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1 INTRODUCTION

In this part we shall consider concepts and approaches for models based on *conservation* principles. Some of the material will be relatively easy, at least for students with some background in fluid and continuum mechanics. Nevertheless, it is important to see that the principles are generally valid and applicable for modeling in many other contexts than traditional mechanics.

It is difficult to discuss conservation principles without getting involved with partial differential equations, but we shall mostly be interested in the qualitative theory and the general behavior of the solutions, and not very specific analytical or numerical solution methods. Below, the term *fluid* is used both for liquids and gases. A *first aid* course about first-order quasi-linear partial differential equations is found in an appendix. It is designed for readers without any knowledge of partial differential equations beyond calculus.

In many models we apply continuous distributions or densities in space where the phenomenon we consider is discrete. Typical examples could be the density of bacteria, people, cars, and the like. In such cases, the models implicitly assume a kind of *continuum hypothesis* similar to the one in continuum mechanics. However, such an approach has obvious limitations, and it is important to be aware what the models are really good for. It leads, *e.g.* to absurdities to insist on mathematical definitions based on limits to ∞ or 0. In the physical world "0" is a few orders of magnitudes below and " ∞ " some orders of magnitudes above where we are located. When we say that " $\Delta x \rightarrow 0$ ", we actually mean that Δx is small compared to the scale where we are located, and not that Δx really goes to 0 in the mathematical sense. This is similar to talking about stationary conditions in time from $-\infty$ and ∞ . In elementary particle physics the eternity could well be 10^{-10} s! Scaling considerations that we have covered earlier, help us to assess the reliability of our assumptions.

We should distinguish between establishing a model and solving the equations after they have been formulated in a mathematical model. The latter is the theme of the courses in analytical and numerical solution of ordinary and partial differential equations. Although enthusiasts advertise numerical software that can solve any differential equation, it is still far from that we can leave to the computer to *understand* what is really happening. As numerical tools are becoming more advanced, it is, on the contrary, and increasing demands for mathematical expertise and analysis of the equations. Today, serious customers require that calculations based on numerical models should be documented to be reliable. Only thorough mathematical and numerical analysis, and not least physical and engineering insight, can help with this. Many of the analytical solutions for idealized problems that are known from the theory of partial differential equations are useful in this respect. Scaling arguments show that the so-called fundamental solution of the heat conduction equation has far greater applicability than is usually mentioned in the mathematics courses. In a way, fundamental solutions and other solutions from idealized mathematical situations are the cornerstones that give us insight and set limits.



Figure 1: Pragmatic definition of *density* at a point in space: The mass over volume ratio is reasonably stable for $r_{\min} < r < r_{\max}$, but the limit when $r \to 0$ does not exist and makes no sense.

2 BASIC CONCEPTS

2.1 Density

Although we perceive water and air as quite homogeneous and uniform physical materials, we all know that this is only when considered from our own length-scale. If we made an imaginary sphere with radius r and center at \mathbf{x} in air and could calculate the mass within the sphere, m(r), the mathematical definition of the density of the air in the point \mathbf{x} would be

$$\rho\left(\mathbf{x}\right) = \lim_{r \to 0} \frac{m\left(r\right)}{4\pi r^3/3} \tag{1}$$

If we really were able to perform this experiment, and plot the ratio in a graph as a function of r, we would however see something like in Fig. 1. When r becomes less than r_{\min} (about 10^{-7} m for the air around us), the ratio begins to fluctuate, and it is certainly no sense in talking about a limit when r goes to 0, as we do in mathematics. Conversely, if r is too large, the ratio will no longer be constant because the air inside the sphere is no longer uniform. As you understand, we must add to the definition of density an assumption that we stop the limit process in the right place, and that our definition of the density of air only has meaning for phenomena with a length scale between r_{\min} and r_{\max} . As applied mathematicians, we have to bear with density not being particularly "well-defined". This does not create major problems for air and water in most of our daily situations, but for high vacuum technology, r_{\min} may well be of the same scale as the apparatus.

Let us consider some quantity that we describe by a density $\varphi(\mathbf{x}, t)$. The amount within a given closed region R of space may be expressed by the volume integral,

$$M(t) = \int_{R} \varphi(\mathbf{x}, t) \, dV.$$
⁽²⁾

Although one immediately think of density as amount per volume unit, there is nothing wrong in defining the density as the amount per of area unit, like $80g/m^2$ for ordinary

writing paper. Similarly, for a thin iron wire the useful density becomes weight per unit length.

In the introduction to [11], the authors have two examples which illustrate how it is possible to think of continuous densities in two quite extreme cases. One example discusses how the spiral structure of galaxies can be modeled as density waves in a gravitational plasma in which the galaxies are modeled as a continuum characterized by the mass density of the stars (C. C. Lin was in fact one of the main contributors to this theory). The second example discusses instabilities in the density of amoebas during food shortages, the density is the number of amoebas per area unit, also regarded as a continuous function of the position on the surface they live (this model and analysis of it was developed by the second author, L. A. Segel).

In mathematical modeling we therefore talk about densities in many other situations than we know from mechanics. The density of various foreign substances, such as contaminants in water, is also a relevant example. Within the air pollution modeling, the most advanced mathematical models consider hundreds of different components, each of which is characterized by its density. In addition, the components interact, decay chemically, are transported with the wind and become mixed in the air masses, or simply fall down. Oil reservoir engineering applies complicated mathematical models for tracing various oil and gas components in porous rocks.

The heat or energy content in materials may be expressed as energy per volume unit. This will in the simplest case with constant specific heat be proportional to the temperature. Entropy density appears in models that deal with heat conduction and heat transfer. Some densities lead us into mathematical problems (so-called *singular densities*) which we shall return to below in the section about sources and sinks.

In continuum mechanics we call quantities that passively follows the flow for material variables. The most common material variables in mechanics are mass, momentum, vorticity and energy, which, in a continuous medium, are described by

ho	mass density	
$ ho \mathbf{v}$	momentum density	(2)
$\nabla \times \rho \mathbf{v}$	Vorticity density	(3)
$e\rho$	energy density	

where \mathbf{v} is the velocity of the medium. Impurities or other additives that passively follow the flow, are also material variable. The concentration of plankton in the water is therefore a material variable as long as it does not move on their own. On the other hand, a school of herring will usually not count as a material variable!

Within biology it is common, as in the example by L. A. Segel, to operate with continuous density functions of animals, bacteria and plants. This allows one to create models which describe the motion of animal herds, bacterial cultures, the spread of epidemics, and the like. We shall later look at a situation where we model the density of cars along a road as a continuum.

2.2 Flux

Flux is about transport or flow of something. The term has actually various meanings in science, but here it is only connected to the motion. If we stand by a road and watch the cars passing, the average number of cars passing per minute will be what we define the *flux* of cars. Flux includes the direction of the flow, so the flux of cars should be separated into flux to the right, and flux to the left.

