of the word “efficient.” In the case of an oil filter, where a longer life might be more important than a high flow rate, a large \( k_0 \) would be indicated. However, in industrial filter applications, such as the filtering of yeast from beer, where large flow rates are economically desirable, a smaller \( k_0 \) would be indicated if the machinery could be designed so that the filter, which would have to be changed more often, is readily accessible.
Figure 8: (x', y') vs. x for various values of k.0 and p(x', y')o.
Section VI: The Three-Dimensional Problem for Steady Flow and No Particles

Next we consider a filter which cannot be reduced to a two-dimensional problem. Here the fluid enters through the top, flows through the filter and leaves through the left side. The perimeter is represented in the figure below by a bold line. The closed walls in the filter unit are represented by brick walls in the figure. As before, this figure actually only shows one portion of a large filter, and the front and back of the figure are planes of symmetry.

![Schematic for three-dimensional problem](image)

Figure 12. Schematic for three-dimensional problem.

For this problem, we use the three-dimensional Navier-Stokes equations in rectangular coordinates for steady flow. These are

\[ \nabla \cdot \ddot{v} = 0 \]  \hspace{1cm} (6.1a)
\( (\tilde{\mathbf{v}} \cdot \nabla)\tilde{\mathbf{v}} = -\frac{1}{\rho} \nabla p + \nu \nabla^2 \tilde{\mathbf{v}} \), \hspace{1cm} (6.1b)

where \( \tilde{\mathbf{v}} = (\tilde{u}, \tilde{v}, \tilde{w}) \) and \( \tilde{w} \) is the velocity in the \( \tilde{z} \) direction. As in the two-dimensional problem, these equations hold for the fluid flow before and after passing through the filter.

Our nondimensionalization process is identical to that of the two-dimensional problem with the addition of

\[ z = \frac{\tilde{z}}{L} \quad \text{and} \quad w = \frac{\tilde{w}}{U}. \] \hspace{1cm} (6.2)

We nondimensionalize \( \tilde{z} \) by \( L \) since we assume \( L \) and \( Z \) to be of the same order. Similarly, we expect \( \tilde{w} \) to be of the same order as \( \tilde{u} \). As before, the nondimensionalization and simplification of equations (6.1) using (6.2) and our other quantities from previous sections lead to the following three-dimensional system of lubrication equations:

\[ \frac{\partial u}{\partial x} + \frac{\partial v}{\partial y} + \frac{\partial w}{\partial z} = 0 \] \hspace{1cm} (6.3a)

\[ \frac{\partial p}{\partial x} = \frac{\partial^2 u}{\partial y^2} \] \hspace{1cm} (6.3b)

\[ \frac{\partial p}{\partial y} = 0 \] \hspace{1cm} (6.3c)

\[ \frac{\partial p}{\partial z} = \frac{\partial^2 w}{\partial y^2}. \] \hspace{1cm} (6.3d)

We consider the region

\[ [0, 1] \times [0, 2] \times [0, \zeta], \]

where \( \zeta \) is defined in section II. Our problem is again divided into two regions determined by the plane \( y = 1 \). In region \( a \),

\[ [0, 1] \times [0, 1^-] \times [0, \zeta], \]

we have the following boundary conditions:

\[ p_o(x, y, \zeta) = 1; \quad u_o(1, y, z) = 0 \] \hspace{1cm} (6.4a)

\[ u_o(0, y, z) = 0; \quad w_o(x, y, 0) = 0 \] \hspace{1cm} (6.4b)

\[ v_o(x, 0, z) = 0; \quad \frac{\partial w_0}{\partial y}(x, 0, z) = 0; \quad \frac{\partial w_0}{\partial y}(x, 0, z) = 0. \] \hspace{1cm} (6.4c)

On the other hand, in region \( i \),

\[ [0, 1] \times [1^+, 2] \times [0, \zeta], \]

the boundary conditions are

\[ w_i(x, y, \zeta) = 0; \quad u_i(1, y, z) = 0 \] \hspace{1cm} (6.5a)

\[ p_i(0, y, z) = 0; \quad w_i(x, y, 0) = 0 \] \hspace{1cm} (6.5b)

\[ v_i(x, 2, z) = 0; \quad \frac{\partial u_i}{\partial y}(x, 2, z) = 0; \quad \frac{\partial w_i}{\partial y}(x, 2, z) = 0. \] \hspace{1cm} (6.5c)
At the filter our permeability law in its nondimensional form is
\[ p_o(x, 1^-, z) - p_i(x, 1^+, z) = k_0 v(x, 1, z). \] (6.6)

Our other boundary conditions at the filter are
\[ u(x, 1, z) = 0 \quad \text{and} \quad w(x, 1, z) = 0. \] (6.7)

Since we are assuming a pure fluid, \( v \) must be continuous across the filter, \textit{i.e.}
\[ v_o(x, 1^-, z, t) = v_i(x, 1^-, z, t). \] (6.8)

We solve this three-dimensional system in exactly the same manner as in the two-dimensional problem. This gives the following:
\[ u_o = \frac{y^2 - 1}{2} \frac{\partial p_o}{\partial x}; \quad u_i = \frac{(2 - y)^2 - 1}{2} \frac{\partial p_i}{\partial x}, \] (6.9)
\[ w_o = \frac{y^2 - 1}{2} \frac{\partial p_o}{\partial z}; \quad w_i = \frac{(2 - y)^2 - 1}{2} \frac{\partial p_i}{\partial z} \] (6.10)

\[ v_o = -\frac{1}{2} \left( \frac{y^3}{3} - y \right) \left( \frac{\partial^2 p_o}{\partial x^2} + \frac{\partial^2 p_o}{\partial z^2} \right) \] (6.11a)
\[ v_i = \frac{1}{2} \left[ \frac{(2 - y)^3}{3} - (2 - y) \right] \left( \frac{\partial^2 p_i}{\partial x^2} + \frac{\partial^2 p_i}{\partial z^2} \right). \] (6.11b)

Using the continuity of \( v \) at the filter and the permeability law we arrive at the following equations:
\[ \frac{\partial^2 p_i}{\partial x^2} + \frac{\partial^2 p_i}{\partial z^2} = - \left( \frac{\partial^2 p_o}{\partial x^2} + \frac{\partial^2 p_o}{\partial z^2} \right) \] (6.12)
\[ p_o - p_i = k_0 v_o = \frac{k_0}{3} \left( \frac{\partial^2 p_o}{\partial x^2} + \frac{\partial^2 p_o}{\partial z^2} \right). \] (6.13)

These equations hold in the rectangle \( 0 < x < 1 \) and \( 0 < z < \zeta \). The boundary conditions are now
\[ \frac{\partial p_o}{\partial x}(1, z) = \frac{\partial p_i}{\partial x}(1, z) = 0 \] (6.14a)
\[ \frac{\partial p_o}{\partial z}(x, 0) = \frac{\partial p_i}{\partial z}(x, 0) = 0 \] (6.14b)
\[ \frac{\partial p_o}{\partial x}(0, z) = p_i(0, z) = 0 \] (6.14c)
\[ p_o(x, \zeta) = 1 \quad \text{and} \quad \frac{\partial p_i}{\partial z}(x, \zeta) = 0. \] (6.14d)

Two attempts were made to solve this system analytically. Neither was successful, as one led to coupled equations and the other to coupled boundary conditions. The most promising method for obtaining a solution seems to be numerical.
Section VII: Future Research

The work presented in this paper may be extended in several directions:

1. A rectangular shape was assumed for the pleats throughout this work. However, the pleat shape is most often not rectangular, but is the result of a folding and crimping process that gives the pleat a characteristic shape and strength, which then determines the behavior. The analysis performed for the rectangular pleat, which assumed a high aspect ratio and slow flow, could be modified to describe the flow in more realistically shaped pleats, such as wedges.

2. The solution obtained for the steady flow in a pleat may be used to calculate the stresses in the filter material. With this information, we may determine deformation in the filter material and whether the yield stress of the material has been exceeded. If the filter undergoes excessive deformation, its performance may be deteriorated, and exceeding the yield stress almost certainly leads to catastrophic failure. These issues are important aspects of filter design.

3. The numerical solution presented in Section V was obtained using LU decomposition techniques. The matrix structure, however, is diagonally sparse, and for sufficiently high resolution, iterative techniques will give superior machine performance. In addition, an explicit Eulerian time integration is used. To avoid excessively small time steps to preserve numerical stability, implicit schemes should be considered.

4. The work presented here assumes the particles are trapped within the filter material. There are applications in which the particles do not penetrate the filter material resulting in the accumulation of particulate matter on the filter. This effectively reduces the permeability of the filter and narrows the pleat width available for fluid flow. A more realistic model would combine a nonrectangular pleat configuration as described in number 1 above and incorporate the effects of a growing layer of particulate matter.

5. Finally, the three-dimensional analysis presented in Section VI is woefully incomplete. Further analytical analysis of the steady, no particle flow may give insight about the qualitative behavior of flow in three-dimensional, pleated filter packs. However, for the transient three-dimensional problem, numerical techniques similar to those discussed in Section V and noted in number 3 above would be used.
Students' Report

#9
Dice Dynamics and Probability

IMA Summer Program for Graduate Students
Mathematical Modeling

Week 3, Group 3
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1 Abstract

This paper addresses the problem of determining the probability for landing on one side of a rod with polygonal cross-section (abbreviated henceforth as die).

2 Introduction

The probability of landing on one side of a regularly shaped die, say for instance a standard six-sided die, at first seems to warrant no further discussion. Given a random throw, the chance of landing on one of the sides is the same as landing on any other. A more delicate question however, is what exactly causes the randomness, or to phrase it another way: at what point in the throwing of the die could the outcome of the roll be fully determined? Even less obvious is the question: if the die is not regularly shaped, then what is the probability distribution of the possible outcomes?

In this paper we address both of these questions by means of analyzing the dynamics of the die. In the process of doing so we will, by necessity, discover more than we need. In fact, we will trace out the entire path of the die being thrown. By doing this, and assuming no random or chaotic events in our ambient universe, we will thus trace back the randomness of the entire process to the initial set of inputs.
3 Nomenclature and Assumptions

We introduce the following symbols, functions, and functionals in the formulation of our model of the die:

\( \alpha, \theta \) : angle
\( \omega \) : angular velocity
\( v \) : vertical velocity
\( u \) : horizontal velocity
\( m \) : mass
\( I \) : moment of inertia
\( J \) : impulse
\( \vec{u} \) : \((u, v)\)
\( \vec{\omega} \) : \( \omega \cdot \vec{k} \) \((\vec{k} = (0, 0, 1)^T)\)
\( u_- \) : horizontal velocity before collision with surface
\( u_+ \) : horizontal velocity after collision with surface
\( (\cdot)_- \) : any entity before collision with surface
\( (\cdot)_+ \) : any entity after collision with surface
\( x_c \) : center of mass
\( a_i \) : length from center of mass to the \( i^{th} \) corner
\( y_0 \) : max \( a_i \)
\( g \) : gravitational constant
\( P_i \) : probability of \( i^{th} \) side landing face down on surface
\( \Omega_i \) : region corresponding to \( i^{th} \) side landing face down on surface
\( \theta_i \) : angle of \( i^{th} \) corner from \( \theta = 0 \)
\( \vec{x} \) : position vector
\( T \) : torque
\( r \) : coefficient of restitution
\( R \) : half the diagonal length of rectangle
\( \vec{n} \) : normal vector
4 Nondimensionalization

Note that the dimensions of the following variables are:

\[ y_0 \quad length \]
\[ v \quad length/time \]
\[ \omega \quad 1/time \]
\[ t \quad time \]
\[ g \quad length/time^2. \]

We nondimensionalize in terms of \( y_0 \) and \( g \) yielding:

\[ \tilde{v} = \frac{v}{\sqrt{g y_0}} \]
\[ \tilde{\omega} = \omega \sqrt{\frac{y_0}{g}} \]
\[ \tilde{t} = t \sqrt{\frac{g}{y_0}}. \]

5 No Surface Dynamics

Before tackling the full problem, it is useful to consider a slightly simplified situation, namely, suppose the surface dynamics are ignored, i.e. once the die lands on the surface its motion, both positional and rotational, come to an instantaneous halt. We will assume throughout that the probability for each side hitting to be nonzero.

**Theorem 1** Suppose the die is thrown into the air from a height \( y_0 \) with an angular velocity \( \omega \) and an upward velocity \( v \). Then the equation for solutions of the die spinning in the air and landing on a corner with the center of mass centered over the corner is as follows:

\[ \tilde{\omega} \tilde{v} \left( 1 + \sqrt{1 + 2 - \frac{a_i}{v^2}} \right) = \frac{3 \pi}{2} - \theta_i + 2n \pi \quad (1) \]

**Proof:**

The equations for motion are given in this case as

\[ \theta = \omega t \]
\[ y = -\frac{1}{2}gt^2 + vt + y_0 \]

Since \( \theta_{Ai} \), represents the angle of vertex \( A_i \) at rest, \( \frac{3 \pi}{2} - \theta_{Ai} + 2n \pi \) represents the angle of rotation needed for the die to land on corner \( A_i \), such that the center of mass is centered over that corner with distance \( a_i \) to the surface. Since both equations of motion must be satisfied at impact, we have

\[ \frac{3 \pi}{2} - \theta_{Ai} + 2n \pi = \omega t \]
\[ a_i = -1/2gt^2 + vt + y_0 \]

Solving both of the before mentioned equations for \( t \), we find that
\[
t = \frac{1}{\omega} \left[ \frac{3\pi}{2} - \theta_{A_i} + 2n\pi \right]
\]

and
\[
t = \frac{v^+ \sqrt{v^2 - 2g(a_i - y_0)}}{g}.
\]

Setting these expressions equal to each other and nondimensionalizing \( \omega \) and \( v \), we arrive at the desired result. \( \square \)

Note: For simplicity, the \textit{tildes} will be removed for the remainder of this section and all equations will be in nondimensionalized form.

**Theorem 2** Let \( p(v,w) \) be a continuous probability density with support in the region \( v > 0 \), \( \omega > 0 \), and let \( \beta \) be a fixed constant satisfying \( 0 \leq \beta \leq \pi/2 \) and \( \theta_{K+1} = 2\pi + \theta_1 \). Then
\[
\lim_{U \to \infty} P_i = \lim_{U \to \infty} \int_{\Omega_{i-1}} p(v - U \cos \beta, \omega - U \sin \beta) \, d\omega \, dv = \frac{\theta_{i+1} - \theta_i}{2\pi}, \quad i = 1, 2, \ldots, K
\]

Note: Thus, given enough initial vertical and angular velocity, the probability that a die will land on any one side (before bouncing and rolling) depends entirely on the angles between successive vertices. **Proof:** For \( 0 \leq \beta < \pi/2 \), we first write the above integral as an iterated integral using (1) to determine the range of \( \omega' = \omega - U \sin \beta \):

\[
P_i = \int_{\Omega_i} p(v,\omega) \, d\omega \, dv = \int_{U \cos \beta}^{\infty} \sum_{n=n_i}^{\alpha_{i,n}(v)-U \sin \beta} p(v - U \cos \beta, \omega') \, d\omega' \, dv
\]

where \( n^* \) is determined by \( U \) and \( \beta \), and \( \alpha_{i,n}(v) = (3\pi/2 - \theta_i + 2n\pi)/\gamma_i(v) \gamma_i(v) = v \left( 1 + \sqrt{1 + \frac{1}{v^2 \beta_i}} \right) \)

For large \( U \), the range of each integral over \( \omega' \) is of length \( \alpha_{i,n}(v) - \alpha_{i+1,n}(v) = \frac{\theta_{i+1} - \theta_i}{\gamma_i(v)} \).

By the mean value theorem, we can approximate each of these integrals by the length of the integral multiplied by the value of the integrand at the right endpoint, \( \alpha_{i,n}(v) - U \sin \beta \). The error in this approximation is \( O(U^{-1}) \). Thus we can rewrite (2) as

\[
P_i = \int_{U \cos \beta}^{\infty} \sum_{n=n_i}^{\alpha_{i,n+1}(v)-U \sin \beta} p(v - U \cos \beta, \alpha_{i,n}(v) - U \sin \beta) \left( \frac{\theta_{i+1} - \theta_i}{\gamma_i(v)} \right) [1 + o(1)] \, dv.
\]

As \( U \) becomes infinite, the sum in (3) converges to \( \frac{\theta_{i+1} - \theta_i}{2\pi} \) times the Riemann integral of \( p \) with respect to \( \omega' \). In order to see this, let us consider the integral

\[
\int_{\alpha_{i,n}(v)-U \sin \beta}^{\alpha_{i,n+1}(v)-U \sin \beta} p(v - U \cos \beta, \omega') \, d\omega' \, dv
\]

Obviously, for \( v \) large, the Taylor expansion of \( p(v - U \cos \beta, \omega') \) about the left endpoint \( \alpha_{i,n}(v) - U \sin \beta \) is \( p(v - U \cos \beta, \omega') = p(v - U \cos \beta, \alpha_{i,n}(v) - U \sin \beta) + O(1/\gamma(v)) \), so
\[
\int_{\alpha_{i,n}(v) - U \sin \beta}^{\alpha_{i,n+1}(v) - U \sin \beta} p(v - U \cos \beta, \omega') dw' = p(v - U \cos \beta, \alpha_{i,n}(v) - U \sin \beta) \frac{2\pi}{\gamma_i(v)}  + O\left(\frac{1}{v\gamma(v)}\right)
\]

combining (3) and (5), and using the fact that \( v \geq U \cos \beta \) we have

\[
P_i = \frac{\theta_{i+1} - \theta_i}{2\pi} \int_{U \cos \beta}^{\infty} \sum_{n=1}^{\infty} p(v - U \cos \beta, \alpha_{i,n}(v) - U \sin \beta) \frac{2\pi}{\gamma_i(v)} [1 + o(1)] dv
\]

\[
= \frac{\theta_{i+1} - \theta_i}{2\pi} \int_{U \cos \beta}^{\infty} \sum_{n=1}^{\infty} \int_{\alpha_{i,n}(v) - U \sin \beta}^{\alpha_{i,n+1}(v) - U \sin \beta} p(v - U \cos \beta, \omega') dw' dv + o(1)
\]

\[
= \frac{\theta_{i+1} - \theta_i}{2\pi} \int_{0}^{\infty} \int_{0}^{\infty} p(v', \omega') dv' = o(1).
\]

Hence,

\[
\lim_{U \to \infty} P_i = \frac{\theta_{i+1} - \theta_i}{2\pi}
\]

since

\[
\int_{0}^{\infty} \int_{0}^{\infty} p(v', \omega') dv' = 1.
\]

For \( \beta = \frac{\pi}{2} \), we introduce \( v' = v - U \sin \beta \), \( \omega' = \omega - U \cos \beta \) and then the proof is similar to that above.