We will meet flux in a lot of different situations. To fix ideas, let us consider the flow of some material in space. Standing at a fixed point \mathbf{x} we observe that it passes, but in order to quantify how much is flowing, we put (an imaginary) open small window frame $d\sigma$ into the stream at \mathbf{x} and observe how much is passing through the frame per second. It is convenient to present the measurements as amount per second and area unit, since a window twice as large and with the same orientation will allow twice as much material to pass through. The orientation of the frame is uniquely defined by a fixed normal vector \mathbf{n} attached to the frame. If we change the orientation and hence the normal vector to the opposite direction, the flux changes sign. The maximum amount will flow through the frame if we align \mathbf{n} with the direction of the flow, and this direction is what we define to be the *direction of the flux*. Flux can therefore be most easily described as a vector field, $\mathbf{j}(\mathbf{x}, t)$, where the direction of \mathbf{j} indicates the transport direction, and the size, $|\mathbf{j}|$, the amount per time and area unit. Nothing passes through the frame if \mathbf{n} is orthogonal to \mathbf{j} . In general, the amount dM that passes through $d\sigma$ (with orientation \mathbf{n}) during a time period dt is thus

$$dM = \mathbf{j} \cdot \mathbf{n} d\sigma dt. \tag{4}$$

The total amount flowing out through a surface Σ in space with normal vector **n** per unit of time is now given by the surface integral,

$$\frac{dM}{dt} = \int_{\Sigma} \mathbf{j} \cdot \mathbf{n} d\sigma.$$
(5)

By means of the *Divergence Theorem* from vector analysis, it is possible to rewrite the surface integrals over the closed surface ∂R of a volume R as

$$\int_{\partial R} \mathbf{j} \cdot \mathbf{n} d\sigma = \int_{R} \nabla \cdot \mathbf{j} dV.$$
(6)

We shall later see that some care must be exercised when applying the Divergence Theorem.

For a material variable with density φ , passively following a continuous flow with a velocity vector field \mathbf{v} , the flux has a particularly simple form, namely, $\mathbf{j} = \varphi \mathbf{v}$. This follows from Fig. 2, where an amount φdV passes through $d\sigma$ during the time dt. Simple vector calculus gives $dV = d\sigma \cdot |\mathbf{v}| dt \cdot \cos \alpha = \mathbf{v} \cdot \mathbf{n} d\sigma dt$. Therefore, the amount passing through $d\sigma$ per time unit will be

$$Q = \frac{\varphi dV}{dt} = \varphi \mathbf{v} \cdot \mathbf{n} d\sigma = \mathbf{j} \cdot \mathbf{n} d\sigma.$$
(7)

The flux for this particular case may be written $\mathbf{j} = \varphi \mathbf{v}$, and the total flow of the material through a surface Σ per time unit is

$$Q = \int_{\Sigma} (\varphi \mathbf{v}) \cdot \mathbf{n} d\sigma.$$
(8)



Figure 2: Derivation of the expression for the flux of a material variable.

There exist a lot of different expressions for flux. In a practical modeling situation it may sometimes be difficult to come up with a good model. The expression for the turbulent dispersion and transport of material considered later in this note is not yet fully resolved, despite more than 100 years of active research. In electricity, we have in the general form of Ohm's law that the flux of electric current, **j**, is given by $\mathbf{j} = \sigma \mathbf{E}$ where σ is the material conductivity and **E** electric field strength. In electromagnetism, there electromagnetic radiation carries energy, the energy flux is given by Poynting vector, $\mathbf{P} = \mathbf{E} \times \mathbf{H}$.

We mentioned in the previous section that plankton could be a material variable. Now it is known that plankton to some extent is attracted by light, therefore, will set up a flux directed towards the light.

Of the more curious models of flux, we have the assumption that schools of fish tend to move along the gradient of its *well-being* function, g, such that

$$\mathbf{j} \propto \nabla g. \tag{9}$$

We shall later return to other models of flux, e.g. diffusion generated flux.

2.3 Sources and Sinks

A source produces a certain amount of substance per time unit, and we may define a sink as a source with negative output, hence we only discuss sources. Mathematically, a study of a source in the point \mathbf{x}_0 could be carried out by considering a ball R of radius r around \mathbf{x}_0 , then computing

$$\int_{\partial R} \mathbf{j} \cdot \mathbf{n} d\sigma, \tag{10}$$

and see what happens when $r \to 0$. Again, we must have the same reservations in mind that we had for definition of density.

One usually distinguishes between *distributed* and *singular* sources. For a distributed source, the limit value of

$$\lim_{r \to 0} \frac{\int_{\partial R} \mathbf{j} \cdot \mathbf{n} d\sigma}{4\pi r^3/3} \tag{11}$$

exists, and when \mathbf{x}_0 varies, it defines a function, a so-called *production density* $q(\mathbf{x}, t)$ that expresses the production per time and volume unit. The production density is related to divergence of flux field if the flux and its divergence are nice and continuous functions. Applying the Divergence and Mean Value Theorems,

$$\int_{\partial R} \mathbf{j} \cdot \mathbf{n} d\sigma = \int_{R} \nabla \cdot \mathbf{j} dV = (\nabla \cdot \mathbf{j}) (\mathbf{x}') \times 4\pi r^{3}/3, \ |\mathbf{x}' - \mathbf{x_{0}}| < r,$$
(12)

and thus,

$$\lim_{r \to 0} \frac{\int_{\partial R} \mathbf{j} \cdot \mathbf{n} d\sigma}{4\pi r^3/3} = \lim_{r \to 0} \left(\nabla \cdot \mathbf{j} \right) \left(\mathbf{x}' \right) = \left(\nabla \cdot \mathbf{j} \right) \left(\mathbf{x_0} \right).$$
(13)

In conclusion,

$$q\left(\mathbf{x},t\right) = \nabla \cdot \mathbf{j}\left(\mathbf{x}\right) \tag{14}$$

Obviously, for a certain production density, the total production in the volume R during the time from t_1 to t_2 , is

$$Q(t) = \int_{t_t}^{t_2} \int_R q(\mathbf{x}, t) \, dV dt.$$
(15)

The simplest singular sources are the *point sources*. For point sources we have, as the name indicates, only production from a single point \mathbf{x}_0 . This is an idealized situation where, in practice, $q(\mathbf{x}, t)$ only differs from zero near \mathbf{x}_0 . For a ball R around \mathbf{x}_0 as considered above,

$$\int_{\partial R} \mathbf{j} \cdot \mathbf{n} d\sigma \tag{16}$$

will stay constant move towards $r \to 0$, or more general be a function of time. If we were to describe a point source at \mathbf{x}_0 by a production density, this would be 0 for $\mathbf{x} \neq \mathbf{x}_0$, while the integral over an arbitrary small region containing \mathbf{x}_0 would be different from 0. Regular functions with this property do not exist, but as you probably know, one has introduced generalized functions (also called distributions) to be used in such situations. A point source at \mathbf{x}_0 can thus be described using a so-called δ -function,

$$q\left(\mathbf{x},t\right) = Q\left(t\right)\delta_{\mathbf{x}_{0}}\left(\mathbf{x}\right).$$
(17)

Here Q(t) denotes the production rate (amount per time unit), and the δ -function states that production occurs in point \mathbf{x}_0 . In general, the δ -function at \mathbf{x}_0 is defined by the property that

$$\int f(x) \,\delta \mathbf{x}_0\left(\mathbf{x}\right) dV = f\left(\mathbf{x}_0\right). \tag{18}$$

for all continuous functions.

Point sources are not completely covering the category of singular sources. Often, one needs to model sources located along a surface or a curve in the area to be considered. For example, one can think of a varying heat production along a curve (think of a electrical resistance wire!) or a surface, as indicated in Fig. 3. This also leads into generalized functions, but one can always model such sources as limits of point sources where these



Figure 3: Illustration of various singular sources.

spreads out along a curve or on a surface. We leave to the reader to find out how the above integral, $\int_{\partial B} \mathbf{j} \cdot \mathbf{n} d\sigma$, will behave when $r \to 0$ for curve and surface sources.

In practice, it is often appropriate also to include the singular sources into the production density, which then, in the mathematical sense, becomes a generalized function.

From physics (or distribution theory in mathematics), *dipole* and *quadrupole* sources are also known. We will not meet these in any of the situations we shall consider here.

2.4 The Universal Conservation Law

Let us consider a geometrically closed, imaginary region R with boundary ∂R in space. In modeling, such a region is often called a *control volume*. No part of the boundary needs to be physical, so that material may flow freely through.

In space we have a material with density $\rho(\mathbf{x},t)$ moving with a flux $\mathbf{j}(\mathbf{x},t,\rho)$, dependent of \mathbf{x} , t and ρ . For the sources and sinks inside R, we prescribe a generalized production density $q(\mathbf{x},t)$, which in general may contain singular sources. From what we have been through, we see that the rate of change rate in the total amount in R may be written

$$\frac{d}{dt} \int_{R} \rho\left(\mathbf{x}, \mathbf{t}\right) dV. \tag{19}$$

Now, this must be equal to *minus* what is disappearing over the boundary of R per time unit (because of the definition of an *outer* unit normal, **n**),

$$-\int_{\partial R} \mathbf{j}(\mathbf{x}, t, \rho) \cdot \mathbf{n} d\sigma \tag{20}$$

plus what is produced (or disappears) in R per time unit,

$$\int_{R} q\left(\mathbf{x}, t\right) dV.$$
(21)

Altogether, we obtain the equation

$$\frac{d}{dt} \int_{R} \rho(\mathbf{x}, t) \, dV + \int_{\partial R} \mathbf{j}(\mathbf{x}, t, \rho) \cdot \mathbf{n} d\sigma = \int_{R} q(\mathbf{x}, t) \, dV.$$
(22)

This is called a *conservation law* in *integral form*. The integrals and the derivative with respect to t in the first term exist under fairly general conditions. Otherwise, the conservation law is the mathematical formulation that "nothing can disappear or arise from nothing", – a law of nature with an overwhelming empirical basis!

If ρ and **v** are sufficiently smooth functions of t and **x**, we can move the derivative with respect to t under the integral sign, and otherwise use the Divergence Theorem,

$$\frac{d}{dt} \int_{R} \rho dV = \int_{R} \frac{\partial \rho}{\partial t} dV,$$

$$\int_{\partial R} \mathbf{j} \cdot \mathbf{n} d\sigma = \int_{R} \nabla \cdot \mathbf{j} dV.$$
 (23)

This means that

$$\int_{R} \left(\frac{\partial \rho}{\partial t} + \nabla \cdot \mathbf{j} - \mathbf{q} \right) dV = 0.$$
(24)

Such a relation would actually hold for all nice R if ρ and \mathbf{v} are smooth and nice functions in the domain we are considering (Mathematically, it is sufficient that it holds for all spheres in the domain). If $\rho_t + \nabla \cdot \mathbf{j} - q$ is continuous, a result from analysis that says that if Eq. 24 hold,

$$\rho_t + \nabla \cdot \mathbf{j} - q = 0. \tag{25}$$

(Suppose that for a fixed t, $f(\mathbf{x}) = \rho_t + \nabla \cdot \mathbf{j} - q$ is different from 0 at the point \mathbf{x}_0 . Then f is different from 0 for all \mathbf{x} a neighborhood $N \subset R$ around \mathbf{x}_0 since f is continuous. Consequently, the integral of f over this neighborhood is also different from 0, contradictory to the assumption). Eq. 25 thus apply when ρ , \mathbf{j} , \mathbf{v} and q are smooth, and this is the conservation law stated in *differential form*.

Since we later will see examples where one cannot move the derivation inside the integration sign, the integral formulation more general and fundamental than the differential formulation.

2.5 Conservation Laws in one Space Dimension

We shall discuss some properties of simple conservation laws, and limit ourselves to a simple one-dimensional situation. The *density*, $\rho(x, t)$, has now the dimension amount per unit length. The *flux* $j(x, t, \rho)$ expresses the amount of material that passes the point x (in the positive x-direction) per time unit, and will in general also be a function of t and ρ . Note that the flux is a *vector* directed along the x-axis. We shall in this discussion for simplicity ignore sources and sinks.

For a finite segment [A, B] of the x-axis, we may, since nothing disappears or is produced in [A, B] write

$$\frac{d}{dt} \int_{A}^{B} \rho(x,t) \, dx + j(B,t,\rho(B,t)) - j(A,t,\rho(A,t)) = 0.$$
(26)

Note that the boundary unit vector **n** is $-\mathbf{i}$ in A and \mathbf{i} in B. If $\rho(x,t)$ is a sufficiently smooth function, we have for all possible subintervals [a, b] of [A, B] that

$$\frac{d}{dt} \int_{a}^{b} \rho\left(x,t\right) dx = \int_{a}^{b} \frac{\partial \rho\left(x,t\right)}{\partial t} dx = \frac{\partial \rho\left(\xi,t\right)}{\partial t} \left(b-a\right), \ \xi \ \epsilon\left(a,b\right).$$
(27)

Thus, we may write

$$\frac{\partial\rho\left(\xi,t\right)}{\partial t} + \frac{j\left(b,t,\rho\left(b,t\right)\right) - j\left(a,t,\rho\left(a,t\right)\right)}{b-a} = 0.$$
(28)

After a Taylor expansion of the second expression, and in the limit $a \rightarrow b$, we obtain the differential equation

$$\frac{\partial \rho}{\partial t} + \frac{\partial j}{\partial x} + \frac{\partial j}{\partial \rho} \frac{\partial \rho}{\partial x} = 0.$$
(29)

This is the conservation law in differential form, which mathematically is a (generally nonlinear) hyperbolic partial differential equation.

The following simple (but important!) example illustrates why one can not in general write

$$\frac{d}{dt} \int_{a}^{b} \rho\left(x,t\right) dx = \int_{a}^{b} \frac{\partial \rho\left(x,t\right)}{\partial t} dx.$$
(30)

A solid medium has a discontinuity in the density from ρ_1 to ρ_2 . The medium moves with uniform speed U along the x-axis. Since the flux in this case is just ρU , the conservation law with the discontinuity between a and b, gives

$$\frac{d}{dt} \int_{a}^{b} \rho dx + \rho_2 U - \rho_1 U = 0, \qquad (31)$$

or,

$$\frac{d}{dt} \int_{a}^{b} \rho dx = \left(\rho_{1} - \rho_{2}\right) U. \tag{32}$$

However, since $\partial \rho / \partial t$ is equal to 0 except at the discontinuity, say at $x = x_g$, we could also write

$$\frac{d}{dt}\int_{a}^{b}\rho dx = \int_{a}^{x_{g}}\frac{\partial\rho_{1}}{\partial t}dx + \int_{x_{g}}^{b}\frac{\partial\rho_{2}}{\partial t}dx = 0 + 0 = 0.$$
(33)

Consequently,

$$\frac{d}{dt} \int_{R} \rho dx \neq \int_{R} \frac{\partial \rho}{\partial t} dx.$$
(34)

This is a situation which may well occur in practice.