\( \square \)

We state the obvious consequence:

**Corollary 1** Suppose a die has uniform mass and \( n \)-edges of equal width. Then

\( \lim_{U \to \infty} P_i = \frac{1}{n} \)

**Proof:**

\( \theta_{i+1} - \theta_i = \frac{2\pi}{n} \)

Dividing by \( 2\pi \) we have our result.

\( \square \)

6 Dynamics with no rolling

In this section, the polygon will be tossed with given initial conditions. The equations of motion will be used for the initial toss and for each bounce. The impact equations will be used to determine the "new" initial conditions for each bounce. To simplify matters, let the polygon (i.e. die) be a uniform rectangle with length \( 2a \) and height 2. For the initial toss of the die, let

\[
\bar{\mathbf{x}}(t = 0) = (x_0, y_0) \\
\bar{\mathbf{u}}(t = 0) = (u_0, v_0) \\
\bar{\theta}(t = 0) = \theta_0 \\
\bar{\omega}(t = 0) = \omega
\]
where $\vec{x}$ and $\vec{u}$ are the position and linear velocity respectively, $\theta$ is the angle shown in figure 1, and $\dot{\theta}$ is the angular velocity.

![Diagram](image)

Figure 1: The angles $\theta$ and $\alpha$; the lengths $a$, $1$, $y$, and $R$; and the normal vector.

The conservation of linear and angular momentum equations are

$$m \ddot{x} = \vec{F} \quad \text{and} \quad I \ddot{\theta} = \vec{T}$$

where $\vec{F}$ is the applied force, $\vec{T}$ is the applied torque, and $I$ is the moment of inertia. For our case, the equations simplify to

$$m \ddot{x} = (0, -mg)$$
$$\dot{\theta} = 0.$$

The above equations of motion and the initial conditions yield

$$x = u_0 t + x_0$$
$$y = \frac{1}{2} gt^2 + u_0 t + y_0$$
$$\theta = \omega t + \theta_0.$$

To determine the landing position and time we need a relationship between $y$ and $\theta$ at impact. Using a geometric argument, we found that $y = a|\sin \theta| + |\cos \theta|$ at impact where $y$ is the distance from the center of mass to the ground when the die first impacts the ground (see figure 1).
Thus, just before impact,
\[ y = a|\sin \theta| + |\cos \theta| \]
\[ y = -\frac{1}{2}gt^2 + v_0t + y_0 \]
\[ \theta = \omega t + \theta_0 \]
so that the angle at impact can be found by solving the following equation:
\[-\frac{\theta}{2\omega^2}(\theta - \theta_0)^2 + \frac{v_0}{\omega}(\theta - \theta_0) + y_0 = a|\sin \theta| + |\cos \theta| \]
Assuming we can numerically solve the above equation for \( \theta \), the time, position, and velocity just before impact can be found using the following equations:
\[ t = \frac{1}{\omega}(\theta - \theta_0) \]
\[ y = -\frac{1}{2}gt^2 + v_0t + y_0 \]
\[ x = u_0t + x_0 \]
\[ u = \dot{x} = u_0 \]
\[ v = \dot{y} = -gt + v_0. \]

Using the notation that \( ()^- \) refers to just before impact and \( ()^+ \) refers to just after impact, the general equations of impact are given by:
\[ \vec{J} = m\vec{u}^+ - m\vec{u}^- \]
\[ T = I\omega^+ - I\omega^- . \]
where \( \vec{J} \) is the change in impulse and \( T \) is the change in torque.

We will now make the assumption that friction is negligible while bouncing. Using a model developed by Poisson we will assume that

\( (\text{impulse after}) = -r(\text{impulse before}) \)
so that
\[ \vec{J} = \text{(impulse after - impulse before)} \]
\[ = m(-1 - r)[(\vec{u}^- + \vec{w}^- \times \vec{R}) \cdot \vec{n}]\vec{n} \]
where \( (\vec{u}^- + \vec{w}^- \times \vec{R}) \cdot \vec{n} \) is the total vertical velocity before impact and \( r \) is the coefficient of restitution.

Similarly (using a point impact),
\[ T = -\vec{J} \times \vec{R} = -J_y R \sin \alpha \]
where \( R \) is the distance from the center of gravity to a corner (i.e. \( R = \sqrt{a^2 + 1} \)) as shown in figure 1. If \( \theta' \) represents the quotient class of the angle, \( \theta \), module \( \pi \) then for \( 0 \leq \theta' \leq \pi/2 \), \( \alpha = (\arctan (1/a) - \theta \), and for \( \pi/2 \leq \theta' < \pi \) \( \alpha = (\arctan (1/a) + \theta - \pi. \)

Thus
\[ mu^+ - mu^- = 0 \]
\[ mv^+ - mv^- = m(-1 - r)(v^- - \omega^- R \sin \alpha) \]
\[ I\omega^+ - I\omega^- = m(1 + r)(v^- - \omega^- R \sin \alpha) R \sin \alpha. \]
Solving the above equations for \( u_+ \), \( v_+ \), and \( \omega_+ \) yields

\[
\begin{align*}
u_+ & = u_- \\
v_+ & = -rv_- + (1 + r)(\omega_- R \sin \alpha) \\
\omega_+ & = \omega_- + \frac{m}{I} \left( 1 + r \right) \left( v_- - \omega_- R \sin \alpha \right) R \sin \alpha.
\end{align*}
\]

Note that the values of \( \theta \), \( x \), \( y \), and \( t \) before and after impact do not change.

Thus the initial conditions for the first bounce are given by:

\[
\begin{align*}
\vec{x}(t = t_+) & = (x_+, y_+) \\
\vec{v}(t = t_+) & = (v_+, v_+) \\
\theta(t = t_+) & = \theta_+ \\
\dot{\theta}(t = t_+) & = \omega_+ 
\end{align*}
\]

and the process can be repeated using the equations of motion and the impact equations to calculate the initial conditions for the next bounce. This method is repeated until it is determined that the die stops bouncing and begins rolling.
7 Dynamics with rolling

In this section, we study the dynamics of our rigid rectangular die landing on the ground after stopping bouncing and then starting rolling. Let’s first analyze the dynamics of the die when it just before and after finishes bouncing. Similar to what we have dealt with bouncing in the last section, we consider one corner of the die hit the ground, and in turn the ground would give an impact to that die. Here we assume there is friction at the corner so that it is held fixed after contact. Thus by doing so, the impulse would generate a torque and make the die rotate about the corner.

Similar to the above section, this dynamical process can be described by

\[ m\dot{u}_+ - m\dot{u}_- = \ddot{J} \]  \hspace{1cm} (6)
\[ I\dot{\omega}_+ - I\dot{\omega}_- = \ddot{T}, \]  \hspace{1cm} (7)

where we again adopt \((.)_+\) to denote the variable before contact and \((.)_-\) as the one after contact; \(\ddot{J}\) is the impulse, \(\ddot{T}\) is the torque generated by the impact, \(\ddot{T} = \ddot{R} \times \ddot{J}\), and \(\ddot{\omega} = \omega \ddot{R}\). Assume side “a” would first hit the ground. The analysis of the \(y\) component of impact \(\ddot{J}\) is the same as above section. The difference lies in the corner has no movement along the horizontal direction due to our assumed friction from the ground. Therefore, the impact \(\ddot{J}\) should be \(\ddot{J} = -m(u_- + \omega_- R \cos \alpha)\ddot{J} - m(1 + r)(v_- - \omega_- R \sin \alpha)\ddot{J}\). And so the torque \(\ddot{T} = \ddot{R} \times \ddot{J} = R(J_x \cos \alpha - J_y \sin \alpha)\ddot{J}\).

Figure 2: Impact from the ground with friction.

Now by solving Equations (6) and (7), we have

\[
\begin{bmatrix}
    u_+ \\
v_+ \\
\omega_+
\end{bmatrix} = 
\begin{bmatrix}
    0 & 0 & -R \cos \alpha \\
    0 & -r & (1 + r)R \sin \alpha \\
    -mR \cos \alpha & mR \sin \alpha (1 + r) & -mR \sin \alpha + mR^2 + mR^2 \sin^2 \alpha
\end{bmatrix}
\begin{bmatrix}
    u_- \\
v_- \\
\omega_-
\end{bmatrix}
\]

We assume the restitution coefficient \(r\) here is chosen such that the die does not jump or
bouncing from the ground. In this case, the vertical velocity at the corner, \( v^+ + (\omega^+ \times \vec{R}) \cdot \vec{j} = v^+ - \omega_+ R \sin \alpha = 0 \). For notational convenience, we let \( \omega^{(0)}_+ = \omega_+ \) with \( r \) taken such a value.

In the above, we analyzed the dynamics during the contact. Since the contact corner of the die is fixed due to the friction, the die would then rotate about the corner and roll. For simplicity we shall assume there is no friction once the die starts rolling so that there is no force along horizontal direction to contribute to the angular momentum. Then the die would have to roll and slide at the same time. And along the vertical direction, from the above analysis, the die has no jump and thus \( v^+ = \omega_+ R \sin \alpha \). While rolling, each face of the die would touch the ground and get an impact. We assume this impact is linear along each point on the face, with the far end to the corner getting the biggest impact. Similar to the above analysis, the impact at each point can be written as \( J(x, t) = \frac{m}{2a} (-1 - r) u_- (x) = \frac{m}{2a} (-1 - r) \omega^{(1)}_- x \delta(t) \), where \( \omega^{(1)}_- = \omega^{(0)}_+ \). Then the average torque acting on the center is,

\[
\bar{T} = \int_{-a}^{a} \int_{0}^{2a} \frac{m}{2a} (-1 - r) \omega^{(1)}_- x \delta(t) \, dx \, dt
\]

\[
= \frac{ma^2}{3} (-1 - r) \omega^{(1)}_-
\]

Figure 3: Impact during rolling.

From \( I \omega_+ - I \omega_- = \bar{T} \) again, we have the angular velocity after side “a” hits the ground.

\[
\omega^{(1)}_+ = \left[ 1 - (1 + r) \frac{ma^2}{3I} \right] \omega^{(1)}_-
= \frac{1 - a^2 r}{1 + a^2} \omega^{(1)}_-
\]

Let \( s_a = \frac{1 - a^2 r}{1 + a^2} \). With this angular velocity, the die would roll ahead. But will it roll over until side “1” hits the ground? If \( \omega^{(1)}_- \geq \omega_a \), where \( \omega_a = \sqrt{\frac{a^2}{a^2 + 1 - 1} \cdot \frac{3}{2} g} \) satisfies

\[
mg \cdot 1 + \frac{1}{2} I_a \omega_a^2 = mg R,
\]

where \( I_a \) is the inertia momentum at the corner, the die will roll over; otherwise, it will fall back and thus side “a” touches the ground.

If side “1” hits the ground, by the same analysis, we can obtain the angular velocity afterwards

\[
\omega^{(2)}_- = s_1 \omega^{(2)}_-
\]
where \( s_1 = \frac{a^2 - \pi}{4 + a^2} \), and we assume \( \omega_{\text{c}}^{(2)} = \omega_{\text{c}}^{(2)} \).

And the critical angular velocity for side “1” continues to roll over is, \( \omega_1 = \sqrt{\frac{a + 1}{a^2 + 1} \cdot \frac{3}{2} g} \).

Therefore, the dynamics of the rolling die can be described by its angular velocity \( \omega = \cdots s_2 s_1 s_1 s_0 \omega_{\text{c}}^{(0)} \). Notice that both \( s_0 \) and \( s_1 \) are less than 1; the die would stop rolling until \( \omega \) is less than one of the critical angular velocities \( \omega_{\text{c}} \) and \( \omega_1 \).

Let us now look at the rolling die from a Ordinary Differential Equation viewpoint. Begin again with the standard torque equation:

\[
T = I \ddot{\theta}
\]

where \( I = \text{inertia}, T = \text{torque}, \) and \( \theta \) is the rotation about the center of mass.

We rewrite this as follows:

\[
T = F d \\
F = mg \\
d = r \cos \omega \theta \\
\text{thus} \\
\ddot{\theta} = \frac{mgr \cos \omega \theta}{I}
\]

We now consider the specific case of a square matrix and add the impulse term described above:

\[
\dot{\theta} = mg \cos 2\theta - J(\dot{\theta})
\]

The \( J \) term represents the impulse for the face of the die hitting the surface. For the square die, this means the \( J \) term will have a value of zero everywhere except at \( \theta = 0, \pi/2, \pi, \ldots \). As indicated by its parameter, the \( J \) term will have a relationship with \( \dot{\theta} \) and in fact will be proportional to it. For the reason of keeping the equation continuous (and also to more accurately match reality), the \( J \) term can be considered to be a ‘rounded’ impulse as opposed to an exact one. \( J \)’s nonzero parts can then be approximated by, for example, \( \sin^2 \dot{\theta} \). A trajectory for these dynamics is shown in Figure 4.

We see that for high \( \dot{\theta} \) the trajectory will oscillate slightly. This corresponds to the die speeding up as it hits the surface and slowing down as it comes off the table. Eventually, the die will not be able to turn over completely. At this point, the die will rock backwards corresponding to \( \dot{\theta} \) going negative. From then on, the die will rock back and forth, its \( \dot{\theta} \) gradually diminishing due to the subtractive impulse. Eventually, the die will come to rest on one of its faces, at which point \( \theta = 0, \pi/2, \pi \ldots \) We note that the total phase plot will in fact have many of these spirals, each occurring around a \( \theta \) corresponding to a face-down position. The only other fixed points of the graph will occur at \( \theta = \pi/4, 3\pi/4, \ldots \). These fixed points will correspond to the die balancing on one of its corners and are both mathematically and physically unstable.

In fact this system is the same as the pendulum with damping, except that the ‘damping’ in our system occurs over specific intervals. The diagram is shown in Figure 5.

Having the phase plot, one can then compute regions of attraction for each of the stable fixed points. This has been done in previous literature for the pendulum but is not generalized to our example in this paper. It will be noted, however, that the trajectories coming out of the unstable fixed points do form the boundaries for the regions of attraction.
8 Probability in rolling

Having studied the mechanics of rolling a “2-dimensional” die with sides $a$ and 1, $a \geq 1$, we now attempt to determine the probability of ending a roll on a particular length side given sufficient initial momentum.

To determine this probability, the ratio of initial angular velocity values leading to side “1” to total velocity values studied is calculated for large values of $\omega$ – angular velocity. This proportion is calculated separately for rolls starting on side “a” and “1”. Then, as $\omega \to \infty$, we take these proportions to be $P(1|a \text{ initial})$ and $P(1|1 \text{ initial})$ respectively. Knowing the probabilities $P_a$ and $P_1$ of starting on side “a” or “1”, respectively, the probability of ending on side “1” is $P(1) = P_1 P(1|1 \text{ initial}) + P_a P(1|a \text{ initial})$.

Now to determine the ending face, starting on side “1”, for different values of $\omega$, we develop the following intervals:

End on “a”: $(\omega_1, \frac{\omega_a}{s_a}), (\frac{\omega_1}{s_1 s_a}, \frac{\omega_a}{s_2 s_1 s_a}), \ldots (\frac{\omega_1}{s_1 s_2 \ldots s_N}, \frac{\omega_a}{s_a (s_1 s_2 \ldots s_N)^n})$

End on “1”: $[0, \omega_1), (\frac{\omega_a}{s_a}, \frac{\omega_1}{s_1 s_a}), \ldots (\frac{\omega_a}{s_1 s_2 \ldots s_N}, \frac{\omega_1}{s_1 s_2 \ldots s_N}^{n-1})$.

So, calculating the ratio for $\omega$ up to $\frac{\omega_a}{(s_1 s_a)^N}$,

\[
P(1|1 \text{ initial}) = \left[ \omega_1 + \left( \frac{\omega_1}{s_1 s_a} - \frac{\omega_a}{s_a} \sum_{n=0}^{N-1} \left( \frac{1}{s_1 s_a} \right)^n \right) \right] \frac{\omega_a}{(s_1 s_a)^N}
\]

\[= \frac{\omega_1}{\omega_a} (s_1 s_a)^N + \left( \frac{\omega_1}{\omega_a} - s_1 \right) \sum_{n=0}^{N-1} (s_1 s_a)^n.
\]

Calculating intervals similarly for rolls starting on side “a”,
Figure 5: Phase Plot of Pendulum Swinging

\[
P(1|a \text{ initial } ) = \left( \frac{\omega}{s_1} - \omega_a \right) \sum_{n=0}^{N-1} \frac{1}{s_1 s_a} \left( \frac{s}{s_1 s_a} \right)^n / \frac{\omega_a}{(s_1 s_a)^N}
\]

\[= s_a \left( \frac{\omega}{\omega_a} - s_1 \right) \sum_{n=0}^{N-1} (s_1 s_a)^n.\]

Now, letting \( N \to \infty \), for \( s_1 s_a < 1 \),

\[P(1|1) = \frac{\omega}{\omega_a} - s_1 / (1 - s_1 s_a)\]

\[P(1|a) = s_a \left( \frac{\omega}{\omega_a} - s_1 \right) / (1 - s_1 s_a)\]

Assuming \( P_1 = P_2 = \frac{1}{2} \), the probability of landing on side “1” is \( P(1) = \frac{1}{2} \left( \frac{\omega}{\omega_a} - s_1 \right) / (1 - s_1 s_a) \).