Without getting too far into the theory of partial differential equations, we shall limit ourselves to a situation where **j** is a known, differentiable function of ρ . The differential equation is then reduced to

$$\frac{\partial \rho}{\partial t} + c\left(\rho\right)\frac{\partial \rho}{\partial x} = 0, \quad c\left(\rho\right) = \frac{dj}{d\rho}.$$
(35)

The quantity $c(\rho)$ has dimension velocity, and is called the *kinematic velocity*. In a way which becomes more clear later, one could say that the kinematic speed represents the speed of information in the problem.

To find the solution of this differential equation, we make the following interesting observation: Suppose that the solution $\rho(x, t)$ is already known. Then we also know $c(\rho(x, t))$. Let us define a vector field in the (x, t)-plane by

$$\mathbf{v}\left(x,t\right) = \left\{c\left(\rho\left(x,t\right)\right),1\right\}$$
(36)

Field curves (with the curve length parameter s) are defined by the equations

$$\frac{dx}{ds} = c\left(\rho\left(x,t\right)\right),$$

$$\frac{dt}{ds} = 1.$$
(37)

Assume that x = p(s) and t = q(s), for $-\infty < s < \infty$ represent the curves. We calculate the variation of ρ along a curve by means of

$$\frac{d\rho}{ds} = \frac{\partial\rho}{\partial t}\frac{dt}{ds} + \frac{\partial\rho}{\partial x}\frac{dx}{ds} = \frac{\partial\rho}{\partial t} \cdot 1 + \frac{\partial\rho}{\partial x} \cdot c\left(\rho\left(x,t\right)\right) = 0.$$
(38)

This means that ρ is constant along the field curves. Consequently, $c = c(\rho)$ is also constant along the curves. But this implies in turn that the curves are straight lines. These fields lines are called *characteristic curves* or simply *characteristics*. Strictly speaking, the field lines are the projection in the (x, t)-plane of the real characteristics in (x, t, ρ) -space, but it is common also to call the projections for characteristics (In general, characteristic curves do not need to be straight lines).

We are now going to find the solution $\rho(x,t)$ for $-\infty < x < \infty$, $0 \le t$, given that

$$\rho\left(x,0\right) = f\left(x\right).\tag{39}$$

With the condition given at t = 0, this is an initial value problem, also called the *Cauchy-problem* in this context.

However, if we are seeking the solution in a point (x_1, t_1) , we first need to find the characteristic curve through the point. Since the characteristics are straight lines, they have equations

$$x = x_0 + c(\rho(x_0, 0)) t = x_0 + c(f(x_0)) t$$
(40)

where $(x_0, 0)$ lies on x-axis. Accordingly, we must first find an x_0 such that

$$x_1 = x_0 + c\left(\rho\left(x_0, 0\right)\right) t_1. \tag{41}$$

Solving Eq. 41 implies solving an implicit (and in general nonlinear) equation in order to find x_0 . Once we know x_0 ,

$$\rho(x_1, t_1) = \rho(x_0, 0) = f(x_0), \qquad (42)$$



Figure 4: The solution of the simplest kinematic wave equation is a fixed function translated along the *x*-axis with constant speed.

since the value of ρ is constant along the characteristic. It is only possible to write the solution in explicit form in simple cases. Let us, as very a simple example, consider the equation

$$\frac{\partial \rho}{\partial t} + \frac{\partial \rho}{\partial x} = 0. \tag{43}$$

Here, $c(\rho) \equiv 1$ so that the characteristics are the lines in (x, t)-plane defined by $x = x_0 + t$. Thus, we get $\rho(x, t) = \rho(x_0, 0) = f(x_0) = f(x - t)$. The variation in the density at t = 0 thus moves without changing the shape towards the right with speed 1 as illustrated in Fig. 4.

2.5.1 The Riemann Problem

Let us again consider the 1D conservation law in integral form,

$$\frac{d}{dt}\int_{a}^{b}\rho\left(x,t\right)dx+j\left(\rho\left(b,t\right)\right)-j\left(\rho\left(a,t\right)\right)=0,$$
(44)

with the differential formulation

$$\frac{\partial \rho}{\partial t} + c\left(\rho\right)\frac{\partial \rho}{\partial x} = 0, \ c\left(\rho\right) = \frac{dj}{d\rho}.$$
(45)

For this conservation law, there are three basic solutions that typically arise, and even if we can find this in most textbooks about Partial Differential Equations, e.g. the book of Whitham [18], we shall for completeness list them here as well. The three cases are solutions to the so-called *Riemann problem*, where we want to determine $\rho(x, t)$ for $-\infty < x < \infty$ and $0 \le t$ when

$$\rho(x,0) = \begin{cases} \rho_1, & x < 0\\ \rho_2, & x > 0 \end{cases}, \ \rho_1 \neq \rho_2.$$
(46)

The characteristics starting at x_0 on the x-axis, in this case, are given by

$$x = x_0 + c(\rho_1)t, \quad x_0 < 0,$$

$$x = x_0 + c(\rho_2)t, \quad x_0 > 0.$$
(47)



Figure 5: Contact discontinuity: The characteristics are parallel.

2.5.2 Contact Discontinuity

If we has $c(\rho_2) = c(\rho_1)$, the characteristics will be parallel for both positive and negative x_0 . The region $-\infty < x < \infty$, $0 \le t$, is now divided into two parts, I and II (see Fig. 5) where the solution ρ to the differential equation are, respectively, ρ_1 and ρ_2 . The solution is called a *contact discontinuity*, since it is discontinuous along the contact of the two parts, i.e. the line $x = c(\rho_1)t = c(\rho_2)t$. Somewhat surprising, this solution does *not* need to be an acceptable solution for the conservation law. We shall see below that the conservation law is only satisfied if, in addition,

$$(\rho_1 - \rho_2) c (\rho_1) + j (\rho_2) - j (\rho_1) = 0$$
(48)

and this does not need be the case even if $c(\rho_1) = j'(\rho_2) = c(\rho_2)$. If this extra condition

is not met, the solution of the conservation law develops in a more complicated way. The basic situation is however when the condition is fulfilled.

2.5.3 Rarefaction Wave

If $c(\rho_1) < c(\rho_2)$, the characteristics that start outside the origin have to go as shown in Fig. 6. The solution in regions I and III are thus ρ_1 and ρ_2 , respectively.

If, $c(\rho)$ is monotonically increasing when ρ goes from ρ_1 to ρ_2 , the solution in region II becomes what is called an elementary rarefaction wave, expansion wave, or expansion fan. Here, all characteristics have to start at the origin. Therefore, the characteristics have all the equation $x = c(\rho) t$, and consequently, the solution for a point (x, t) in region II is given implicitly by

$$\rho(x,t) = c^{-1}(x/t) \tag{49}$$

(The inverse function c^{-1} exists under the above assumption of monotonicity). We leave to the reader to show that this solution really fulfil the conservation law.

Consider the following simple example where $c(\rho) = \rho$, and $\rho_1 = 0$ $\rho_2 = 1$. Then the characteristics for $x_0 < 0$ is simply $x = x_0$, whereas $x = x_0$ for $x_0 > 0$ 0 In region II defined



Figure 6: The rarefaction wave.



Figure 7: The situation when $c(\rho_1) > c(\rho_2)$ requires the introduction of a shock.

by $\{(x,t); 0 < x < t\}$ the solution is given by $x = \rho t$, i.e. $\rho = x/t$. Thus, the solution for t > 0 becomes

$$\rho(x,t) = \left\{ \begin{array}{ll}
1, & x < 0, \\
x/t, & 0 \le x \le t, \\
0, & t < x.
\end{array} \right\}$$
(50)

Try some other possibilities for $c(\rho)$ and make sketches to see how things come out!

2.5.4 Shock Solution

If we have the reverse situation from above, namely that $c(\rho_1) > c(\rho_2)$, the characteristics will cross, as illustrated in Fig. 7 to the left. Although the solution outside the collision area can be found using the characteristic method, this is of little help in the area where the characteristics crosses. In order to resolve the situation, we have to go back to the original conservation law and introduce a *discontinuity*, x = s(t), called a *shock*, as illustrated in Fig. 7 to the right.

In order to determine the speed U = ds/dt of the shock, we consider interval [a, b] such that it includes discontinuity. By calculating the change of the contents in [a, b], as outlined



Figure 8: A control volume enclosing a discontinuity in the density. The change in the content during a time interval Δt is $(\rho_2 - \rho_1) U \Delta t$.

in Fig.8, we obtain

$$\frac{d}{dt} \int_{a}^{b} \rho\left(x,t\right) dt = \lim_{\Delta t \to 0} \frac{-\left(\rho_{2} - \rho_{1}\right) \times U\Delta t}{\Delta t} = \left(\rho_{1} - \rho_{2}\right) U.$$
(51)

The conservation law will now only be satisfied if

$$\frac{d}{dt} \int_{a}^{b} \rho(x,t) \, dx + j\rho(b,t) - j\left(\rho(a,t)\right) = (\rho_{1} - \rho_{2}) \, U + j\left(\rho_{2}\right) - j\left(\rho_{1}\right) = 0.$$
(52)

(recall the situation for the contact discontinuity). Thus we derive that the shock speed must be

$$U = \frac{j(\rho_2) - j(\rho_1)}{\rho_2 - \rho_1},$$
(53)

and the solution for t > 0 is thus

$$\rho\left(x,t\right) = \left\{\begin{array}{l}
\rho_{1}, \quad x < Ut\\
\rho_{2}, \quad x > Ut\end{array}\right\}$$
(54)

We shall finally show a simple example where the same differential equation may come from different conservation laws. Let the density and the flux depend of another function u such that

$$\rho(x,t) = \frac{1}{n} u(x,t)^{n}$$

$$j(x,t) = \frac{1}{n+1} u(x,t)^{n+1}$$
(55)

The differential formulation follows the conservation law $\frac{\partial \rho}{\partial t} + \frac{\partial j}{\partial x} = 0$, leading to

$$\frac{\partial \rho}{\partial t} + \frac{\partial j}{\partial x} = u^{n-1} \frac{\partial u}{\partial t} + u^n \frac{\partial u}{\partial x} = u^{n-1} \left(\frac{\partial u}{\partial t} + u \frac{\partial u}{\partial x} \right) = 0.$$
(56)

The differential equation for u is therefore essentially the same regardless the value of n we had the conservation law. The characteristics are the same in all cases, but the shock speeds are different for different n-s:

$$U = \frac{n}{n+1} \frac{u_2^{n+1} - u_1^{n+1}}{u_2^n - u_1^n}$$
(57)

The example shows that if the solutions develop shocks, the shock can *not* be found from the differential equation alone. The position of the shock must be determined from the original conservation laws. In some cases it is also necessary to bring in additional conditions in order to determine a physically acceptable solution (This is more thoroughly covered in courses in non-linear partial differential equations).

3 MODELING OF ROAD TRAFFIC

Systematic studies of road traffic started about 70 years ago in the homeland of the cars, USA. During the 1950s also mathematicians began to get stuck in rush hour traffic, and more theoretical work appears in mathematical journals. An article by M. J. Lighthill and G.B. Whitham in the Proceedings of the Royal Society entitled "On kinematic waves II. A theory of traffic flow on long, crowded roads" from 1955 is one of the milestones in the development. Mathematical modeling of road traffic is a relatively wide field, and there is much information on the Internet and in several textbooks.

The present material has been based on lectures and seminars in mathematical modeling at NTNU over several years. The report published by US Transportation Research Board, *Traffic Flow Theory* is, as of this writing, available free of charge from the Internet [7].

Research claims that between 20–30 percent of traffic jams on Norwegian roads would disappear if each motorist is driving more efficiently. Researchers at NTNU have in controlled trials managed to double the flux from 1800 to 3600 vehicles per hour just by adjusting the drivers' behavior. Interestingly enough, it appears that sometimes the flux of cars may be larger when the traffic is kept at 60km/h, compared to 90km/h. On the ringroad around London, M25, the speed limits are constantly adjusted in order to optimize the traffic flow.

Traffic modeling can be approached from many sides and applying many different mathematical and statistical tools. It is reasonable to think of models based of individual vehicles on a road where the speed is expressed as a function of road conditions and other vehicles nearby. The models may contain stochastic elements such as variations in the drivers' perception of what is a *safe speed*, a *safe distance to the vehicle in front*, and an *acceptable overtaking margin*. Such models quickly become analytically complicated, but are suitable for computer simulations. Queuing theory and other statistical models that describe the randomness of real traffic, are also widely used.

The article of Lighthill and Whitham suggests a continuum model for car traffic. Traffic flow is described in terms of density, flux, sources and sinks, which consequently leads to hyperbolic conservation laws. This theory is called the *kinematic theory* of road traffic. The models can be refined by including the drivers' ability to respond to changes in traffic density, and how quickly they can adjust according to road conditions. The material below is mainly taken from the books of Whitham and Haberman stated in the reference list.

3.1 Kinematic Theory

In kinematic traffic theory, traffic is modeled by means of a simple conservation law. The density $\rho(x,t)$ of cars on the road is expressed as the number of cars per unit length. The term must of be considered somewhat pragmatic, as is often the case when we model a collection of highly discrete objects as a continuous medium. We consider ρ as a piecewise continuous function of position and time. Because of the car's finite size, it is reasonable to assume that

$$0 \le \rho \le \rho_{\max},\tag{58}$$

where ρ_{max} is the maximum density as calculated from the cars' average length.