Substituting for \( s_1 \) and \( s_a \) with \( \frac{\omega}{\omega_a} = \sqrt{\frac{1 + a^2 - r}{1 + a^2}} \),

\[P(1) = \frac{1}{2} \left( \frac{(1 + a^2) \omega_a - (a^2 - r) \cdot [(1 + a^2) + (1 - a^2 r)]}{(1 + a^2)^2 - (a^2 - r)(1 - a^2 r)} \right).\]

<table>
<thead>
<tr>
<th>P(1)</th>
<th>( r = 0 )</th>
<th>( r = 0.5 )</th>
<th>( r = 1 )</th>
</tr>
</thead>
<tbody>
<tr>
<td>( a = 75/74 )</td>
<td>0.4751</td>
<td>0.4786</td>
<td>0.4787</td>
</tr>
<tr>
<td>( a = 75/73 )</td>
<td>0.4502</td>
<td>0.4573</td>
<td>0.4574</td>
</tr>
<tr>
<td>( a = 75/70 )</td>
<td>0.3762</td>
<td>0.3941</td>
<td>0.3944</td>
</tr>
</tbody>
</table>
Figure 6: Probability of Landing on Face 1 vs Length of Side a

Figure 7: Elasticity vs Length of Side a

Notice that in the calculation of interval lengths, \( \frac{\omega_1}{\omega_1} \) is assumed to be greater than \( \omega_a \). This will occur for \( r > a^2 - (1 + a^2) \frac{\omega_1}{\omega_2} \), plotted for \( a = 1 \) to 2 below. For combination of \( a \) and \( r \) which do not satisfy this inequality, the chance of side "1" occurring is zero (seen negative on \( P(1) \) vs \( a \) plot). This error (zero or negative probability) arises in our model from the assumption that \( s_1(a, r) \) and \( s_2(a, r) \) are multiplicative constants rather than operators which should include momentum change due to potential energy changes as the die rolls from
face to face. Incorporating gravity, the momentum with which the two sides will strike down, based on what they hit on, is $s^*\omega = \sqrt{(s_0\omega)^2 + \frac{mg(1-a)}{I_0}}$ and $s^1\omega = \sqrt{(s_1\omega)^2 + \frac{mg(a-1)}{I_0}}$. By taking these considerations, the problem of negative probability and such would be eliminated.

9 Conclusions

In this report, we have studied the dynamics of throwing, bouncing and rolling a die and other shapes in an attempt to deterministically model these physical processes. We then calculated probabilities of certain events occuring by determining the fractions of initial values corresponding to these events for large initial conditions.

Using this method for calculating probability, we proved several theorems involving the landing orientation of a tossed polygonal 2-dimensional body into the air for large vertical initial velocities. We then applied the technique to the posed problem of a shaved die, and for small differences in lengths for a 2-dimensional rolling problem we found the advantages gained in probability of landing on a desired side.

10 Future work

First and foremost, future work on this project must include an extension to 3-dimensions for the die problem. Since rolling is inherently 2-dimensional, this part of our work should be easily extendable with each orientation of the axis of rotation studied independently.

Other work must be done in correcting the rolling section to use the full operators $s_1$ and $s_a$ rather than the multiplicative constants as assumed in our calculations.

Also, we suggest that the effects of friction be examined and incorporated in the model as needed and that the bouncing problem continue to be studied perhaps to include bouncing (off a wall) after rolling begins.

11 Reference

Modeling an Automobile Bumper

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Week 4, August 24–28, 1992

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1 Introduction

We wish to model the response of an automobile bumper to forces such as might be experienced in a collision. Several different models will be presented. The bumper will be described as a spring with large spring constant and as a beam.

The United States government mandates that bumpers on all cars sold here must be of a sufficient design and strength that they can be struck by a pendulum traveling 2.5 mph and the car will sustain no damage which must be repaired. The pendulum mass is equal to that of the car. Our various models will contain parameters which describe the stiffness, length, cross-sectional area, and shape of the bumper. We will also discuss the bumper's effect on the survivability of automobile crashes at higher speeds.

2 Nomenclature

The following notation will be used to describe quantities in our models.

\( a_i(t) \) position of object \( i \), units m

\( m_i \) mass of object \( i \), units kg

\( m_s \) mass of spring, units kg

\( m_b \) mass of bumper, units kg

\( u_i(t) \) length of spring \( i \), units m

\( h_i \) uncompressed length of spring \( i \), units m

\( v_i \) initial (collision) velocity of object \( i \), units m/s

\( k_i \) spring constant of spring \( i \), units kg/m \( ^2 \)

\( b(t) \) position of bumper, units m

\( d \) coefficient of friction, units kg/s

\( t \) time, units s

3 Pendulum Test

In the simplest case we imagine a car at rest with mass, \( m \), being struck by a pendulum of equal mass traveling with a speed, \( v \). See Fig. 1. We will assume there are no frictional forces on the car. The bumper of the car will be modeled as a spring with spring constant, \( k \), and uncompressed length \( h \). There is no loss of generality if we replace the pendulum with a second car of the same mass
and initial velocity. In this case the equations describing the interaction of the two vehicles are

\[ mc_1''(t) = k(u(t) - h) \]  \hspace{1cm} (1)
\[ mc_2''(t) = -k(u(t) - h). \] \hspace{1cm} (2)

The function \( u(t) \) is the length of the bumper as a function of time. The initial conditions of this problem are

\[ c_1(0) = 0, \quad c_1'(0) = 0, \quad c_2(0) = h, \quad c_2'(0) = -v. \]

Adding equations (1) and (2) and solving the resulting second ODE subject to the initial conditions above yields the following solution.

\[ c_1(t) + c_2(t) = -vt + h \] \hspace{1cm} (3)

From the geometry of the problem we also have the relation

\[ u(t) = c_2(t) - c_1(t). \] \hspace{1cm} (4)

Substituting equation (4) into equation (3) and differentiating twice with respect to \( t \) and using equation (1) yields the following ODE in terms of \( u(t) \),

\[ u''(t) + \frac{2k}{m} u(t) = \frac{2hk}{m} \] \hspace{1cm} (5)

with initial conditions

\[ u(0) = h \text{ and } u'(0) = -v. \]

We choose to simplify and nondimensionalize by letting

\[ \tilde{t} = \sqrt{\frac{2k}{m}} t \text{ and } u = \tilde{u} \sqrt{\frac{m}{2k}}. \]
Applying these transformations to the variables in equation (5) produces the following nondimensional ODE

$$\ddot{\tilde{u}} + \tilde{u} = 0$$  \hspace{1cm} (6)

and the following boundary conditions

$$\tilde{u}(0) = 0 \text{ and } \dot{\tilde{u}}(0) = -1.$$  

Solving the ODE produces

$$\tilde{u}(\tilde{t}) = -\sin \tilde{t}.$$  \hspace{1cm} (7)

The maximum magnitude of deflection of the bumper occurs when $\tilde{u} = \tilde{u}_{\text{max}} = -1$. In terms of the dimensioned quantities, the maximum energy stored in the spring is

$$\frac{1}{2} k (h - u_{\text{min}})^2 = \frac{1}{2} k \left( h - \left( h + \tilde{u}_{\text{max}} v \sqrt{\frac{m_1}{2k}} \right) \right)^2 = \frac{1}{4} mv^2.$$  

In other words, the spring can store at maximum only one half of the kinetic energy of the pendulum at the time of collision.

A conservative design for an automobile bumper might call for it to absorb an amount of energy equal to $\frac{1}{4} mv^2$ while only deforming by an amount $\delta$ where $\delta$ is determined by the car’s designers. In that case the bumper must absorb energy equal to the amount

$$\frac{1}{2} k \delta^2 = \frac{1}{4} mv^2$$

which allows us to calculate the desired spring constant.

$$k = \frac{1}{2} \frac{m v^2}{\delta^2}$$  \hspace{1cm} (8)

For instance if $m = 1000 \text{ kg}$, $v = 2.5 \text{ mph}$, and $\delta = 0.01 \text{ m}$ then $k \approx 6 \times 10^6 \text{ kg/s}^2$.

4 Friction

Assuming that $m_1 = m_2 = m$ and that friction is non-zero, the governing equations become:

$$mc_1''(t) = -dc_1'(t) + k(u(t) - h)$$  \hspace{1cm} (9)

$$mc_2''(t) = -k(u(t) - h)$$  \hspace{1cm} (10)

$$c_1(t) = c_2(t) - u(t)$$  \hspace{1cm} (11)

where $d$ is the coefficient of friction. The initial conditions are

$$c_1(0) = 0$$
$$c_1'(0) = 0$$
$$c_2(0) = h$$
$$c_2'(0) = -v.$$
Substituting \( c_2'(t) - u'(t) \) for \( c_1'(t) \) and \( c_2''(t) - u''(t) \) for \( c_1''(t) \) into equation (9) yields
\[
mc_2''(t) - mu''(t) = -dc_2'(t) + du'(t) + k(u(t) - \bar{h}). \tag{12}
\]
Substituting equation (10) into equation (12) and simplifying results in
\[
mu''(t) = -du'(t) - 2ku(t) + 2kh + dc_2'(t).
\]
Differentiating the above equation with respect to \( t \) and substituting \( c_2''(t) = -(k/m)(u(t) - \bar{h}) \) yields
\[
mu'''(t) = -du'''(t) - 2ku'(t) - \left( \frac{dk}{m} \right) u(t) + \left( \frac{dkh}{m} \right)
\]
with initial conditions
\[
\begin{align*}
u(0) &= h \\
u'(0) &= -v \\
u''(0) &= 0.
\end{align*}
\]
To simplify and nondimensionalize let
\[
\begin{align*}
u &= \bar{h} + v \sqrt{\frac{m}{2k}} \tilde{u} \\
t &= \sqrt{\frac{m}{2k}} \tilde{t}.
\end{align*}
\]
Then equation (13) becomes:
\[
\tilde{u}_{\tilde{t}\tilde{t}\tilde{t}} + \tilde{u}_{\tilde{t}} + \tilde{d}\tilde{u}_{\tilde{t}\tilde{t}} + \left( \frac{\tilde{d}}{2} \right) \tilde{u} = 0
\]
where
\[
\tilde{d} = \frac{d}{2k} \left( \frac{2k}{m} \right)^{1/2}.
\]
The nondimensionalized initial conditions are
\[
\begin{align*}
\tilde{u}(0) &= 0 \\
\tilde{u}'(0) &= 0 \\
\tilde{u}''(0) &= -1.
\end{align*}
\]
Since \( k \approx 6 \times 10^6 \text{ kg/s}^2, m = 1000 \text{ kg}, \text{ and } d \approx 6672 \text{ kg/s}^1, \tilde{d} \approx 0.06. \) Thus \( \tilde{d} \) is considered to be a small parameter and perturbation theory can be used. Dropping the tilde notation on \( u \) and \( t \) and letting
\[
u(t) = u_0(t) + u_1(t)\tilde{d} + O(\tilde{d}^2)
\]
\( ^1 \) is approximated using \( F = vd \) with \( F = 50 \text{ lbs} \) and \( v = 2 \text{ miles/hr} \)
results in

\[(u_0'' + u_0') + (u_1'' + u_1' + u_0'' + \frac{u_0}{2}) \tilde{d} + O(\tilde{d}^2) = 0.\]

Thus

\[
\begin{align*}
    u_0'' + u_0' &= 0 \\
    u_0(0) &= 0 \\
    u_0'(0) &= -1 \\
    u_0''(0) &= 0
\end{align*}
\]  

and

\[
\begin{align*}
    u_1'' + u_1' + u_0'' + \frac{u_0}{2} &= 0 \\
    u_1(0) &= u_1'(0) = u_1''(0) &= 0.
\end{align*}
\]  

The solution to equation (14) is given by

\[u_0 = A + Be^{it} + Ce^{-it}.\]

Applying the initial conditions and simplifying results in

\[u_0 = -\sin t.\]

Then equation (15) becomes

\[u_1'' + u_1' + \frac{\sin t}{2} = 0.\]

Integrating once results in

\[u_1'' + u_1 = \frac{\cos t}{2} + c.\]  

The solution to equation (16) is given by:

\[u_1 = A\cos t + B\sin t + (1/4)\ t\sin t + c.\]

Using the initial conditions results in

\[u_1 = (1/2)\cos t + (1/4)\ t\sin t - (1/2).\]

Thus

\[u(t) = -\sin t + \left[\frac{1}{2}\cos t + \frac{1}{4}t\sin t - \frac{1}{2}\right] \tilde{d} + O(\tilde{d}^2).\]  

The graphs of \(-\sin t\) (no friction) and \(u(t)\) shown above (with friction) are shown in Fig. 2. The dimensionless maximum deflection is obtained by substituting \(t = (\pi/2) + O(\tilde{d})\) in equation (17), and retaining terms of order \(\tilde{d}\). This gives

\[u_{max} = -1 + \left(\frac{\pi}{8} - \frac{1}{2}\right) \tilde{d} + O(\tilde{d}^2).\]

The final result is that the original model with the simplifying assumption of no friction is a reasonable model.
Figure 2: The graphs of bumper deflection versus time for the models without friction (top curve) and with friction (bottom curve).
5 Effect of Bumper Mass

5.1 Governing Equations

We now consider the significance of the mass of the bumper with respect to the mass of the car. In particular, we will analyze the motion of a spring with point mass.

![Figure 3: Bumper with Mass](image)

We begin by constructing the free body diagrams for the three objects in our diagram: the car, the wall, and the point mass of the spring.

![Figure 4: Freebody Diagram](image)

The resulting equations are as follows:
\[ m_1 \ddot{c}_1 = k_1(u_1 - h_1) \]
\[ m_2 \ddot{b} = -k_1(u_1 - h_1) + k_2(u_2 - h_2) \]
\[ m_2 \ddot{c}_2 = k_2(h_2 - u_2) \]

where
\[ u_1(t) = b(t) - c_1(t) \]
\[ u_2(t) = c_2(t) - b(t) \]

The initial conditions will be:

\[
\begin{align*}
    c_1(0) &= 0 \\
    c_1(0) &= 0 \\
    c_2(0) &= h_1 + h_2 \\
    c_2(0) &= -v_2 \\
    b(0) &= h_1 \\
    b(0) &= 0
\end{align*}
\]

We will make the following simplifying assumptions:
\[ m_1 = m_2 = m, k_1 = k_2 = k, h_1 = h_2 = h/2 \]

The equations thus become:
\[ m_1 \ddot{c}_1 = k(u_1 - h/2) \]
\[ m_2 \ddot{b} = -k(u_1 - h/2) + k(u_2 - h/2) \]
\[ m_2 \ddot{c}_2 = k(h/2 - u_2) \]

where
\[ u_1(t) = b(t) - c_1(t) \]
\[ u_2(t) = c_2(t) - b(t) \]

and the new initial conditions will be:

\[
\begin{align*}
    c_1(0) &= 0 \\
    \dot{c}_1(0) &= 0
\end{align*}
\]
\[ \begin{align*}
    c_2(0) &= h \\
    \dot{c}_2(0) &= -v_2 \\
    b(0) &= h/2 \\
    \dot{b}(0) &= 0
\end{align*} \]

5.2 Nondimensionalization

We choose the characteristic time scale \( \sqrt{\frac{m}{2k}} \) from our earlier solution, and a characteristic length scale \( U \) whose exact value will be determined later. The nondimensionalized values become:

\[ \tilde{t} = \sqrt{\frac{2k}{m}} \]

\[ \tilde{c}_1 = \frac{c_1}{U} \]

\[ \tilde{c}_2 = \frac{c_2 - h}{U} \]

\[ \tilde{u}_1 = \frac{u_1 - h/2}{U} \]

\[ \tilde{u}_2 = \frac{u_2 - h/2}{U} \]

\[ \tilde{b} = \frac{b - h/2}{U} \]

Our governing equations become:

\[ \begin{align*}
    \ddot{\tilde{c}}_1 &= \frac{1}{2} \tilde{u}_1 \\
    \ddot{\tilde{c}}_2 &= -\frac{1}{2} \tilde{u}_2 \\
    \frac{m_{\text{eff}}}{m} \ddot{\tilde{b}} &= \frac{1}{2} (\tilde{u}_1 + \tilde{u}_2)
\end{align*} \]

where

\[ \tilde{u}_1(t) = \tilde{b}(t) - \tilde{c}_1(t) \]

\[ \tilde{u}_2(t) = \tilde{c}_2(t) - \tilde{b}(t) \]

The nondimensionalized initial conditions will be:

\[ \tilde{c}_1(0) = 0 \]
\[
\begin{align*}
\dot{c}_1(0) &= 0 \\
\dot{c}_2(0) &= 0 \\
\dot{c}_2(0) &= -\frac{v_2}{U} \sqrt{\frac{m}{2k}} \\
b(0) &= 0 \\
\dot{b}(0) &= 0
\end{align*}
\]

Examining the above equations we choose \( U = v_2 \sqrt{\frac{m}{2k}} \). From here on, we will assume nondimensionalized equations and will exclude the tildes.

Consider the ratio \( \frac{ma}{m} \) to be a small parameter say \( \epsilon^2 \) (in actual physical situations, this ratio is approximately 0.05). The equations now become:

\[
\begin{align*}
\ddot{c}_1 &= 1/2u_1 \\
\ddot{c}_2 &= -1/2u_2 \\
\epsilon^2 \ddot{b} &= 1/2(-u_1 + u_2)
\end{align*}
\]

where

\[
\begin{align*}
u_1(t) &= b(t) - c_1(t) \\
u_2(t) &= c_2(t) - b(t)
\end{align*}
\]

with initial conditions:

\[
\begin{align*}
c_1(0) &= 0 \\
\dot{c}_1(0) &= 0 \\
c_2(0) &= 0 \\
\dot{c}_2(0) &= -1 \\
b(0) &= 0 \\
\dot{b}(0) &= 0
\end{align*}
\]

5.3 Zeroth Order Solution

If we set \( \epsilon = 0 \), that is if we ignore the effect of the mass of the bumper, then from the above equations we get \( u_1 = u_2 \).

Let \( u_1 = u_2 = u/2 \) so that \( u_1 + u_2 = u \).

Also, \( \ddot{c}_1 = -\ddot{c}_2 \) whose solution

\[
c_1 + c_2 = -t
\]
But we know that $c_2 - c_1 = u$. Therefore, $c_1 = \frac{-t + u}{2}$ and $c_2 = \frac{-t - u}{2}$

Let $b_0(t)$ be our zeroth order approximation to $b(t)$.

Then, $b_0(t) = c_1(t) + u_1(t) = c_1(t) + u(t)/2 = -t/2$

### 5.4 Perturbation

The zeroth order solution $b_0(t)$ describes the gross movement of the bumper as it is pushed by the pendulum. But for our model, we know that the bumper vibrates around a mean position even as it is being pushed by the pendulum. To analyze these vibrations we need to introduce a smaller time scale into the problem.