The car velocity v is assumed to be a function of car density, $v(\rho)$, so that $v(0) = v_{\text{max}}$ and $v(\rho_{\text{max}}) = 0$. Thus, v decreases as ρ increases. A clear-cut relation between the cars' velocity and density may only be reasonable on one-lane roads, but is also used for multilane highways, where the car velocities vary both individually and from lane to lane. In this case, one interprets v as the average speed, and measurements indicate this is a reasonable assumption, at least for parts of the interval between 0 and ρ_{max} .

If we assume that the speed of the cars is a function of ρ , $v(\rho)$, a small argument gives us that the flux of cars, *i.e.* the number of cars passing a given point on the road per time unit, can be expressed as

$$J = \rho v(\rho). \tag{59}$$

In the traffic literature flux is often designated with the symbols k, or F, and the graph of J as a function of ρ is called the *fundamental diagram*. Normally, $J(\rho)$ tends to 0 when ρ approaches 0 or ρ_{max} , and is a concave function with a maximum value somewhere between 0 and ρ_{max} . The conservation law becomes as before

$$\frac{d}{dt} \int_{a}^{b} \rho(x,t) dx + J(b,t) - J(a,t) = \int_{a}^{b} q(x,t) dx,$$
(60)

where the source term expresses cars entering or leaving the road. The differential formulation leads to a first order hyperbolic equation, and since J is only a function of ρ , we can write the equation

$$\frac{\partial \rho}{\partial t} + \frac{\partial J}{\partial x} = \frac{\partial \rho}{\partial t} + \frac{dJ}{d\rho} \frac{\partial \rho}{\partial x} = q.$$
(61)

If q = 0, the characteristics will be straight lines with slope (kinematic velocity) equal to $c(\rho) = \frac{dJ}{d\rho}$.

By applying the equations 60 and 61, we can examine what is happening around a traffic light crossing, when we have a varying density of traffic, how the individual cars are moving, etc. The car's own motion is determined by differential equation

$$\frac{dx}{dt} = v(\rho(x,t)). \tag{62}$$



Figure 9: Speed, flux and kinematic velocity as a function of car density for the standard model.

Usually, $c(\rho)$ will be a decreasing function of ρ . This will typically lead to situations developing shocks if the traffic is moving in the positive x-direction and ρ increases with x. From the conservation law, a shock x = s(t) will have to satisfy

$$\frac{ds}{dt} = \frac{J(s+,t) - J(s-,t)}{\rho(s+,t) - \rho(s-,t)},$$
(63)

Changes in traffic conditions can be incorporated in several ways. If the road has a narrowing, e.g., goes from two to one lane, it is reasonable that ρ_{\max} is reduced, whereas v_{\max} remains the same. This changes the fundamental diagram. At the start of the narrowing, the flux has to be continuous, whereas ρ will have a discontinuity.

If the road is slippery and the visibility is poor due to rain or fog, then v_{max} will decrease whereas ρ_{max} remains unchanged. This changes the fundamental diagram in a different way.

A very common kinematic model that is reasonably easy to work with analytically, is to assume that v is a decreasing, linear function of ρ . After scaling, we obtain the equations

$$v(\rho) = 1 - \rho,$$

$$J(\rho) = \rho(1 - \rho),$$

$$c(\rho) = 1 - 2\rho,$$

$$\frac{\partial \rho}{\partial t} + (1 - 2\rho) \frac{\partial \rho}{\partial x} = 0.$$
(64)

Fig. 9 shows how the car velocity, the flux and the kinematic velocity change for the this model. Note that $c(\rho) = \frac{d}{d\rho}(\rho v) = v + \rho v'(\rho)$, and therefore $c(\rho) \neq v(\rho)$ when $\rho \neq 0$. Below we shall use this model to analyze some simple situations.

3.1.1 Traffic Lights

Assume that at x = 0, there has a been a red light for the cars for t < 0. To the left of the light (x < 0), there is a dense queue of cars, $\rho = 1$, while at the the right (x > 0), there are



Figure 10: Junction at x = 0, where the light changes from red to green.

no cars and $\rho = 0$. In all such problems, it is useful to outline a so-called x/t-chart that describes the conditions, in particular how the characteristics behave, as shown in Fig. 10. When t > 0, we have three regions. To the left is an area where $\rho = 1$, to the right a region where $\rho = 0$, while in the middle there is an expansion wave with characteristics starting at the origin,

$$x = c(\rho)t = (1 - 2\rho)t.$$
(65)

Within the central area $\rho = \frac{1}{2} \left(1 - \frac{x}{t}\right)$, and the complete solution becomes for $t = t_0$

$$\rho(x, t_0) = \begin{cases}
1, & x \le t_0, \\
\frac{1}{2} \left(1 - \frac{x}{t_0} \right) & -t_0 < x < t_0, \\
0 & x \ge t_0.
\end{cases}$$
(66)

Suppose you are sitting in a car at x = -1 for t = 0. What will be your own motion for t > 0? From Fig. 10 we observe that you will start to drive at t = 1, and then your own path, y(t), will be controlled by the differential equation

$$\frac{dy}{dt} = v(\rho) = 1 - \frac{1}{2} \left(1 - \frac{y}{t} \right)
= \frac{1}{2} \left(1 + \frac{y}{t} \right), \quad y(1) = -1.$$
(67)

The equation is thus $2t\dot{y} - y = t$, with general solution $y(t) = At^{1/2} + t$. Since y(1) = -1, $y(t) = t - 2t^{1/2}$. It is worth noting that the distance to the front car at x = t becomes greater as time passes.

The situation we have analyzed, resembles what you encounter in a big running event: if you have ambitions of fighting in the lead, it pays to have a position as close as possible to the head of the queue before the start.



Figure 11: The situation with an increase in the car density.

3.1.2 Traffic Clogging Up

Assume that there is a line of traffic on the road where the density at t = 0 has the form

$$\rho(x,0) = \begin{cases}
\rho_1, & x \le a, \\
\rho_1 + \frac{x-a}{b-a}(\rho_2 - \rho_1) & a < x < b, \\
\rho_2 & b \le x.
\end{cases}$$
(68)

where $\rho_1 < \rho_2$. Between x = a and x = b, the car density increases linearly from ρ_1 to ρ_2 . The characteristics are given by $x = x_0 + (1 - 2\rho)t$, and for characteristics between a and b this amounts to

$$x = x_0 + t - 2\left(\rho_1 + \frac{x_0 - a}{b - a}\left(\rho_2 - \rho_1\right)\right)t$$

= $x_0 + (1 - 2\rho_1)t - 2\frac{x_0 - a}{b - a}\left(\rho_2 - \rho_1\right)t.$ (69)

By inserting the time $t_s = \frac{1}{2} \frac{b-a}{\rho_2 - \rho_1}$, we see that x_0 vanishes. This means that all characteristics starting from the interval [a, b] meet in the point (x_s, t_s) ,

$$x_s = a + (1 - 2\rho_1) \frac{1}{2} \frac{b - a}{\rho_2 - \rho_1} = b + (1 - 2\rho_2) \frac{1}{2} \frac{b - a}{\rho_2 - \rho_1}.$$
 (70)

The situation is sketched in Fig. 11.