Let $\tau = t/\epsilon$, and set $b(t) = b_0(t) + \epsilon b_1(\tau, t)$.

Retaining only order one terms, our equations become:

$$\frac{d^2 c_1}{d\tau^2} = 0$$
$$\frac{d^2 c_2}{d\tau^2} = 0$$
$$\frac{d^2 b}{d\tau^2} = 1/2(-2b + c_1 + c_2)$$

The initial conditions on $c_1(\tau)$ and $c_2(\tau)$ are the same as before. The initial conditions on $b_1(t, \tau)$ are obtained as follows:

Since $b_0(t) = c_1(t) + u_1(t) = c_1(t) + u(t)/2 = -t/2$, it follows that $b(0) = b_0(0) + \epsilon b_1(0, 0)$ or $b_1(0, 0) = 0$.

Now

$$\dot{b}(t) = \dot{b}_0(t) + \epsilon \left[ \frac{\partial b_1(\tau, t)}{\partial t} + \frac{1}{\epsilon} \frac{\partial b_1(\tau, t)}{\partial \tau} \right]$$

i.e.,

$$\dot{b}(t) = \dot{b}_0(t) + \frac{\partial b_1(\tau, t)}{\partial \tau} + O(\epsilon)$$

It follows that $\frac{\partial b_1}{\partial \tau}(0, 0) = \frac{1}{2}$.

Solving the above equations, we get

$$b_1(\tau, t) = \frac{1}{2} \sin \tau$$

so that

$$b(t) = -\frac{t}{2} + \frac{\epsilon}{2} \sin \left( \frac{t}{\epsilon} \right)$$

or

$$b(t) = -\frac{t}{2} + \frac{1}{2} \sqrt{\frac{m_h}{m}} \sin \left( \sqrt{\frac{m}{m_h}} t \right)$$
Thus, the bumper vibration amplitude is \( \frac{1}{2} \sqrt{\frac{m_b}{m}} \). Hence, provided the ratio of the bumper mass to the mass of the car is small, the bumper's contribution to the motion of the system will be negligible.

6 The Beam Model

In this section we consider the front bumper of the car to be a beam. To be specific, we assume that the undisplaced bumper (beam) occupies the region \([0, L] \times [-T/2, T/2]\) in the \((x, y)\)-plane and is subject to a vertical force density \(F(x)\) which is independent of \(y\).

![Beam Model Diagram]

Here \(L\) is the length and \(T\) is the thickness of the bumper. Suppose the bumper is 'thin' and the deformation is small, then we can impose the following assumptions:

1) the vertical displacement only depends on \(x\);

2) the midplane \(y = 0\) is not displaced horizontally;

3) the vertical fibers \(x = \)constant remain to be perpendicular to the deformed midplane.

Let \(V_y\) be the vertical force (shear force) and \(M_z\) the bending moment. It is well known that, from the balances of forces and moments,

\[
\frac{dV_y}{dx} = -F(x) - \mu \frac{\partial^2 w}{\partial t^2}, \tag{18}
\]

\[
\frac{dM_z}{dx} = -V_y, \tag{19}
\]

where \(\mu\) is the mass density of the beam and \(w\) is the vertical displacement of the bumper. Combining the above equation yields

\[
\frac{d^2 M_z}{dx^2} = F(x) + \mu \frac{\partial^2 w}{\partial t^2}.
\]

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To find the expression for $M_z$, we note that the strain in the $x$-direction is

$$
\epsilon_{xx} = -\frac{y}{R},
$$

where $R$ is the radius of curvature of the middle 'neutral' plane and $y$ is the distance from the neutral surface in the undeformed geometry to an arc of the beam under consideration. By the Hooke's law, we have

$$
\tau_{xx} = E\epsilon_{xx},
$$

where $E$ is the Young's Modulus. Obviously, we took the stresses $\tau_{yy}$ and $\tau_{zz}$ to be zero based on the assumption we made about the bumper (beam) above. Next, by definition

$$
M_z = \int \int_A \tau_{xx} y \, d\omega,
$$

and with

$$
I_{zz} = \int \int_A y^2 \, d\omega,
$$

we obtain

$$
M_z = \frac{EI_{zz}}{R}.
$$

Here $I_{zz}$ is the second moment of inertia of the cross-sectional area about the neutral axis and $A$ is the cross section region. Because of the small deformation assumption, we conclude that $I_{zz}$ is independent of $z$ and does not differ from the inertia when the beam is undeformed.

From basic calculus we know

$$
\frac{1}{R} = \frac{w''(x)}{(1 + w'(x)^2)^{3/2}} \approx w''(x),
$$

in which $w$ is the vertical displacement of each point on the mindplane and we assume that $y(x)^2$ is very small. Using this result and the equations above we finally obtain

$$
\frac{d^4w}{dx^4} = -\frac{F(x) + \mu \frac{\partial^2 w}{\partial t^2}}{EI_{zz}}.
$$

In this place, we will only consider the static situation, so the above equation becomes

$$
\frac{d^4w}{dx^4} = -\frac{F(x)}{EI_{zz}}.
$$

For our problem, the beam is hard clamped at its two ends, so

$$
w(0) = w'(0) = w(L) = w'(L) = 0
$$

are the boundary conditions.
Now we will solve the fourth order ordinary differential equation when the load desity is
\[ F(x) = F_0, \text{ for } (L-l)/2 \leq x \leq (L+l)/2, \text{ and} \]
\[ F(x) = 0, \text{ otherwise.} \]
This density represents e.g. the situation, when a block of width \( l \) and weight \( F_0 \cdot l \) is laid on the center of the beam. Solving the boundary value problem and using the symmetry of the solution, we get
\[
\begin{align*}
w(x) &= ax^3 + bx^2, \quad & \text{for } 0 \leq x < \frac{(L-l)}{2}, \\
w(x) &= -P \left( \frac{(x-L/2)^4}{24} + c(x-L/2)^2 + d \right), \quad & \text{for } \frac{(L-l)}{2} < x < \frac{(L+l)}{2}, \\
w(x) &= a(L-x)^3 + b(L-x)^2, \quad & \text{for } \frac{(L+l)}{2} < x \leq L,
\end{align*}
\]
where
\[
P = \frac{F_0 l}{EI_{zz} l'}
\]
in which \( F_0 \cdot l \) is the total force exerted on the beam, and
\[
\begin{align*}
a &= \frac{P l}{12}, & b &= \frac{P l (-3L^2 + l^2)}{48L}, \\
c &= -\frac{4(3L^2 - 3Ll + l^2)}{48L}, & d &= \frac{2L^3 l - 2Ll^3 + l^4}{384}.
\end{align*}
\]
(20) (21)
The displacement at each position \( x \) is obviously linear in the total force. Since we are only interested in the maximal displacement, which we get from \( w(L/2) \) we may replace the beam model by a spring model with a spring just at \( x = (L/2) \). The corresponding spring constant - according to Hooke’s law - is then:
\[
k = \frac{F_0 l}{P d} = \frac{EI_{zz} l}{d} = \frac{384EI_{zz}}{2L^3 - 2Ll^3 + l^3}
\]
7 Bumper Design
The real-world designing of a bumper for a given car model will consist, at its core, as a minimization problem with given constraints.
The usual design problem will be to minimize the mass of the bumper, \( m_b \), while maintaining its integrity, controlling the maximum deformation, \( \delta_b \), during the pendulum test, and conforming the bumper to some general outer shape.
Viewing the bumper as a beam of some form, the length between supports, \( L \), will generally be dictated by other car design constraints. Also, for each considered bumper material, the density, \( \rho \), will be known. Thus, the problem of minimizing the mass \( m_b = \rho L A \) becomes the same as minimizing the actual bumper cross-sectional area.

A first constraint to the design problem is a given clearance, \( \delta_c \), between the bumper and the car. This value will correspond to the maximum allowable deflection, \( \delta_b \). Often this constraint value may be adjusted with the overall car designer to achieve lighter weight or better safety performance.

One of the most important design questions is the choice of material for our bumper. This choice will specify such parameters as \( \rho \), \( E \) - Young's Modulus, and \( Y \) - the yield stress. Generally, the design calculations must be repeated for each choice being considered.

The material choice is central to insuring the integrity of the beam. The design of the beam must include the constraint that the maximum stress felt anywhere within the beam, \( |\tau_{xx}| = |-(E/R)y'| \) be less than the yield stress \( Y \). Knowing \( |y'| \leq (h/2) \), this implies that \( (h/R) \leq (2Y/E) \) which relates the geometric quantity \( h/R \) to the known physical parameter \( Y/E \) for each material. Thus, the design shape of the beam within the general outer shape constraints must insure a correct maximum \( h/R \). In fact, a safety factor is invariably used in the modeling so as to keep the actual maximum stress well below the yield stress. Thus, for some materials and beam shapes, the yield stress may dictate \( \delta_b \) rather than the stated clearance \( \delta_c \).

Since the effective spring constant, \( k \), of a beam is proportional to \( EI_{zz} \) where \( I_{zz} \) is the moment of inertia, the design of the beam shape is a critical step in the design process. By maximizing \( I_{zz} \), \( k \) is maximized which decreases \( \delta_b \) since \((1/2)k\delta_b^2 = (1/4)mv^2 \), \( m \) and \( v \) known, in the pendulum test. Therefore, either the mass, and so \( I_{zz} \), may be reduced further until \( \delta_b = \delta_c \) or a greater safety margin can be achieved.

Clearly, \( k \) proportional to \( E \) also emphasizes the dependence of the entire design problem on material selection.

Though closely tied together, other design problems may arise including the designing of the beam under general shape constraints to minimize bumper weight with specified bumper performance.

8 Design of the Bumper Beam

Now we solve a design problem for the case, that we have a given design \( h(z) \) outside, which is symmetrical to the centroidal line, and want to know where to fill material in \( (f(z)) \) in order to minimize weight but conserve a given stiffness.

Since we assume that the bumper material has constant density and the stiffness can be expressed in terms of the cross sectional inertia, we get the
The following optimization problem:

$$\min \int \int \int \frac{dA}{x}$$

s.t. $\int \int \int \frac{y^2 dA}{x} = I_o$, $I_o = constant$
and $h - y \geq 0$

Evaluating the inner integrals we get:

$$\min \int_0^T h(x) - f(x) dx$$

s.t. $\int_0^T h^3(x) - f^3(x) dx = 3I_o$
and $h(x) - f(x) \geq 0$
The Lagrangian of this Optimization Problem is:

\[ L(f, \lambda, \mu) = \int_0^T h(x) - f(x) dx - \lambda \left\{ \int_0^T h^3(x) - f^3(x) dx - 3I_0 \right\} - \int_0^T \mu(x)[h(x) - f(x)] dx, \quad \mu \geq 0 \]

Necessary for Optimality is the Stationarity of the Langrangian, i.e.

\[ \frac{\partial L}{\partial f}(f) \delta f = \int_0^T [-\delta f(x) + 3\lambda f^2(x)\delta f(x) + \mu(x)\delta f(x)] dx = 0, \quad \forall \delta f \]

\[ \Rightarrow f^2(x) = \frac{1 - \mu(x)}{3\lambda}, \quad a.e. \]

and the complementarity conditions:

\[ \int_0^T \mu(x)[h(x) - f(x)] dx = 0 \]

So for \( h(x) - f(x) > 0 \): \( f(x) \) is constant.

The solution is now:

\[ f(x) = \min\{h_0, h(x)\} \]

with \( h_0 \) such that \( \int_0^T [h(x) - h_0]^2 dx = I_0 \)

Since such a solution is practically not very promising, one should slightly change the inequality condition to \( h(x) - f(x) \geq h_{min} \). The solution is then obviously:

\[ f(x) = \min\{h_0, h(x) - h_{min}\} \]

with \( h_0 \) such that \( \int_0^T (h(x) - h_{min} + [h(x) - h_{min} - h_0]^+) dx = I_0 \)
Since in general symmetric bumpers like the one above are not very realistic one can also treat nonsymmetric bumpers, where the centroidal line $y_0$ is defined by:

$$\int_{A} \int_{y} dA = y_0 A$$

Then one gets one additional variable and one additional constraint, where the solution can be found analogously.

9 Collision of Two Cars

Throughout the collision, the bumper are assumed to remain elastic and meet the pendulum test with an 1 cm maximum deformation. We also assume that the friction and spring masses can be neglected. Using a free body diagram, we have the following equations

\begin{align*}
    m_1 \ddot{c}_1(t) &= -k_1(h_1 - u_1(t)) \tag{22} \\
    m_2 \ddot{c}_2(t) &= k_2(h_2 - u_2(t)) \tag{23} \\
    k_1(h_1 - u_1(t)) &= k_2(h_2 - u_2(t)) \tag{24} \\
    u_1 + u_2 &= c_2 - c_1 \tag{25}
\end{align*}

with the initial conditions

\begin{align*}
    c_1(0) &= 0 & c_2(0) &= h_1 + h_2 & u_1(0) &= h_1 \\
    \dot{c}_1(0) &= v_1 & \dot{c}_2(0) &= -v_2 & u_2(0) &= h_2
\end{align*}

Using equation (24) and combining equation (22) and (23), we obtain that

$$\ddot{c}_2(t) - \ddot{c}_1(t) = k_2 \left( \frac{1}{m_1} + \frac{1}{m_2} \right) (h_2 - u_2)$$
Hence, from equation (25) and (24), we have a decoupled equation
\[
\left(\frac{1}{k_1} + \frac{1}{k_2}\right)\ddot{u}_2 = \left(\frac{1}{m_1} + \frac{1}{m_2}\right)(h_2 - u_2)
\]

Denote the equivalent mass \(m\) and stiffness \(k\) of the system as follows.
\[
\frac{1}{m} = \frac{1}{m_1} + \frac{1}{m_2}, \quad \frac{1}{k} = \frac{1}{k_1} + \frac{1}{k_2}
\] (26)

From equation (24) and (25), it's easy to see that
\[
\dot{u}_2(0) = -\frac{k}{k_2}(v_1 + v_2)
\] (27)

So,
\[
u_2(t) = h_2 - \frac{\sqrt{mk}}{k_2}(v_1 + v_2)\sin\sqrt{\frac{k}{m}}t
\] (28)

By the symmetry of the system, we have
\[
u_1(t) = h_1 - \frac{\sqrt{mk}}{k_1}(v_1 + v_2)\sin\sqrt{\frac{k}{m}}t
\] (29)

Since
\[
m_i\ddot{c}_i = (-1)^i\sqrt{mk}(v_1 + v_2)\sin\sqrt{\frac{k}{m}}t \quad i = 1, 2
\]
for \(0 \leq t \leq \pi\sqrt{\frac{k}{m}}\), the maximum accelerations for both cars occurs at time \(t = \frac{\pi}{2}\sqrt{\frac{k}{m}}\) with
\[
\ddot{c}_{i,\text{max}} = (-1)^i\frac{\sqrt{mk}}{m_i}(v_1 + v_2)
\] (30)

From the Pendulum Test,
\[
\frac{1}{2}k_i\delta^2 = \frac{1}{4}m_i\nu^2
\]
where \(\nu = 2.5\text{mph}\) and \(\delta = 1\text{cm}\) is the maximum allowed deformation, we have
\[
\beta = \frac{k_i}{m_i} = \frac{1}{2}\frac{\nu^2}{\delta^2} = 6242.5/\text{sec}^2
\] (31)

Let
\[
\alpha = \frac{m_2}{m_1}
\] (32)

then
\[
m = \frac{\alpha}{1 + \alpha}m_1, \quad k = \frac{\alpha\beta}{1 + \alpha}m_1
\]
Hence, from equation (30), the maximum accelerations for the two cars are

\[
\ddot{c}_{1,\text{max}} = -\frac{\alpha}{1+\alpha}\sqrt{\beta}(v_1 + v_2)
\]

\[
\ddot{c}_{2,\text{max}} = \frac{1}{1+\alpha}\sqrt{\beta}(v_1 + v_2)
\]

When \(\alpha = 1\), i.e. when the two cars have the same mass, \(|\ddot{c}_{1,\text{max}}(\alpha = 1)| = |\ddot{c}_{2,\text{max}}(\alpha = 1)| = \frac{\sqrt{\beta}}{2}(v_1 + v_2)\). Therefore,

\[
\ddot{c}_{1,\text{max}}(\alpha)/\ddot{c}_{1,\text{max}}(1) = \frac{2\alpha}{1+\alpha}
\]

\[
\ddot{c}_{2,\text{max}}(\alpha)/\ddot{c}_{2,\text{max}}(1) = \frac{2}{1+\alpha}
\]

We can also observe that the ratio of maximum acceleration felt by car 1 to that by car 2 is \(-\alpha\). In other word, the ratio of maximum accelerations is inversely proportional to the ratio of masses.

### 9.1 Survivability Analysis

For survivability analysis, the important criterion is the maximal acceleration since this acts as a measure of the acceleration of the driver forward the dash or steering wheel. To convert these accelerations into "g-force" divide the total mass by the gravitation constant \(g = 9.8\text{m/s}^2\). For critical values of "g-force" a plot of effective velocity \(v_1 + v_2\) versus mass ratio \(\alpha\) can be computed showing "safe" and "dangerous" condition for the driver in each car during the accident.

For car 1:

\[
(v_1 + v_2) = \frac{1+\alpha}{\alpha}(\frac{ng}{\sqrt{\beta}}) \quad \text{n "g-forces"}
\]

For car 2:

\[
(v_1 + v_2) = (1+\alpha)(\frac{ng}{\sqrt{\beta}}) \quad \text{n "g-forces"}
\]

where \(g/\sqrt{\beta} = 0.124\text{m/s}\). Again, these curves are plotted for different "g-force" for each car.

Now we turn our attention to deciding the minimum failure stress that the car's material should have for the occupants of the car to remain safe. We also calculate the maximum acceleration experienced by the occupants during a crash. We will consider the case of a car crashing headlong into a wall.

For the remainder of this section we will introduce the following additional notation.

\(\rho\) density of the car, units kg/m\(^3\)

\(m_i(t)\) mass of the intact portion of the car, units kg
\( l(t) \) distance from the wall to the back of the car, units m

\( \ell_0 \) original length of the car, units m

\( d(t) \) distance from the wall to the boundary between the intact and crushed parts of the car, units m

\( A \) effective cross-sectional area of the car, units \( m^2 \)

\( Y \) failure stress

We can see that the following holds.

\[
m_i(t) = \rho A (l(t) - d(t))
\]  \((37)\)

By conservation of energy the kinetic energy of the car just before hitting the wall should equal the sum of the kinetic energy of the intact portion and the potential energy stored in the crushed portion. Therefore

\[
\frac{1}{2} m v^2 = \frac{1}{2} m_i(t)(l'(t))^2 + Y A d(t)
\]  \((38)\)

Substituting equation (37) into (38) we get the following ODE

\[
(l'(t))^2 = \frac{1}{\rho (l(t) - d(t))} \left[ \frac{m v^2}{A} - 2 Y d(t) \right]
\]  \((39)\)

Since \( l(t) \) is a decreasing function then

\[
l'(t) = -\sqrt{\frac{1}{\rho (l(t) - d(t))} \left[ \frac{m v^2}{A} - 2 Y d(t) \right]}
\]  \((40)\)
By conservation of momentum the rate of change of momentum of the intact portion equals the sum of the force exerted on the intact portion by the crushed portion and the rate at which momentum is lost due to mass being consumed into the crushed portion. Therefore

\[
\frac{d}{dt} [\rho A (l(t) - d(t))l'(t)] = -YA - \rho Ad'(t)l'(t) \quad (41)
\]

Simplifying yields

\[
(l'(t))^2 + (l(t) - d(t))l''(t) = -\frac{Y}{\rho} \quad (42)
\]

Equations (40) and (42) can be solved subject to the following initial conditions:

\[ l(0) = l_o, \quad l'(0) = -v, \quad d(0) = 0. \]

We can solve the above system numerically and calculate the maximum acceleration experienced by the car’s occupants. In the final state of the crash there is no velocity and hence from our kinetic energy equation we get

\[
\frac{1}{2}mv^2 - YA_{final} = 0. \quad (43)
\]

From this relation we can calculate the desired value of the failure stress for a given value of \( d_{final} \), which is the length of the hood of the car under consideration.

10 Conclusions and Future Research

By modeling the bumper of a car as a spring with spring constant \( k \) determined from beam theory, we were able to analyze the performance of the bumper. In this analysis, we discovered that omission of frictional forces had negligible effect and that the mass of the “spring”-bumper could be ignored with a known error effect.

By using calculus of variations, we determined optimal interior bumper shape for a specific design problem. Finally, we examined factors contributing to survivability in high speed crashes and postulated a model for this study.

Future work should include a much more detailed analysis of the actual crash mechanism as far as how the car bends, compacts and absorbs energy. Also, using beam theory, an analysis could be attempted for impacts to the bumper on the supports or from the sides. Finally, the whole issue of criteria for survivability needs to be examined to direct future analysis on this question.
Students' Report

#11
Flow Improvement in Hydrofractured Reservoirs

IMA Summer Program for Graduate Students
Mathematical Modeling

Week 4, Group 2
August 24-28, 1992

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Section I: Introduction and Assumptions

Introduction

A common problem in the oil industry is the discovery of oil or gas in tight (low permeability) formations. This problem is often surmounted by hydrofracturing the well. In this process, the borehole is perforated along a vertical segment at the same depths as the gas bearing strata, and a fracturing fluid is pumped down the borehole at extremely high pressures. This high-pressure fluid fractures the formation, usually creating a (roughly) straight fracture centered at the borehole. The fracture is usually held open by "packers" - sand or gravel that flows into the fracture along with the fluid. Typically the vertical extent of the fracture roughly matches the top and bottom of the gas bearing strata (see figures 1a and 1b), that is, the top and bottom of the permeable layer. Although these fractures are very thin, usually no more than a few millimeters across, the permeability within the fractures is radically larger than the permeability of the surrounding formation. We will consider how the productivity (flow rate through borehole) changes due to hydrofracturing.

Advances in hydrofracturing techniques promise to yield wider, longer, and more permeable fractures. In fact, it appears possible to generate multiple fractures. So we will also consider how increasing the number of fractures changes the productivity of the well.

Assumptions

In modeling this problem, we make the following assumptions:

- The pay zone is cylindrical.
- The temperature within the pay zone and fracture is constant.
- The atmospheric pressure is so small in comparison to the pressure inside the pay zone that we consider it to be zero.
- The pressure on the edge of the pay zone is constant.
- The fracture is straight and centered at the borehole.
- The top and bottom of the pay zone are impermeable, and we will have no variation in the vertical direction.
- This is a steady-state problem.
- We consider the gas to be ideal.
- We consider the problem to be governed by Darcy's law.
Figure 1a. Nondimensional schematic of pay zone, side view.
Figure 1b. Nondimensional schematic of pay zone, top view.
Section II: Nomenclature

$a$: width of fracture (perturbation model), value $2 \times 10^{-3}$ m.
$a_j(\tilde{r})$: width of fracture $j$ (variational model), units m.
$A_j$: constants used in equations ($j = 1, 2, 3, 4, 5$).
$\tilde{C}_0(x), \tilde{C}_f(x)$: concentration of gas at position $x$ in the pay zone, fracture. Units mol/m$^2$.
$\tilde{C}_0^{(o)}(x), \tilde{C}_0^{(u)}(x)$,
$\tilde{C}_0^{(v)}(x)$: outer, uniform, and variational approximations to $\tilde{C}_0(x)$. Units mol/m$^2$.
$\tilde{C}_f^{(j)}(x)$: $j$th term in the perturbation expansion for $\tilde{C}_f(x)$. Units mol/m$^2$.
$d$: constant used in conclusion.
$D$: diffusion coefficient for gas (units m$^2$/sec), defined as

\[ D = \frac{RTk}{\mu}. \tag{2.1} \]

$E_1(s)$: the first exponential integral at value $s$, defined by

\[ E_1(s) = \int_{s}^{\infty} \frac{e^{-t}}{t} \, dt = \int_{1}^{\infty} \frac{e^{-st}}{t} \, dt. \tag{2.2} \]

$f(r, \theta)$: nondimensional test function (variational model).
h: height of the pay zone. Units m.
$j$: indexing variable.
$\tilde{J}(x)$: flux of gas at position $x$. Units mol/(m-sec).
k: permeability constant in Darcy's law. Units mol/m$^2$.
m: constant.
n: constant.
$N$: number of fractures.
$\tilde{p}(x)$: pressure of gas at position $x$. Units kg/(m-sec$^2$).
$\tilde{P}_0$: pressure of gas at $\tilde{r} = \tilde{r}_0$. Units kg/(m-sec$^2$).
g: nondimensional flux constant.
$\tilde{Q}$: flux of gas (units mol/sec) through borehole, defined as

\[ \tilde{Q} = -\tilde{r} \int_{0}^{2\pi} \tilde{J}(x) \, d\theta. \tag{2.3} \]

Note that the radius of the circle around which you integrate this is arbitrary due to Gauss' law.
$\tilde{r}$: radius from axis of pay zone. Units m.
$\tilde{r}_0$: radius of pay zone, value 300 m.
\( \tilde{r}_b \): radius of borehole, value \( 5 \times 10^{-2} \) m.
\( \tilde{r}_f \): radius of fracture, value 50 m.
\( \bar{R} \): gas law constant, value \( 8.314 \times 10^3 \) kg\( \cdot \)m\(^2\)/\((\text{sec}\cdot\text{K})\).
\( \Re \): the real part of a complex expression.
\( s \): dummy variable.
\( t \): integration variable.
\( T \): temperature of gas, units K.
\( u(\hat{x}, \hat{\zeta}) \): difference of nondimensional concentration in inner boundary layer from minimum value.
\( v(\lambda, \hat{\zeta}) \): Fourier cosine transform of \( u \), given by the transform pair

\[
v(\lambda, \hat{\zeta}) = \sqrt{\frac{2}{\pi}} \int_0^\infty u(\hat{x}, \hat{\zeta}) \cos(\lambda \hat{x}) \, d\hat{x} \tag{2.4a}
\]

\[
u(\hat{x}, \hat{\zeta}) = \sqrt{\frac{2}{\pi}} \int_0^\infty v(\lambda, \hat{\zeta}) \cos(\lambda \hat{x}) \, d\lambda. \tag{2.4b}
\]

\( \hat{x} \): distance along fracture axis from axis of pay zone. Units m.
\( \hat{y} \): distance (in fracture) from fracture axis. Units m.
\( \hat{z} \): distance along axis of pay zone. Units m.
\( \alpha \): ratio of radius of pay zone to radius of fracture, defined by \( \alpha = \tilde{r}_0 / \tilde{r}_f \).
\( \beta \): nondimensional parameter, defined by \( \beta = 1/\epsilon_0 \).
\( \gamma \): Euler’s constant, value 0.577.
\( \epsilon_0 \): perturbation expansion parameter, defined by

\[
\epsilon_0 \equiv \frac{a D_f}{2 \tilde{r}_0 D_0} = 3 \times 10^{-2}. \tag{2.5}
\]

\( \epsilon_f \): perturbation expansion parameter, defined by

\[
\epsilon_f \equiv \frac{a}{2 \tilde{r}_0} = 3 \times 10^{-6}. \tag{2.6}
\]

\( \eta \): small nondimensional parameter used in equations.
\( \lambda \): Fourier transform variable.
\( \mu \): dynamic viscosity of gas, units kg/(m\cdot sec).
\( \tau(r) \): function (units m) used in variational method, defined by

\[
\tau(r) \equiv \sum_{j=1}^{N} 2\beta_j(r). \tag{2.7}
\]

\( \theta \): angle measured from fracture axis.
\( \Upsilon \): function to be minimized in variational method.
\( \hat{\zeta} \): nondimensionalized distance (in pay zone) from fracture axis.
\( \Omega \): the cylindrical pay zone region.

Nondimensionalized variables will have no tildes. The subscript 0 refers to the rock region, while the subscript \( f \) refers to the fracture. Parenthesized supberscripts indicate terms in the perturbation expansion. Hats refer to inner expansion variables.
Section III: Governing Equations

We begin by writing the form of Darcy's law which we wish to use:

$$\tilde{J} = -\frac{k}{\mu} \nabla \tilde{p}. \quad (3.1)$$

In addition, we will use Fick's diffusion law:

$$\frac{\partial \tilde{C}}{\partial t} = -\nabla \cdot \tilde{J}, \quad (3.2)$$

and the ideal gas law:

$$\tilde{p} = \tilde{C}RT, \quad (3.3)$$

where we assume $T$ to be constant in our region. Combining equations (3.1)-(3.3), we have the following expression for $\tilde{C}$:

$$\frac{\partial \tilde{C}}{\partial t} = -\nabla \cdot \left( -\frac{k}{\mu} \nabla \tilde{p} \right)$$

$$= \frac{k}{\mu} \nabla^2 (\tilde{C}RT)$$

$$= D \nabla^2 \tilde{C}. \quad (3.4)$$

Note that equation (3.4) holds in either the fracture or the pay zone.

We now assume that the only quantity which fundamentally changes from the pay zone to the fracture is $k$, and hence $D$. We assume the pay zone to be a cylinder with height $h$, inner radius $\tilde{r}_b$ (the radius of the bore hole), and outer radius $\tilde{r}_0$. We assume that the pressure on the outer radius of the cylinder is constant, i.e.,

$$\tilde{p}_0(\tilde{r}_0, \theta, \tilde{z}) = P_0. \quad (3.5)$$

The pressure at the bore hole is atmospheric pressure, which is so much smaller than $P_0$ that we assume it to be 0. Hence, we have

$$\tilde{p}_0(\tilde{r}_b, \theta, \tilde{z}) = 0. \quad (3.6)$$

We assume as well that the top and bottom ends of our tube are impermeable. Then, since neither equation (3.5) nor (3.6) depend on $\tilde{z}$, and since no flow can come in from above or below our tube, we conclude that our entire solution is independent of $\tilde{z}$ and reduce our problem to a two-dimensional system. We also are looking for steady-state solutions, so we set our time derivatives equal to 0.
Writing equation (3.4) in polar coordinates in the pay zone, we have

\[ D_0 \left( \frac{\partial^2 \tilde{C}_0}{\partial \tilde{r}^2} + \frac{1}{\tilde{r}} \frac{\partial \tilde{C}_0}{\partial \tilde{r}} + \frac{1}{\tilde{r}^2} \frac{\partial^2 \tilde{C}_0}{\partial \theta^2} \right) = 0. \] (3.7)

We assume the fracture to be so thin that we may assume it to be in rectangular coordinates, so we rewrite equation (3.4) in that region:

\[ D_f \left( \frac{\partial^2 \tilde{C}_f}{\partial x^2} + \frac{\partial^2 \tilde{C}_f}{\partial y^2} \right) = 0. \] (3.8)

Now we nondimensionalize our equations. We nondimensionalize \( \tilde{r}, \tilde{x}, \) and all our associated constant radii by \( \tilde{r}_0, \) our pay zone radius. We normalize our concentrations by the maximal concentration at the boundary, which is given by (3.3) and (3.5) to be \( P_0/RT. \) We nondimensionalize \( \tilde{y} \) by \( a/2, \) half the width of our fracture. Summarizing, we have the following:

\[ r = \frac{\tilde{r}}{\tilde{r}_0}, \quad x = \frac{\tilde{x}}{\tilde{r}_0}, \quad r_f = \frac{\tilde{r}_f}{\tilde{r}_0}, \quad r_b = \frac{\tilde{r}_b}{\tilde{r}_0}, \] (3.9a)

\[ C_0 = \frac{\tilde{C}_0 RT}{P_0}, \quad C_f = \frac{\tilde{C}_f RT}{P_0}, \quad y = \frac{2\tilde{y}}{a}. \] (3.9b)

Using equations (3.9) in (3.7), we have

\[ \frac{P_0 D_0}{RT \tilde{r}_0^2} \left( \frac{\partial^2 C_0}{\partial \tilde{r}^2} + \frac{1}{\tilde{r}} \frac{\partial C_0}{\partial \tilde{r}} + \frac{1}{\tilde{r}^2} \frac{\partial^2 C_0}{\partial \theta^2} \right) = 0 \]

\[ \frac{\partial^2 C_0}{\partial \tilde{r}^2} + \frac{1}{\tilde{r}} \frac{\partial C_0}{\partial \tilde{r}} + \frac{1}{\tilde{r}^2} \frac{\partial^2 C_0}{\partial \theta^2} = 0. \] (3.10)

Using equations (3.9) in (3.8), we have

\[ \frac{P_0 D_f}{RT} \left( \frac{1}{\tilde{r}_0^2} \frac{\partial^2 C_f}{\partial x^2} + \frac{4}{a^2} \frac{\partial^2 C_f}{\partial y^2} \right) = 0 \]

\[ \varepsilon_f \frac{\partial^2 C_f}{\partial x^2} + \frac{\partial^2 C_f}{\partial y^2} = 0. \] (3.11)

Now we need to complete our boundary conditions for our system of equations (3.10) and (3.11). In the rest of this report, if no range is listed for an independent variable, it is assumed to be the entire range. We have let \( y = 0 \) be the centerline of our fracture, so since the problem is symmetric, we have

\[ \frac{\partial C_f}{\partial y}(x,0) = 0, \] (3.12)
and we only need to solve in the region $0 \leq y \leq 1$. In addition, since the fracture splits in two directions, we know that the concentration in the pay zone must be symmetric in each of the four quadrants; hence we only need to solve in the region $0 \leq \theta \leq \pi/2$ and we have

$$\frac{\partial C_0}{\partial \theta} \left( r, \frac{\pi}{2} \right) = 0$$  \hspace{1cm} (3.13a)

$$\frac{\partial C_0}{\partial \theta} (r,0) = 0, \quad r_f \leq r \leq 1. \hspace{1cm} (3.13b)$$

Along the boundary between the fracture and the rock we want the concentration to be continuous. We approximate the top of the fracture in the pay zone coordinates by $(r, \tan^{-1}(\alpha \epsilon_f))$ for $r_b \leq r \leq r_f$. However, since $\epsilon_f$ is small, $\tan^{-1}(\alpha \epsilon_f) \approx \alpha \epsilon_f$ and we have

$$C_0(r, \alpha \epsilon_f) = C_f(x, 1), \quad r_b \leq r \leq r_f. \hspace{1cm} (3.14a)$$

Similarly, along the end of the fracture we have

$$C_0(r_f, \theta) = C_f(r_f, y), \quad 0 \leq \theta \leq \alpha \epsilon_f. \hspace{1cm} (3.14b)$$

In addition, we want the normal flux to be continuous there. First we note that $\mathbf{J} = -D \nabla \tilde{C}$. Therefore, to balance along the top of the fracture we have to set the angular flux into the fracture equal to the flux in the $y$ direction inside the fracture, which we write as

$$-\frac{D_0}{\tilde{r}} \frac{\partial C_0}{\partial \theta} (\tilde{r}, \alpha \epsilon_f) = -D_f \frac{\partial \tilde{C}_f}{\partial y} \left( \tilde{x}, \frac{\alpha}{2} \right), \quad \tilde{r}_b \leq \tilde{r} \leq \tilde{r}_f$$

$$\frac{D_0 P_0}{\tilde{r}_0 RT} \frac{1}{r} \frac{\partial C_0}{\partial \theta} (r, \alpha \epsilon_f) = \frac{2D_f P_0}{aRT} \frac{\partial C_f}{\partial y} (x, 1), \quad r_b \leq r \leq r_f$$

$$\frac{\beta \epsilon_f^2}{r} \frac{\partial C_0}{\partial \theta} (r, \alpha \epsilon_f) = \frac{\partial C_f}{\partial y} (x, 1), \quad r_b \leq r \leq r_f. \hspace{1cm} (3.15a)$$

To balance along the end of the fracture we have to set the radial flux into the fracture equal to the flux in the $x$ direction inside the fracture, which we write as

$$-D_0 \frac{\partial \tilde{C}_0}{\partial \tilde{r}} (\tilde{r}_f, \theta) = -D_f \frac{\partial \tilde{C}_f}{\partial \tilde{x}} (\tilde{r}_f, \tilde{y}), \quad 0 \leq \theta \leq \alpha \epsilon_f$$

$$\frac{D_0 P_0}{\tilde{r}_0 RT} \frac{\partial C_0}{\partial r} (r_f, \theta) = \frac{D_f P_0}{\tilde{r}_0 RT} \frac{\partial C_f}{\partial x} (r_f, y), \quad 0 \leq \theta \leq \alpha \epsilon_f$$

$$\beta \epsilon_f \frac{\partial C_0}{\partial r} (r_f, \theta) = \frac{\partial C_f}{\partial x} (r_f, y), \quad 0 \leq \theta \leq \alpha \epsilon_f. \hspace{1cm} (3.15b)$$