For $t > t_s$, we get a jump in density, a *shock*. The speed of the shock, has to be determined from the shock condition, as discussed above,

$$U = \frac{J(\rho_2) - J(\rho_1)}{\rho_2 - \rho_1}$$

= $\frac{\rho_2 (1 - \rho_2) - \rho_1 (1 - \rho_1)}{\rho_2 - \rho_1}$
= $1 - \rho_1 - \rho_2.$ (71)

Region	ρ	$v\left(ho ight)$	$J\left(ho ight)$	$c\left(ho ight)$
x < 1	$[0 \ 1]$	$1-\rho$	$\rho\left(1-\rho\right)$	$1-2\rho$
x > 1	$\begin{bmatrix} 0 \ \frac{1}{2} \end{bmatrix}$	$1-2\rho$	$\rho \left(1 - 2\rho \right)$	$1-4\rho$

Table 1: The conditions surrounding a narrowing of the road..

One may wonder what is happening around such a shock, and in practice, the cars will try to avoid colliding. However, when driving through the shock, the car velocity has a discontinuity, and it is limited how fast it is possible to react!

3.1.3 When is the First Shock Formed?

The shock is formed when two characteristics collide. Let us look at two characteristics starting at x_0 and $x_0 + \Delta t$, respectively, and meeting at (x_s, t_s) :

$$x_0 + c(x_0)t_s = x_0 + \Delta t + c(x_0 + \Delta t)t_s.$$
(72)

Thus,

$$t_{s} = -\frac{1}{(c(x_{0} + \Delta t) - c(x_{0}))/\Delta t}.$$
(73)

If we let $\Delta t \to 0$, the limit is

$$t_s = -\frac{1}{\frac{dc}{dx}\Big|_{x_0}}.$$

For a shock to form for t > 0, there has to be some x_0 where $\frac{dc}{dx}\Big|_{x_0} < 0$, and the first time this happens is

$$\min t_s = -\frac{1}{\min_x \frac{dc}{dx}}.$$
(74)

3.1.4 Narrowing the Road

On a road with two lanes for x < 1, one of the lanes is closed for x > 1, so that the maximum car density for x > 1 is only half of the original. Table 1 shows how the flux varies with the density of each of the two parts of the road. There is no storage for cars at x = 1. Therefore, the flux around x = 1 must be continuous,

$$J(\rho(1-,t)) = J(\rho(1+,t)).$$
(75)

This means that the density is discontinuous (if different from 0). If the number of vehicles passing x = 1 is as large as possible, the flux is J = 1/8, and densities immediately to the left and right of x = 1 are given by

$$J(\rho^{-}) = \rho^{-}(1-\rho^{-}) = J(\rho^{+}) = \rho^{+}(1-2\rho^{+}).$$
(76)

Thus,

$$\rho^+ = 1/4, \tag{77}$$



Figure 12: Narrowing of the road after a traffic light.

whereas there are two possibilities for ρ^- :

$$\rho^{-} = \frac{1}{2} \left(1 \pm \frac{\sqrt{2}}{2} \right). \tag{78}$$

To see how both possibilities can occur, we connect this situation with a traffic light at x = 0, as in the first example. The situation is illustrated in Fig. 12.

We get a shock at x = 1 until the density ρ on the left side reaches the value $\rho_1^- = \frac{1}{2} (1 - 2^{-1/2})$. Then we get a sudden jump in the density up to $\rho_2^- = \frac{1}{2} (1 + 2^{-1/2})$. Before the narrowing, we get a queue where the density is ρ_2^- . At the end of this queue another shock is formed. We leave it to readers to consider how it is to drive through such a situation.

3.1.5 Research Project: A Green Wave in Infinity Street?

In a long straight street the pedestrian crossings are organizes\d with traffic lights. If the traffic lights are uncoordinated, the cars will need to drive and stop at uneven interval, and the resulting average flux of cars may be quite low. However, sometimes we hear that it is possible arrange the lights in a so-called green wave, so that the cars may "surf" through the street without having to stop. Is it really possible to streamline the traffic by using

the green waves, and what is the maximum possible average flux? In this study we will consider an idealized situation of this problem.

At Infinity Street pedestrian crossings are located at a constant distance L. There are no side streets with opportunities for for the cars to leave or enter the street. The crossings have all traffic lights with a cycle of length S. This means that it is *red* in the period $[0, r^*)$, then it is green in the period $[r^*, S]$. The cycle repeats itself continuously. To facilitate the driving, the light cycles may be displaced in time in relation to each other, so that cycle of crossing k + 1 starts some time before or after the cycle of crossing k. The maximum vehicles density is ρ_{max} , and the velocity is v_{max} . Traffic follows the simple kinematic model considered above. By scaling x and ρ the usual way, and using the time scale L/v_{max} we obtain Eq. 64.

The length of the red period is denoted r and green period g. Here r = 1 correspond to the shortest time it takes to drive between two traffic lights separated by a length 1, and the cycle length is r + g. The traffic goes around the clock, and the problem is to maximize the average flux, \overline{J} . If the red period starts in x = 0 at t = 0, the average flux will be

$$\bar{J} = \frac{1}{r+g} \int_0^{r+g} J(0,t) dt = \frac{1}{r+g} \int_r^{r+g} \rho(0,t) [1-\rho(0,t)] dt.$$
(79)

It is clear that the theoretical maximum average flux will be

$$\bar{J}_{\max} = \frac{g}{r+g} J_{\max} = \frac{g}{r+g} \frac{1}{4},\tag{80}$$

since the maximum number of cars passes the crossing during the green period, and anything better than that is impossible.

We shall first analyze a simpler situation with one traffic light. Until time t = -g there has been red light at x = 0. To the left of x = 0 there is a queue of cars. The light is green up to t = 0, where it again changes to red. From the point (0, -g) there is now an expansion wave which collides with the shock from (0, 0) in both positive and negative x-directions, as shown in Fig. 13. The shock speed in this case is

$$U = \frac{J_2 - J_1}{\rho_2 - \rho_1} = 1 - (\rho_1 + \rho_2).$$
(81)

The density of the two characteristics that are symmetrical about the *t*-axis are $\rho^- = \frac{1}{2} - \rho$ and $\rho^+ = \frac{1}{2} + \sigma$, respectively. Thus, the two shock speeds the same with the opposite sign:

$$U^{+} = 1 - (0 + \frac{1}{2} - \sigma) = \frac{1}{2} + \sigma,$$

$$U^{-} = 1 - (1 + \frac{1}{2} + \sigma) = -\left(\frac{1}{2} + \sigma\right).$$
(82)

Consequently, the two shock curves are also symmetrical about the origin. We can calculate



Figure 13: The expansion wave from (0, -g) collides with the shocks that start at t = 0. The characteristics in the regions where $\rho = 0$ and 1 have speed 1 and -1, respectively.

the shock curve x_c from

$$\frac{dx_s}{dt} = U^+(x_s, t) = 1 - \rho^+
= 1 - c^{-1} \left(\frac{x_s}{t+g}\right)
= 1 - \frac{1}{2} \left(1 - \frac{x_s}{t+g}\right),$$
(83)

or

$$2(t+g)\dot{x}_s = (t+g) + x_s.$$
(84)

The solution is

$$x_s(t) = t + g - g^{1/2}(t+g)^{1/2}.$$
(85)

The shocks follow this curve until they meet the characteristics that have started in t = r, in other words, immediately after the red period from t = 0 to r is over. The areas with $\rho = 0$ and $\rho = 1$ are therefore also *symmetric* about the y-axis.