We end this section by nondimensionalizing equations (3.5) and (3.6) and converting them to concentration values:

$$C_0(1, \theta) = 1 \hspace{1cm} (3.16)$$

$$C_0(r_b, \theta) = 0. \hspace{1cm} (3.17)$$

Since the fracture also abuts the bore hole, we have

$$C_f(r_b, y) = 0. \hspace{1cm} (3.18)$$
Section IV: No Fracture

The first model we consider is that of gas flow with no fracture in the pay zone. Hence we only have region 0 to consider, and there is no fracture to break radial symmetry. Hence equation (3.10) with its remaining relevant boundary conditions (3.16) and (3.17) become

\[
\frac{d^2 C_0}{dr^2} + \frac{1}{r} \frac{dC_0}{dr} = 0 \tag{4.1}
\]

\[C_0(1) = 1 \tag{4.2}\]

\[C_0(r_b) = 0. \tag{4.3}\]

The solution of equation (4.1) is \(C_0(r) = A_1 + A_2 \log r\), where the \(A_j\) are constants. Solving for them, we have

\[C_0(r) = \frac{\log(r/r_b)}{\log(1/r_b)}. \tag{4.4}\]

Now we wish to know the flux through the borehole. The flux is only in the radial direction, so we have

\[\bar{Q} = \bar{r}_b \int_0^{2\pi} D_0 \frac{\partial \tilde{C}_0}{\partial r}(\bar{r}_b) \, d\theta. \]

Nondimensionalizing, we have the following:

\[
\frac{\bar{Q}RT}{D_0 P_0} \equiv Q = r_b \int_0^{2\pi} \frac{\partial C_0}{\partial r}(r_b) \, d\theta \]

\[= -\frac{2\pi}{\log(r_b)}. \tag{4.5}\]
Section V: Fracture Included

Now we wish to examine the more difficult case of the full set of equations derived in section III. Since $\varepsilon_f \ll 1$ and $\varepsilon_f$ only appears in conjunction with $C_f$ terms, we postulate the following perturbation expansion in $\varepsilon_f$:

$$C_f = \sum_{j=0}^{\infty} \varepsilon_f^j C_f^{(j)}, \quad (5.1)$$

where $n$ is as yet undetermined. Substituting equation (5.1) into the equations with $\varepsilon_f$ explicitly in them, namely (3.11), (3.15a), and (3.15b), we have the following:

$$\sum_{j=0}^{\infty} \varepsilon_f^n \left[ \varepsilon_f^2 \frac{\partial^2 C_f^{(j)}}{\partial x^2} + \frac{\partial^2 C_f^{(j)}}{\partial y^2} \right] = 0 \quad (5.2)$$

$$\frac{\beta \varepsilon_f^2}{r} \frac{\partial C_0}{\partial \theta} (r, \alpha \varepsilon_f) = \sum_{j=0}^{\infty} \varepsilon_f^n \frac{\partial C_f^{(j)}}{\partial y} (x, 1), \quad r_b \leq r \leq r_f \quad (5.3)$$

$$\frac{\beta \varepsilon_f}{\partial r} (r_f, \theta) = \sum_{j=0}^{\infty} \varepsilon_f^n \frac{\partial C_f^{(j)}}{\partial x} (r_f, y), \quad 0 \leq \theta \leq \alpha \varepsilon_f. \quad (5.4)$$

We see that equation (5.4) provides the strongest criterion for $n$, namely that $n = 1$. For the remaining equations in our system, we simply match term-by-term. We now begin our consideration of our system of equations in the fracture. From equations (5.3) and (5.4) we see that to obtain boundary conditions for $C_0$, we have to solve our equations up to order $\varepsilon_f^2$.

Order 0 in Fracture

Using the fact that $n = 1$ and taking the zeroth order terms from (5.2), (3.12), (5.3), and (3.18), we have

$$\frac{\partial^2 C_f^{(0)}}{\partial y^2} = 0 \quad (5.5)$$

$$\frac{\partial C_f^{(0)}}{\partial y} (x, 0) = 0 \quad (5.6)$$

$$\frac{\partial C_f^{(0)}}{\partial y} (x, 1) = 0 \quad (5.7)$$
\[ C_f^{(0)}(r_b, y) = 0. \]  

(5.8)

The solution of equations (5.5)-(5.8) is \( C_f^{(0)}(x, y) = C_f^{(0)}(x) \). Note that there is now no variance in the \( y \) direction, and hence no variance across \( 0 \leq \theta \leq \alpha \epsilon_f \). Since \( \epsilon_f \ll 1 \), we then approximate our boundary conditions there by \( \theta = 0 \) and allow (5.4) to become a point boundary condition. This causes the rest of the zeroth-order equations [namely (3.14a), (3.14b), and (5.4)] to become

\[ C_f^{(0)}(x) = C_0(r, 0), \quad r_b \leq r \leq r_f \]  

(5.9)

\[ C_f^{(0)}(r_f) = C_0(r_f, 0) \]  

(5.10)

\[ C_f^{(0)'}(r_f) = 0. \]  

(5.11)

**Order 1 in Fracture**

Now taking the first order terms of our fracture equations (5.2), (3.12), and (5.3), we have

\[ \frac{\partial^2 C_f^{(1)}}{\partial y^2} = 0 \]  

(5.12)

\[ \frac{\partial C_f^{(1)}}{\partial y}(x, 0) = 0 \]  

(5.13)

\[ \frac{\partial C_f^{(1)}}{\partial y}(x, 1) = 0. \]  

(5.14)

The solution of equations (5.12)-(5.14) is \( C_f^{(1)}(x, y) = C_f^{(1)}(x) \). However, since equation (3.14a) becomes \( C_f^{(1)}(x, 1) = 0 \), we have \( C_f^{(1)}(x, y) \equiv 0 \). Hence the first-order term of equation (5.4), which is the real equation of interest for this order, becomes

\[ \frac{\partial C_0}{\partial r}(r_f, 0) = 0. \]  

(5.15)

**Order 2 in Fracture**

Now taking the second order terms of our fracture equations (5.2), (3.12), and (3.14a), we have

\[ \frac{\partial^2 C_f^{(2)}}{\partial y^2} + C_f^{(0)''} = 0 \]  

(5.16)

\[ \frac{\partial C_f^{(2)}}{\partial y}(x, 0) = 0 \]  

(5.17)

\[ C_f^{(2)}(x, 1) = 0. \]  

(5.18)
The solution of equations (5.16)-(5.18) is

\[ C_f^{(2)}(x, y) = C_f^{(0)''}(x) \frac{1 - y^2}{2}. \]  

(5.19)

Also, equations (3.18), (3.14b), (5.3), and (5.4) become

\[ C_f^{(2)}(r_b, y) = 0 \]  

(5.20)

\[ C_f^{(2)}(r_f, y) = 0 \]  

(5.21)

\[ \frac{\beta}{r} \frac{\partial C_0}{\partial \theta}(r, 0) = \frac{\partial C_f^{(2)}}{\partial y}(x, 1), \quad r_b \leq r \leq r_f \]  

(5.22)

\[ \frac{\partial C_f^{(2)}}{\partial x}(r_f, y) = 0. \]  

(5.23)

Note that equation (5.23) is a third boundary condition for a two-point boundary value problem; hence it becomes a consistency condition. Using equation (5.19) in equations (5.20)-(5.23), we have the following system:

\[ \frac{\beta}{r} \frac{\partial C_0}{\partial \theta}(r, 0) = -C_f^{(0)''}(x), \quad r_b \leq r \leq r_f \]  

(5.24)

\[ C_f^{(0)''}(r_b) = C_f^{(0)''}(r_f) = C_f^{(0)''}(r_f) = 0. \]  

(5.25)

However, since \( r = x \) on \( \theta = 0 \), (5.24) is also a boundary condition for equation (3.10). Hence, we now have a solvable system of equations for \( C_0 \):

\[ \frac{\partial^2 C_0}{\partial r^2} + \frac{1}{r} \frac{\partial C_0}{\partial r} + \frac{1}{r^2} \frac{\partial^2 C_0}{\partial \theta^2} = 0 \]  

(5.26)

\[ C_0(1, \theta) = 1 \]  

(5.27)

\[ C_0(r_b, \theta) = 0 \]  

(5.28)

\[ \frac{\partial C_0}{\partial \theta}(r, \frac{\pi}{2}) = 0 \]  

(5.29)

\[ \frac{\beta}{r} \frac{\partial C_0}{\partial \theta}(r, 0) = -\frac{\partial^2 C_0}{\partial r^2}(r, 0), \quad r_b \leq r \leq r_f \]  

(5.30)

\[ \frac{\partial C_0}{\partial \theta}(r, 0) = 0, \quad r_f \leq r \leq 1 \]  

(5.31)

\[ \frac{\partial C_0}{\partial r}(r_f, 0) = 0. \]  

(5.32)
Section VI: Singular Perturbation Solution

Outer Solution

Now we wish to solve our system of equations (5.26)-(5.32) using a singular perturbation approach. We begin by assuming the following perturbation expansion of $C_0$ in $\varepsilon_0$:

$$C_0 = C_0^{(o)} + o(1), \quad (6.1)$$

where the superscript $(o)$ indicates that this is the outer solution. Using equation (6.1) in equation (5.30), we have the following:

$$\frac{\partial C_0^{(o)}}{\partial \theta}(r, 0) = -r\varepsilon_0 \frac{\partial^2 C_0^{(o)}}{\partial r^2}(r, 0), \quad r_b \leq r \leq r_f. \quad (6.2)$$

(Since $\varepsilon_f \ll \varepsilon_0$, our assumption that we may approximate the boundary condition by $\theta = 0$ still holds true.) Now letting $\varepsilon_0 \to 0$ and combining (6.2) with (5.31), we have a new system for $C_0^{(o)}$:

$$\frac{\partial^2 C_0^{(o)}}{\partial r^2} + \frac{1}{r} \frac{\partial C_0^{(o)}}{\partial r} + \frac{1}{r^2} \frac{\partial^2 C_0^{(o)}}{\partial \theta^2} = 0 \quad (6.3)$$

$$C_0^{(o)}(1, \theta) = 1 \quad (6.4)$$

$$C_0^{(o)}(r_b, \theta) = 0 \quad (6.5)$$

$$\frac{\partial C_0^{(o)}}{\partial \theta}(r, \frac{\pi}{2}) = 0 \quad (6.6)$$

$$\frac{\partial C_0^{(o)}}{\partial \theta}(r, 0) = 0 \quad (6.7)$$

$$\frac{\partial C_0^{(o)}}{\partial r}(r_f, 0) = 0. \quad (6.8)$$

However, we now note that there is no longer any $\theta$ dependence in the problem and our solution immediately reduces to (4.4):

$$C_0^{(o)}(r, \theta) = \frac{\log(r/r_b)}{\log(1/r_b)}. \quad (6.9)$$
To check our assumption, we plug in our solution (6.9) into (6.2):

$$0 = \frac{\varepsilon_0}{r \log(1/r_b)}. \quad (6.10)$$

Unfortunately, \(r_b = 1.67 \times 10^{-4} = O(\varepsilon_0^2)\). Hence the right-hand side is no longer negligible in a region near the bore hole. Thus, we must try a singular perturbation approach by introducing an inner expansion variable scaling where the two terms in equation (6.2) are of the same order. Our outer expansion still holds true for the outer region, so we lose one boundary condition and our outer solution becomes the following:

$$C_0^{(o)}(r, \theta) = 1 + A_3 \log r, \quad (6.11)$$

where \(A_3\) is yet to be determined.

### Inner Solution

We expect \(C_0^{(o)}\) to be \(O(1)\) in the region, so we introduce the following scalings in the independent variables only:

$$\hat{r} = \frac{r}{\varepsilon_0^m}, \quad \hat{\theta} = \frac{\theta}{\varepsilon_0^n}, \quad \hat{C}_0(\hat{r}, \hat{\theta}) = C_0^{(o)}(r, \theta), \quad m \geq 0, \quad n \geq 0. \quad (6.12)$$

Then, for the proper choices of \(m\) and \(n\), these variables will have the unique quality that

$$\lim_{r \to \infty} \hat{C}_0(\hat{r}, \hat{\theta}) = \lim_{r \to r_b} C_0^{(o)}(r, \theta). \quad (6.13)$$

We also approximate our small radius \(r_b\), which is \(O(\varepsilon_0^2)\), by the origin. Using that fact and equations (6.12) in (6.3), we have the following:

$$\varepsilon_0^{-2m} \frac{\partial^2 \hat{C}_0}{\partial \hat{r}^2} + \varepsilon_0^{-2m} \frac{1}{\hat{r}} \frac{\partial \hat{C}_0}{\partial \hat{r}} + \varepsilon_0^{-2m-2n} \frac{1}{\hat{r}^2} \frac{\partial^2 \hat{C}_0}{\partial \hat{\theta}^2} = 0, \quad 0 \leq \hat{r} < \infty. \quad (6.14)$$

Note that if \(n > 0\), then the leading order in equation (6.14) implies that \(\hat{C}_0\) is a linear function of \(\hat{\theta}\), which we cannot match to our outer expansion \(C_0^{(o)}\). Hence we find that \(n = 0\), and we will drop the hat on \(\theta\) in the rest of the section.

Next we introduce our scalings into equation (6.2):

$$\frac{\partial \hat{C}_0}{\partial \theta}(\hat{r}, 0) = -\hat{r} \varepsilon_0^{1-m} \frac{\partial^2 \hat{C}_0}{\partial \hat{r}^2}(\hat{r}, 0), \quad 0 \leq \hat{r} < \infty. \quad (6.15)$$

This implies that \(m = 1\). Now, in order to make the problem easier to solve, we convert from \((\hat{r}, \theta)\) to \((\hat{x}, \hat{\zeta})\), where the standard transformations are used:

$$\hat{C}_0(\hat{r}, \theta) = \hat{C} \left( \sqrt{\hat{x}^2 + \hat{\zeta}^2}, \tan^{-1} \left( \frac{\hat{\zeta}}{\hat{x}} \right) \right). \quad (6.16)$$
Doing so, equation (6.14) becomes the following:

\[
\frac{\partial^2 \hat{C}}{\partial \hat{x}^2} + \frac{\partial^2 \hat{C}}{\partial \hat{\zeta}^2} = 0, \quad 0 \leq \hat{x} < \infty, \quad 0 < \hat{\zeta} < \infty. \tag{6.17}
\]

Here the \( \hat{\zeta} \) has a strict inequality since we have the differential equation (6.15) for a boundary condition there. Since we are approximating \( r_b \) by the origin, equation (6.5) becomes

\[
\hat{C}(0,0) = 0. \tag{6.18}
\]

Continuing with our boundary conditions, we have from equation (6.6) that

\[
\frac{\partial \hat{C}}{\partial \hat{x}}(0, \hat{\zeta}) = 0, \quad \hat{\zeta} > 0. \tag{6.19a}
\]

Note that equation (6.19a) has a strict inequality. This is because at the fracture (which we have now taken to be the line \( \hat{\zeta} = 0 \)), the flux is not 0. In fact, taking the derivative of equation (3.14a) with respect to \( f \) on the left-hand side and with respect to \( x \) on the right-hand side (since \( r = x \) on the line \( \theta = 0 \), which is our approximate fracture boundary), we have

\[
\frac{\partial \hat{C}_f}{\partial \hat{x}}(0,0) = \frac{\partial \hat{C}_0}{\partial \hat{r}}(0,0).
\]

Then nondimensionalizing and solving together, we have

\[
\frac{\partial C_0}{\partial r}(0,0) = \frac{\partial C_f}{\partial x}(0,0) \tag{6.19b}
\]

\[
\frac{1}{\varepsilon_0} \frac{\partial \hat{C}_0}{\partial \hat{r}}(0,0) = \frac{\partial C_f}{\partial x}(0,0)
\]

\[
\frac{\partial \hat{C}}{\partial \hat{x}}(0,0) = \varepsilon_0 \frac{\partial C_f}{\partial x}(0,0) \equiv q.
\]

In our solution, we solve as if \( q = O(1) \), since we now expect a large flux at the borehole. Continuing with our boundary conditions, from equation (6.15) we have

\[
\frac{\partial \hat{C}}{\partial \hat{\zeta}}(\hat{x},0) = - \frac{\partial^2 \hat{C}}{\partial \hat{x}^2} (\hat{x},0). \tag{6.20}
\]

Our matching condition (6.13) gives us the following:

\[
\hat{C}(\infty, \hat{\zeta}) = C_0^{(o)}(r_b) \tag{6.21a}
\]

\[
\hat{C}(\hat{x}, \infty) = C_0^{(o)}(r_b). \tag{6.21b}
\]
We wish to solve equations (6.17)-(6.21) using a Fourier cosine transform method. To use that method, however, our boundary conditions at \( \hat{x} \) and \( \hat{\zeta} \) equal to \( \infty \) must be 0. Hence we introduce the following transformation:

\[
\hat{C}(\hat{x}, \hat{\zeta}) = C_0^{(o)}(r_b) \left[ 1 - u(\hat{x}, \hat{\zeta}) \right].
\]  
(6.22)

Using equation (6.22) in equations (6.17), we have the following:

\[
\frac{\partial^2 u}{\partial \hat{x}^2} + \frac{\partial^2 u}{\partial \hat{\zeta}^2} = 0, \quad 0 \leq \hat{x} \leq \infty, \quad 0 < \hat{\zeta} < \infty.
\]  
(6.23)

Equation (6.21a) becomes

\[
u(\infty, \hat{\zeta}) = 0,
\]  
(6.24)

while equation (6.19a) becomes

\[
\frac{\partial u}{\partial \hat{x}}(0, \hat{\zeta}) = 0, \quad \hat{\zeta} > 0.
\]  
(6.25)

Continuing to rewrite our boundary conditions, equation (6.20) becomes

\[
\frac{\partial u}{\partial \hat{\zeta}}(\hat{x}, 0) + \frac{\partial^2 u}{\partial \hat{x}^2}(\hat{x}, 0) = 0,
\]  
(6.26)

equation (6.19b) becomes

\[
\frac{\partial u}{\partial \hat{x}}(0, 0) = -\frac{q}{C_0^{(o)}(r_b)},
\]  
(6.27)

and equation (6.21b) becomes

\[
u(\hat{x}, \infty) = 0.
\]  
(6.28)

Lastly, we may rewrite our boundary condition at the origin given by (6.18) as

\[
u(0, 0) = 1.
\]  
(6.29)

Applying the Fourier cosine transform to equation (6.23) subject to (6.24) and (6.25), we have the following, where we assume \( \lambda \) to be a constant:

\[-\lambda^2 v + v''(\hat{\zeta}) = 0.
\]  
(6.30)

Applying the Fourier cosine transform to equation equation (6.26) subject to (6.24) and (6.27), we have

\[
\frac{q}{C_0^{(o)}(r_b)} \sqrt{\frac{2}{\pi}} - \lambda^2 v(0) + v'(0) = 0.
\]  
(6.31)

Equation (6.28) now becomes

\[
u(\infty) = 0,
\]  
(6.32)
and equation (6.29) is not used. Solving (6.30) subject to (6.31) and (6.32), we have

\[ v(\lambda, \dot{\zeta}) = \frac{qe^{-\lambda \dot{\zeta}}}{\lambda(\lambda + 1)C_0^{(o)}(r_b)\sqrt{2\pi}}, \]

from which we have

\[ u(\dot{x}, \dot{\zeta}) = \frac{2q}{\pi C_0^{(o)}(r_b)} \int_0^\infty \frac{e^{-\lambda \dot{\zeta}} \cos(\lambda \dot{x})}{\lambda(\lambda + 1)} d\lambda. \]  

(6.33)

We note that the integral diverges. We move into the complex plane and treat the lower limit formally.

\[ u(\dot{x}, \dot{\zeta}) = \frac{2q}{\pi C_0^{(o)}(r_b)} \Re \left[ \lim_{\eta \to 0} \int_\eta^\infty \frac{e^{-\lambda \dot{\zeta} + i\lambda \dot{x}}}{\lambda} d\lambda - \int_0^\infty \frac{e^{-\lambda \dot{\zeta} + i\lambda \dot{x}}}{\lambda + 1} d\lambda \right] \]

\[ = \frac{2q}{\pi C_0^{(o)}(r_b)} \Re \left[ \lim_{\eta \to 0} \int_\eta^\infty \frac{e^{-t}}{t} dt - e^{i\dot{\zeta} - i\dot{x}} \int_1^\infty \frac{e^{-t(\dot{\zeta} - i\dot{x})}}{t} dt \right]. \]

Using equations (2.2), which define the exponential integral, we have the following:

\[ u(\dot{x}, \dot{\zeta}) = \frac{2q}{C_0^{(o)}(r_b)\pi} \Re \left\{ \lim_{\eta \to 0} E_1[\eta(\dot{\zeta} - i\dot{x})] - e^{i\dot{\zeta} - i\dot{x}} E_1(\dot{\zeta} - i\dot{x}) \right\} \]  

(6.34)

At this juncture it is appropriate to write down asymptotic expansions for \( E_1(s) \):

\[ E_1(s) \sim -\gamma - \log s, \quad s \to 0; \quad E_1(s) \sim \frac{e^{-s}}{s}, \quad s \to \infty. \]  

(6.35)

Rewriting \( u \) in terms of \( \hat{C}_0(\hat{r}, \theta) \), we have

\[ \hat{C}_0(\hat{r}, \theta) = C_0^{(o)}(r_b) - \frac{2q}{\pi} \Re \left[ \lim_{\eta \to 0} E_1(-\eta i \hat{r} e^{i\theta}) - \exp(-i \hat{r} e^{i\theta}) E_1(-i \hat{r} e^{i\theta}) \right]. \]  

(6.36)

Again we note that our first integral, now represented by

\[ \lim_{\eta \to 0} E_1(-\eta i \hat{r} e^{i\theta}) \]

is divergent. For our problem this is not physically reasonable. Since we wished to use a cosine transform, we extended the \( \dot{x} \) and \( \dot{\zeta} \) to a semi-infinite range. However, \( \dot{x} \) and \( \dot{\zeta} \) are only \( O(\epsilon_0^{-1}) \) at our boundary \( r = 1 \). A more correct but more complicated method would involve a discrete eigenfunction expansion. In this case, the difference between subsequent eigenvalues would be \( O(\epsilon_0) \) because our region is \( O(\epsilon_0^{-1}) \). Since the problem is not isotropic in the \( \dot{x} \) direction, the first eigenvalue \( \lambda_1 \) would be greater than zero. This would indicate that our limit \( \eta \) (which corresponds to \( \lambda_1 \)) remains small, but never reaches 0.
Using (6.35), we know that
\[
\lim_{\eta \to 0} E_1(-\eta i e^{i\theta}) = -\log \hat{r} - \gamma - \log \eta.
\]

We use the above in equation (6.36) to obtain a new representation for our inner solution:
\[
\hat{C}_0(\hat{r}, \theta) = \frac{2q}{\pi} \left\{ \log \hat{r} + A_4 + \mathbb{R} \left[ \exp(-i\hat{r} e^{i\theta}) E_1(-i\hat{r} e^{i\theta}) \right] \right\},
\]  
(6.37)

where \(A_4 = \gamma + \log \eta - \pi c_0^{(o)}(r_b)/2q\).

**Boundary and Matching Conditions**

We now need to solve our matching conditions while satisfying the boundary condition \(\hat{C}_0 = 0\) at the borehole. We begin with the condition at the borehole. Using (6.35) again, we see that equation (6.37) becomes
\[
\hat{C}_0(\hat{r}, 0) = \frac{2q}{\pi} (A_4 - \gamma).
\]  
(6.38)

Setting the above equal to 0, we have \(A_4 = \gamma\). Using that fact and equation (6.35) in equation (6.37), we see that
\[
\hat{C}_0(\hat{r}, \theta) \sim \frac{2q}{\pi} (\log \hat{r} + \gamma) \text{ as } \hat{r} \to \infty
\]

(6.39a)

Writing the outer solution (6.11) in terms of the inner variable \(\hat{r}\), we have
\[
C_0^{(o)}(\hat{r}, \theta) = 1 + A_3 \log \varepsilon_0 \hat{r}
\]

(6.39b)

Matching the inner solution (6.39a) and the outer solution (6.39b) as \(\hat{r} \to \infty\) yields
\[
A_3 = \frac{2q}{\pi}, \quad \frac{2q\gamma}{\pi} = 1 + A_3 \log \varepsilon_0
\]

(6.40)

Solving the two parts of (6.40) together, we have
\[
q = \frac{\pi}{2(\gamma - \log \varepsilon_0)}, \quad A_3 = \frac{1}{\gamma - \log \varepsilon_0}
\]

(6.41)

Using equations (6.41) in equations (6.37) and (6.39b), we now have our inner and outer solutions:
\[
\hat{C}_0(\hat{r}, \theta) = \frac{1}{\gamma - \log \varepsilon_0} \left\{ \log \hat{r} + \gamma + \mathbb{R} \left[ \exp(-i\hat{r} e^{i\theta}) E_1(-i\hat{r} e^{i\theta}) \right] \right\}
\]

(6.42a)
\[ C_0^{(o)}(\hat{r}, \theta) = 1 + \frac{\log r}{\gamma - \log \varepsilon_0}. \]  

(6.42b)

However, note that using equation (6.35) as \( \hat{r} \to \infty \), the inner solution reduces to the outer solution. Hence, (6.42a) is the uniformly valid solution. We rewrite it in terms of the outer variables and denote it by the subscript \( (u) \) for uniform.

\[ C_0^{(u)}(r, \theta) = \frac{\log(r/\varepsilon_0e^{-\gamma})}{\log(1/\varepsilon_0e^{-\gamma})} + \frac{1}{\log(1/\varepsilon_0e^{-\gamma})} \Re \left[ \exp \left( \frac{-i\varepsilon_0 e^{i\theta}}{\varepsilon_0} \right) E_1 \left( \frac{-i\varepsilon_0 e^{i\theta}}{\varepsilon_0} \right) \right]. \]  

(6.43)

**Verification of Uniform Solution**

Now, since we have performed several steps in our analysis without rigorous mathematical justification, we check that equation (6.43) satisfies our system of equations (5.26)-(5.32) to \( O(\varepsilon_0) \). To show that it satisfies Laplace’s equation, we note that if we move into the complex plane, the logarithm is an analytic function everywhere except at the origin. However, equation (6.38) shows us that the singularity in the logarithm is exactly canceled by the singularity for the \( E_1 \) term, and the function is analytic there as well. So (5.26) is satisfied.

As \( r \to 1 \), the second term in equation (6.43) decays algebraically while the first term goes to 1, so we have \( C_0^{(u)}(1, \theta) = 1 + O(\varepsilon_0) \). As \( r \to r_b \), which we have assumed to be small, our asymptotics in equation (6.38) show that we yield the correct solution to \( O(\varepsilon_0) \). For equations (5.29)-(5.32), we calculate the necessary derivatives using equation (6.42a):

\[ \frac{\partial C_0^{(u)}}{\partial \theta} = \Re \left[ \hat{r} e^{i\theta} \exp(-i\hat{r} e^{i\theta}) E_1(-i\hat{r} e^{i\theta}) - i \right] \]  

(6.44)

\[ \frac{\partial C_0^{(u)}}{\partial \hat{r}} = \Re \left[ -i e^{i\theta} \exp(-i\hat{r} e^{i\theta}) E_1(-i\hat{r} e^{i\theta}) \right] \]  

(6.45)

\[ \hat{r} \frac{\partial^2 C_0^{(u)}}{\partial \hat{r}^2} = -\hat{r} \Re \left[ e^{2i\theta} \exp(-i\hat{r} e^{i\theta}) E_1(-i\hat{r} e^{i\theta}) - \frac{i e^{i\theta}}{\hat{r}} \right]. \]  

(6.46)

Using equation (6.44) at \( \theta = \pi/2 \) to satisfy (5.29), we have

\[ \Re \left[ i \hat{r} \exp(\hat{r}) E_1(\hat{r}) - i \right] = 0, \]

which is trivially satisfied. Using equation (6.15) with \( m = 1 \) instead of (5.30), and then using equations (6.44) and (6.46) at \( \theta = 0 \), we have

\[ \Re \left[ \hat{r} \exp(-i\hat{r}) E_1(-i\hat{r}) \right] = \hat{r} \Re \left[ \exp(-i\hat{r}) E_1(-i\hat{r}) - \frac{i}{\hat{r}} \right], \]

which is again trivially satisfied. We use equation (6.44) at \( \theta = 0 \) for equation (5.31):

\[ \Re \left[ \hat{r} \exp(-i\hat{r}) E_1(-i\hat{r}) \right] = 0. \]
Asymptotically expanding the above for large $\tilde{r}$ using equation (6.35), we have

$$\Re[-i + O(\varepsilon_0)] = 0.$$  

For equation (5.32), we use (6.45) evaluated at $\theta = 0$:

$$\Re[-i \exp(-i\tilde{r}) E_1(-i\tilde{r})] = 0.$$  

Once again asymptotically expanding for large $\tilde{r}$ using equation (6.35), we have

$$O(\varepsilon_0) = 0.$$  

Hence we have satisfied our entire system of equations, and (6.42) is the solution of our problem to $O(\varepsilon_0)$.

**Flux Calculation**

As a first guess, we surmise that all the flux is coming from the fracture, so we integrate our flux there over the width of both fractures, yielding

$$\dot{Q} = 2aD_f \frac{\partial \tilde{C}_f}{\partial \tilde{x}}(0,0)$$

$$= \frac{2aP_0 D_f q}{RT \tilde{r}_0 \varepsilon_0}$$

$$Q = \frac{a\pi}{\tilde{r}_0 \varepsilon f \log(1/\varepsilon_0 e^{-\gamma})}$$

$$= \frac{2\pi}{\log(1/\varepsilon_0 e^{-\gamma})}. \quad (6.47)$$

To actually calculate the flux, we integrate around $r = 1$:

$$Q = r \int_0^{2\pi} \frac{1}{r \log(1/\varepsilon_0 e^{-\gamma})} \, d\theta \bigg|_{r=1}$$

$$= \frac{2\pi}{\log(1/\varepsilon_0 e^{-\gamma})}. \quad (6.48)$$

Since the two equations agree, we see that our intuition was correct and that to leading order all the flux comes from the fracture.
Section VII: Variational Principle Solution

For this section, each fracture only extends in one radial direction; hence, in the notation of this section, the perturbation computations were for two fractures.

From the perturbation analysis we determined that the zeroth order approximation $C_0$ is the solution to the problem:

$$\nabla^2 C_0(r, \theta) = 0, \quad C_0(1, \theta) = 1, \quad C_0(r_b, \theta) = 0,$$

with the additional boundary condition that

$$\frac{\partial}{\partial r} \left[ \beta_j(r) \frac{\partial C_0}{\partial r} \right] + \frac{1}{r} \frac{\partial C_0}{\partial \theta} = 0$$

(7.2)

along the $j$th fracture at $\theta = \theta_j$ and

$$\beta_j(r) = \frac{D_f a_j(r)}{2D_0 r_0},$$

(7.3)

where $a_j(r)$ is the width of the $j$th fracture as a function of $r$ and is set equal to zero from the end of the fracture up to $r = 1$. We shall now construct a variational formulation of the same problem. We define the functional $\Upsilon$ by

$$\Upsilon(C) = \int_\Omega |\nabla C|^2 \, d\Omega + \sum_{j=1}^N 2 \int_{r_b}^1 \beta_j(r) \left( \frac{\partial C}{\partial r} \right)^2 \, dr \Bigg|_{\theta = \theta_j},$$

(7.4)

where $N$ is the number of fractures. We were able to prove that our initial problem is equivalent to the following variational formulation:

$$\min_{C(r_b, \theta) = 0, C(1, \theta) = 1} \Upsilon(C) = Q.$$

(7.5)

The proof is easily obtained by differentiating $\Upsilon(C_0 + \delta f)$ with respect to $\delta$ at $\delta = 0$, where $f(r, \theta)$ is an arbitrary perturbation of the minimizing function $C_0$ which satisfies $f = 0$ at $r = r_b$ and $r = 1$. The derivative has to be equal to zero for all $f$, i.e.,

$$\frac{d}{d\delta} \left[ \Upsilon(C_0 + \delta f) \right] \bigg|_{\delta = 0} = \int_\Omega \nabla C_0 \cdot \nabla f \, d\Omega + 2 \sum_{j=1}^N \int_{r_b}^1 \beta_j(r) \frac{\partial C_0}{\partial r} \frac{\partial f}{\partial r} \, dr \bigg|_{\theta = \theta_j}. $$

...
Integrating by parts, we obtain

\[ -2 \sum_{j=1}^{m} \int_{r_b}^{1} f \left[ \frac{1}{r} \frac{\partial C_0}{\partial \theta} + \frac{\partial}{\partial r} \left( \beta_j \frac{\partial C_0}{\partial r} \right) \right] dr \bigg|_{\theta = \theta_j} - \int_{\Omega} f \nabla^2 C_0 \, d\Omega. \]  

(7.6)

Since (7.7) has to be equal to zero for arbitrary \( P \), \( C_0 \) must be the solution to

\[ \nabla^2 C_0 = 0 \text{ in } \Omega \]

with the boundary conditions

\[ C_0(r_b, \theta) = 0, \ C_0(1, \theta) = 1 \]

and

\[ \frac{1}{r} \frac{\partial C_0}{\partial \theta} + \frac{\partial}{\partial r} \left( \beta_j \frac{\partial C_0}{\partial r} \right) = 0, \ \theta = \theta_j. \]

We note here that the value of \( \Upsilon \) at its actual minimum \( \Upsilon(C_0) \) is

\[ \Upsilon(C_0) = \int_{0}^{2\pi} \frac{\partial C_0(1, \theta)}{\partial r} \, d\theta = Q. \]  

(7.7)

The proof is a straightforward, but messy, calculation. In order to obtain an approximate value for \( \Upsilon(C_0) \), we restrict the class of functions over which we are minimizing to functions which depend on \( r \) only. When we introduce \( C(r) = C_0(r) + \delta f(r) \) into the variational problem, we obtain the following ordinary differential equation:

\[ 2\pi \frac{d}{dr} \left( r \frac{dC_0}{dr} \right) + \frac{d}{dr} \left[ \tau(r) \frac{dC_0}{dr} \right] = 0, \ r_b < r < 1 \]

\[ C_0(r_b) = 0, \ C_0(1) = 1, \]

where

\[ \tau(r) = \sum_{j=1}^{N} 2\beta_j(r). \]  

(7.8)

The solution is easily obtained and is found to be

\[ C_0(r) = A_5 \int_{r_b}^{r} \frac{dt}{2\pi t + \tau(t)}, \]  

(7.9a)

where

\[ A_5 = \left[ \int_{r_b}^{1} \frac{dt}{2\pi t + \tau(t)} \right]^{-1}. \]  

(7.9b)
Let us now compute the total flux $Q$. Since $\tau(1) = 0$,

$$Q = \int_0^{2\pi} \frac{dC}{dr}(1, \theta) d\theta = \int_0^{2\pi} \frac{A_5 d\theta}{2\pi + \tau(1)} = A_5.$$  \hspace{1cm} (7.10)

Thus,

$$Q = \left[ \int_{\tau_b}^{1} \frac{dt}{2\pi t + \tau(t)} \right]^{-1}. \hspace{1cm} (7.11)$$

We now consider the particular case when all cracks have the same length $r_f$, and the same constant value $\beta$. Thus,

$$\tau(r) = \sum_{j=1}^{m} 2\beta_j(r) = 2m\beta, \hspace{1cm} (7.12)$$

and $Q$ is given by

$$Q = 2\pi \left[ \log \left( \frac{\tau_f + \tau/2\pi}{\tau_b + \tau/2\pi} \right) \right]^{-1}. \hspace{1cm} (7.13)$$

We then normalize $Q$ by the flow rate with no fracture, which is given by (4.5). In figure 7a, we plot the normalized flow rate with respect to $\tau(r)$. In this special case, $\tau(r) = 2m\beta$. In figure 7b, we plot the normalized flow rate, which is proportional to the grosse revenue, versus the number of fractures for a constant value of $\beta = 1/30$. From these graphs we conclude that it is highly profitable to hydrofracture the porous medium with up to four cracks.
Fig 7a: Hydrofracture flow rate

Fig. 7b: Hydrofracture flow rate, beta = 1/30
Section VIII: Conclusions and Future Research

Conclusions

In this report, we have studied a steady-state model for gas flow in a hydrofractured oil field. Without the fracture, equation (4.4) becomes

\[ C_0(r) = \frac{\log(r/r_b)}{\log(1/r_b)}, \quad \text{(8.1)} \]

so the effective radius of the borehole is \( r_b = 1.7 \times 10^{-4} \). However, when we introduce our fracture, the new flow for moderate \( r \) is given by equation (6.43), and is

\[ C_0^{(\omega)}(r, \theta) \sim \frac{\log(r/\varepsilon_0 \varepsilon^{-\gamma})}{\log(1/\varepsilon_0 \varepsilon^{-\gamma})} \quad \text{(8.2)} \]

Note that here our effective radius is \( \varepsilon_0 \varepsilon^{-\gamma} = 1.7 \times 10^{-2} \), an increase of two orders of magnitude. Hence, it is easy to see the usefulness of producing hydrofractures.

Note from equation We employed a perturbation analysis to find out the flow rate through the borehole with two fractures:

\[ Q = \frac{2\pi}{\gamma - \log \varepsilon_0}, \]

where Euler's constant \( \gamma = 0.5771 \).

The above result shows how the amount of gas flowing out of the borehole depends on the width and permeability of the fracture.

Using a variational principle, we obtained an approximation to the flow rate with multiple fractures. In the case of two fractures and taking the radius of the borehole to be approximately zero, the variational method gives us the flow rate

\[ Q = \frac{2\pi}{d - \log \varepsilon_0}, \]

where \( d = \log(\pi/2) + \log(1 + 2\varepsilon_0 / \pi r_f) \). The second term in \( d \) would be generated by calculating the perturbation result to higher order. Discarding the second term in \( d \), we get \( d = \gamma - 0.125 \), so the two results agree very well, seldom differing by more than 6%. Thus, we conclude that the variational method has given us a surprisingly good approximation considering the crudeness of our trial functions.

Considering the case of multiple fractures, especially the case of an odd number of fractures, we would encounter great difficulties using a perturbation method since we would not be able to use the symmetry property to solve the Laplacian problem in our
perturbation analysis. Therefore, the variational method is superior in solving multi-fracture problems where asymptotic solutions cannot be obtained. We also believe the variational method will render a better approximation when the number of fractures is increased.

**Future Research**

In the future, it will be important to extend our steady-state model to a transient one. In the transient model, the pressure will change with time, from which we can extract the relation between the flow rate of gas in the borehole and the pressure in the fractured field. This will then allow one to determine the actual fracture widths and permeabilities from the measured flow rate vs. pressure curve.

Another important area to work on is the extraction rate in fields with many interacting oil and gas wells. The work will be to model several hydrofractured wells with interactions between each other (see figure 8a).

![Figure 8a. Pay zone with multiple fractures, top view.](image-url)
Students' Report
#12
IMA Summer Program for Graduate Students

Mathematical Modeling

The Perpetual Motion of a Thermobile

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1 Introduction

With the rising financial and environmental costs of current energy production, there is a great desire for alternate sources of energy. In this paper we present a model to examine the operation and efficiency for the Thermobile engine which operates by extracting heat from its environment and converting it to mechanical energy. The primary component of the engine is the metal alloy Nitinol which was developed around 1960. This alloy consists of 53 to 57 weight percent nickel, balance titanium, and have the unusual property that it can be plastically deformed, but upon heating return to its original shape.

The thermobile engine considered here consists of a Nitinol wire wrapped around two pulleys of different sizes as indicated in Figure 1. Pulley B has a radius of 12 mm and is made of a metal with high thermal conductivity. Pulley A has a radius of 38 mm and is made of plastic. When Pulley B is given an initial angular velocity in the presence of a heat source, it continues to spin and drive the engine indefinitely and the perpetual motion of this machine is accounted for as follows. When the wire encounters Pulley B, it is plastically deformed. Heat influx from Pulley B and the environment causes a phase transition in the wire to an elastic state. Therefore, upon leaving Pulley B, energy is added to the system as a result of the wire’s tendency to return to its original straight shape. This output of energy causes the entire system to continue spinning.

Many factors such as composition, prior heat treatment, and cold working, can affect the wire properties. We assume the wire is composed of 55 percent nickel, 45 percent titanium and has had no previous cold working. We ignore friction in the pulleys and assume a no slip condition for the wire. This enables us to derive general equations for steady state motion.

![Figure 1: Thermobile](image_url)
2 Nomenclature

We introduce the following symbols in the formulation of our model:

\( \rho = \) density \quad \text{[kg/m}^3]\)
\( \omega_1 = \) angular velocity of top pulley \quad \text{[rad/sec]}\)
\( \omega_2 = \) angular velocity of bottom pulley \quad \text{[rad/sec]}\)
\( R_1 = \) radius of top pulley \quad \text{[m]}\)
\( R_2 = \) radius of bottom pulley \quad \text{[m]}\)
\( T_1 = \) tension on the left \quad \text{[N/m}^2]\)
\( T_2 = \) tension on the right \quad \text{[N/m}^2]\)
\( \theta = \) angle from the point the wire first touches the lower pulley to the present point \quad \text{[rad]}\)
\( \sigma = \) stress \quad \text{[N/m}^2]\)
\( \varepsilon = \) strain \quad \text{[nondim]}\)
\( E = \) Young's modulus in cold state \quad \text{[N/m}^2]\)
\( F = \) Young's modulus in warm state \quad \text{[N/m}^2]\)
\( r = \) radius of wire \quad \text{[m]}\)
\( \varphi = \) angle from the point the wire first touches the top pulley to the present point \quad \text{[rad]}\)
\( T(\varphi) = \) tension along the top pulley \quad \text{[N/m}^2]\)
\( k = \) thermal conductivity of wire \quad \text{[J/sec-m-K]}\)

3 Force Balance Equation

We have assumed a no slip condition for the wire, so that the linear velocities on both pulleys are equal which gives us

\[ \omega_2 R_2 = \omega_1 R_1. \] (1)

We use Newton's Law, \( F = ma \), to derive the equations of motion for our pulley system.

The forces on the left hand side are

- For the tension \( T_2: -T(\varphi) \cos \left( \frac{\varphi}{2} \right) \cdot i + T(\varphi) \sin \left( \frac{\varphi}{2} \right) \cdot j \)
3 FORCE BALANCE EQUATION

![Figure 2: Forces acting on the wire](image)

- For the tension $T_1$: $T(\varphi + d\varphi) \cos\left(\frac{d\varphi}{2}\right) \cdot i + T(\varphi + d\varphi) \sin\left(\frac{d\varphi}{2}\right) \cdot j$
- Normal force: $N \cdot j$
- Frictional force: $-\mu N \cdot j$

The force on the right hand side is

- centrifugal force: $\rho(R_1 d\varphi)R_1\omega^2 \cdot j$.

Summing the forces we find

$$[-T(\varphi)\cos\left(\frac{d\varphi}{2}\right) + T(\varphi + d\varphi)\cos\left(\frac{d\varphi}{2}\right) - \mu N] \cdot i + [T(\varphi)\sin\left(\frac{d\varphi}{2}\right) + T(\varphi + d\varphi)\sin\left(\frac{d\varphi}{2}\right) - N] \cdot j = \rho(R_1 d\varphi)R_1\omega^2 \cdot j.$$

Using Taylor series expansions for $T(\varphi)$, $\cos(\varphi)$, and $\sin(\varphi)$, we have the following relations

$$T(\varphi + d\varphi) = T(\varphi) + \frac{\partial T}{\partial \varphi} d\varphi + O(d\varphi^2)$$

$$\sin\left(\frac{d\varphi}{2}\right) = \frac{d\varphi}{2} + O(d\varphi^3)$$

$$\cos\left(\frac{d\varphi}{2}\right) = 1 + O(d\varphi^2).$$

Substituting and keeping only the linear terms yields

$$\left[-T + T + \frac{\partial T}{\partial \varphi} d\varphi - \mu N \right] \cdot i + \left\{T + T + \frac{\partial T}{\partial \varphi} d\varphi \left(\frac{d\varphi}{2}\right) - N \right\} \cdot j = \rho R_1^2 \omega^2 d\varphi \cdot j.$$
Upon comparing coefficients of the unit vectors, we find

\[
\frac{\partial T}{\partial \varphi} d\varphi - \mu N = 0
\]

\[
T d\varphi - N = \rho R_1^2 \omega_1^2 d\varphi .
\]

Substituting

\[
N = \frac{1}{\mu} \frac{\partial T}{\partial \varphi} d\varphi
\]

into the second equation gives

\[
\frac{\partial T}{\partial \varphi} - \mu T = -\mu \rho R_1^2 \omega_1^2 .
\]

Solving this first order O.D.E for \( T \) in terms of \( \varphi \):

\[
T(\varphi) = A \exp(\mu \varphi) + \rho R_1^2 \omega_1^2 .
\] (2)

Our initial condition at \( \varphi = 0 \) is \( T(0) = T_2 \) and therefore

\[
A = T_2 - \rho R_1^2 \omega_1^2 .
\]

The tension at \( \varphi = \varphi_2 \) is defined to be \( T_1 \) which gives the following relation between \( T_1 \) and \( T_2 \):

\[
T_1 = (T_2 - \rho R_1^2 \omega_1^2) \exp(\mu \varphi_2) + \rho R_1^2 \omega_1^2 .
\] (3)

We now have the following two equations from the conservation of linear momentum

\[
\omega_1 R_1 = \omega_2 R_2
\]

\[
T_1 = (T_2 - \rho R_1^2 \omega_1^2) \exp(\mu \varphi_2) + \rho R_1^2 \omega_1^2 .
\]

4 Rotational Equilibrium Equation

The pulleys are in rotational equilibrium, i.e. the sum of the torques is equal to zero. There are four components to the net torque on the the lower pulley. These are the two tensile torques and the torques caused by bending and unbending the wire. The sum of the tensile torques is

\[-T_1 R_2 + T_2 R_2 .\]
Now we need to find the torques, $M_1$ and $M_2$ caused by the bending and unbending so that we have

$$-T_1R_2 + T_2R_2 - M_1 + M_2 = 0.$$  

Note that since $T_1 < T_2$, we must have $M_2 > M_1$ for the device to work.

To calculate $M_1$ we need to study the bending process. We consider a small length of wire which will be bent over an angle $d\theta$. We assume the center of the wire is not stressed by bending; therefore, we have

$$l = (R_2 + r)d\theta.$$  

The work done by bending a unit volume is the area below the graphs in the stress-strain diagram. For our engine, the wire is bent in the cold state and mostly exhibits plastic behavior, whereas for unbending it is warm and its behavior is totally elastic. The stress-strain diagram in these cases looks like this:

![Stress-Strain Diagram](image)

Figure 3: Stress-Strain Diagram

We study a fiber at a distance $y$ from the center of the wire:

![Fiber in Wire](image)

Figure 4: Fiber in Wire

The final strain on this fiber after bending is

$$\varepsilon(y) = \frac{y}{R_2 + r},$$
where \( r \) is the radius of the wire. So, when the wire is cold, the stress is

\[
\sigma(y) = \begin{cases} 
\frac{E \frac{y}{R_2 + r}}{R_2 + r} & \text{if } 0 \leq y \leq y^* \\
\sigma^* = \frac{E \frac{y^*}{R_2 + r}}{R_2 + r} & \text{if } y^* \leq y \leq r
\end{cases}
\]

where \( |y^*| \) is the distance from the center of the wire where the fibers start showing plastic behavior. In case of a warm wire, we have

\[
\sigma(y) = \frac{F \frac{y}{R_2 + r}}{R_2 + r} \quad \text{for all } y.
\]

In these expressions, \( E \) and \( F \) are Young's moduli associated with the cold state's elastic part and the warm state respectively. The work done by bending a unit volume of the narrow fiber is the area \( A \) under the graph for cold wire and is given by

\[
A = \begin{cases} 
\varepsilon(y)\sigma^* - \frac{1}{2}\varepsilon^*\sigma^* & \text{if } \varepsilon(y) \geq \varepsilon^* \\
\frac{1}{2}\sigma(y)\varepsilon(y) & \text{if } \varepsilon(y) \leq \varepsilon^*.
\end{cases}
\]

The cross-sectional area of the fiber is

\[
dA = 2\sqrt{r^2 - y^2} \, dy.
\]

So, by integrating over all fibers, the work \( W \) done by a unit length of wire in the cold state is (for reasons of symmetry)

\[
W = 2 \left[ \int_0^{y^*} \frac{1}{2} \sigma(y)\varepsilon(y) 2\sqrt{r^2 - y^2} \, dy + \int_{y^*}^r (\varepsilon(y)\sigma^* - \frac{1}{2}\varepsilon^*\sigma^*) 2\sqrt{r^2 - y^2} \, dy \right],
\]

which works out to be

\[
\frac{2E}{(R_2 + r)^2} \left[ -\frac{\pi}{4} y^* r^2 + \frac{5}{12} y^* \sqrt{(r^2 - y^2)^3} + \frac{1}{8} r^2 (4y^2 + r^2) \arcsin \left( \frac{y^*}{r} \right) + \frac{1}{8} y^* (4y^2 + r^2) \sqrt{r^2 - y^2} \right].
\]

Therefore, the work required to bend a wire of length \( l \) is

\[
WL = W(R_2 + r) \, d\theta,
\]

so that the necessary torque is

\[
M_1 = W(R_2 + r) =
\frac{2E}{R_2 + r} \left[ -\frac{\pi}{4} y^* r^2 + \frac{5}{12} y^* \sqrt{(r^2 - y^2)^3} + \frac{1}{8} r^2 (4y^2 + r^2) \arcsin \left( \frac{y^*}{r} \right) + \frac{1}{8} y^* (4y^2 + r^2) \sqrt{r^2 - y^2} \right] (4)
\]

In the warm state the calculation is the same but the result is much simpler. In fact,

\[
M_2 = \frac{F \pi r^4}{8(R_2 + r)}
\]

Therefore the rotational equilibrium equation now reads

\[
R_2(T_1 - T_2) =
\frac{F \pi r^4}{8(R_2 + r)} - \frac{2E}{R_2 + r} \left[ -\frac{\pi}{4} y^* r^2 + \frac{5}{12} y^* \sqrt{(r^2 - y^2)^3} + \frac{1}{8} r^2 (4y^2 + r^2) \arcsin \left( \frac{y^*}{r} \right) + \frac{1}{8} y^* (4y^2 + r^2) \sqrt{r^2 - y^2} \right].
\]
5 Maximum Angular Speed

A limiting factor for the speed of the wire is the rate at which the wire can absorb energy. Assuming that the wire completes the phase transition between \( \theta = 0 \) and \( \theta = \theta_2 \), the minimum heat required is

\[
A[l \rho C(T^* - T_0) + \Delta H],
\]

where the first term is the heat required to raise a wire of cross-sectional area, \( A \), length \( l \), and density \( \rho \) from room temperature, \( T_0 \), to the transition temperature \( T^* \). The second term is the heat required for the wire to go through the transition phase.

The rate at which the wire absorbs heat (per unit surface area) is given by

\[
Q = k \frac{\partial T}{\partial R} \bigg|_{R=r}.
\]

For a rough estimate, we will assume that average temperature gradient at the wire surface is

\[
\frac{\partial T}{\partial R} \bigg|_{R=r} = \frac{3(T_w - T^*)}{r}.
\]

Hence the total heat is given by

\[
QAf = kAf \left[ \frac{2T_w - T_0 - T^*}{2r} \right],
\]

where \( t \) is the time the wire is in contact with the water.
Using

- \( k = \) thermal conductivity = 0.8 Watt cm\(^{-1}\) °C\(^{-1}\)
- \( A = 0.00209 \text{ cm}^2 \)
- \( T_w = 80^\circ \text{C} \)
- \( T_0 = 22^\circ \text{C} \)
- \( T^* = 55^\circ \text{C} \)
- \( \Delta H = 8 \text{ cal cm}^{-3} \)
- \( \rho = 6.45 \text{ g cm}^{-3} \)
- \( l = R_2 \theta_2 = 3.8 \text{ cm} \)
- \( C = \) specific heat = 0.109 cal g\(^{-1}\) °C\(^{-1}\)
- \( r = \) radius of wire = 0.0257 cm

we find that the minimum time required is

\[
t = l \left\{ \frac{\rho C (T^* - T_0) + \Delta H}{k (2T_w - T_0 - T^*)} \right\} \cdot 4.2r = 0.214 \text{ sec}
\]

Using this to calculate the angular velocity of the lower pulley tells us the maximum speed is 13.7 rad/sec. This is obviously an upper limit since we have neglected all frictional forces.

6 Conclusions and Future Research

In this report we have attempted to determine a mathematical model for the Thermobile engine. Due to the lack of available information on Nitinol, quantitative information is difficult to generate. Clearly these equations could be used to model an ideal engine once the material properties are known.

Our analysis has used many assumptions and simplifications whose validity should be studied further. Future work includes:

- Determine whether the friction resisting the turning of the pulley is negligible. In this device the bottom pulley does not turn freely.
• The heating process has been greatly simplified. For instance, the phase transition may not take place through the entire width of the wire, but only near the surface.

• The bending and unbending of the wire passing over the top pulley has been ignored. If the wire satisfies Hooke's law near that pulley, then the net work is zero and this is appropriate. We need to determine whether the wire is elastic or plastic in this region.

• Additional data is required to determine the exact curve of the stress-strain diagram, especially in the cold state.

• In the model presented here, we have assumed that the wire coincides with the lines which are tangent to both pulleys. Observation shows that this is not the case in our device.

Beyond understanding this device, it would be interesting to study how changes in design affect engine performance. For instance we could vary the radii of the pulleys and the distance between them. An especially interesting factor to study is the shape of the wire. A larger surface area would increase the rate of heat transfer but would also increase friction. More cross-sectional area far from the center would increase the mechanical energy released by the unbending process. We assume that much of this research is currently underway.