Let us now look at a situation where the red period from x = 0 has lasted so long that the areas in Fig. 13 reaches out to $x = \pm \frac{1}{2}$. We find out where $(\pm \frac{1}{2}, t_0)$ is by observing that

$$\frac{1}{2} = 0 + c(0)(t_0 - r),$$

that is,

$$t_0 = r + \frac{1}{2} \frac{1}{c(\rho = 0)} = r + \frac{1}{2}.$$
(86)



Figure 14: Sketch of the complete solution. Note that we get a stationary shock at x = 1/2.

Then we put this into the equation for the shock:

$$\frac{1}{2} = (t_0 + g) - g^{1/2} (t_0 + g)^{1/2}$$
$$= \left((r + \frac{1}{2}) + g \right) - g^{1/2} \left((r + \frac{1}{2}) + g \right)^{1/2},$$
(87)

or

$$g = \frac{r^2}{\frac{1}{2} - r}.$$
 (88)

The solution requires that r < 1/2, and otherwise that g = r for r = 1/4. For these combinations of g and r, we can now construct complete solutions for *Infinity Street* that for any given ratio $r/g \in \mathbb{R}^+$ provide maximum throughput. The construction is best described on a figure, see Fig. 14. Note that we have got a motionless shock for half integers (the shock speed is 0, since the sum of the densities on both sides is 1 at any time). If we want r/g to be large, this gives very short cycles. Even the maximum red period, r = 1/2, which corresponds to the time it takes to cover half the distance between two traffic lights at maximum speed, seems to be rather short for practical purposes.

It appears that the symmetric structure may be generalized:

• At shorter distances between the crossings, the "leaves" are cut and meet in the middle.



Figure 15: Is this a possible solution?

• For larger distances the "leaves" are extended with two shocks that also meet in the middle.

Is it possible to have a solution that is looking like the one in Fig. 15?

3.2 Generalizations of the Kinetic Theory

In practice, drivers try to compensate for changes in traffic density by adjusting the speed according to surrounding conditions. To avoid the development of shocks and thus extremely rapid changes in density, they will tend to slow down somewhat more than the relationship $v = v(\rho)$ suggests, and therefore avoid strong gradients in density build up. Whitham models this by assuming that the drivers adjust the speed as

$$v = v_k(\rho) - \kappa \frac{\partial \rho / \partial x}{\rho},\tag{89}$$

where v_k is the speed according to the kinematic theory above. This seems to be a reasonable model since $v = v_k(\rho)$ if ρ is constant, whereas v is less than v_k if ρ increases in the driving direction, and the opposite when ρ decreases. The best part of the model, and probably the reason why Whitham selected the particular form in Eq. 89, is that it leads to a famous 2nd order parabolic equation for ρ , since $J = \rho v = \rho v_k(\rho) - \kappa \rho_x$:

$$\frac{\partial \rho}{\partial t} + c(\rho)\frac{\partial \rho}{\partial x} - \kappa \frac{\partial^2 \rho}{\partial x^2} = 0, \ c(\rho) = \frac{d(\rho v_k)}{d\rho}.$$
(90)

For the special case where $c(\rho) = 1 - 2\rho$ we may use c instead of ρ as the dependent variable, leading to the equation

$$\frac{\partial c}{\partial t} + c \frac{\partial c}{\partial x} - \kappa \frac{\partial^2 c}{\partial x^2} = 0, \qquad (91)$$

called *Burgers Equation*. Burgers equation is one of the most studied non-linear partial differential equations and is extensively described in, e.g. [18], Ch. 4.

It turns out that Burgers equation has solutions in the form of "migrating fronts":

$$c(x,t) = C(x - x_0 - at) = C(s), \ s = x - x_0 - at.$$
$$\lim_{s \to -\infty} C(s) = c_1, \ \lim_{s \to \infty} C(s) = c_2.$$
(92)

The front thus has a constant value on the curves $x = x_1 + at$, and well-defined limits as x tend to $\pm \infty$. We find such a solution by entering C in the equation:

$$-aC' + CC' - \kappa C'' = 0. (93)$$

By one integration we obtain

$$(C-a)^2 = 2\kappa C' + A, (94)$$

where A is another integration constant. Since we expect that also the derivative goes to 0 when $x \to \pm \infty$, we see that

$$a = \frac{c_1 + c_2}{2},$$

$$A = \left(\frac{c_1 - c_2}{2}\right)^2.$$
(95)

We now insert this and separate the variables:

$$-\frac{ds}{2\kappa} = \frac{dC}{\left(\frac{c_2-c_1}{2}\right)^2 - (C-a)^2}.$$
(96)

This gives

$$-\frac{s-s_0}{2\kappa} = \frac{2}{c_2 - c_1} \operatorname{arctanh} \left(2\frac{C-a}{c_2 - c_1} \right),$$
(97)

which may be turned around to

$$C(s) = \frac{c_1 + c_2}{2} - \frac{c_2 - c_1}{2} \tanh\left(\frac{c_2 - c_1}{4\kappa}(s - s_0)\right)$$
$$= c_1 + (c_2 - c_1) \left[1 + \exp\left(\frac{c_2 - c_1}{2\kappa}(s - s_0)\right)\right]^{-1}.$$
(98)

The function is a sigmoid (recall the equation for logistic growth). If $c_2 < c_1$, then C(s) is a monotone decreasing front moving at velocity

$$U = a = \frac{c_1 + c_2}{2} \tag{99}$$

from to left to right. Note that since $c = 1 - 2\rho$ in this model, $\rho(x, t)$ will be a monotone *increasing* front moving with the same velocity. Moreover,

$$\lim_{x \to -\infty} \rho(x, t) = \rho_1 = \frac{1 - c_1}{2},$$

$$\lim_{x \to \infty} \rho(x, t) = \rho_2 = \frac{1 - c_2}{2},$$

$$U = \frac{c_1 + c_2}{2} = 1 - (\rho_1 + \rho_2).$$
(100)

The transition between $\rho = \rho_1$ and $\rho = \rho_2$ becomes sharper the smaller κ is, but U is independent of κ . We see further that U is just the shock speed for the equation

$$\rho_t + \rho \rho_x = 0 \tag{101}$$

for the initial conditions $\rho(x,0) = \rho_1$ for x < 0, and $\rho(x,0) = \rho_2$ for x > 0, and $\rho_1 < \rho_2$. The behaviour in the limit $\kappa \to 0$ is therefore reasonable.

Whitham take the theory a step further by studying what happens when the cars need some time to adjust to the proper speed. A driver has some finite reaction time. If we look at the speed of a particular car, v_B , in a situation where traffic density changes, the car velocity could probably follow the equation

$$\frac{dv_B}{dt} = \frac{1}{\tau} \left(V - v_B \right),\tag{102}$$

where V is the ideal speed of the drivers wants to follow, as given by Eq. 102. This is a well-known equation from control theory. If $v_B = v_0$ at time t = 0 and V is a given function of t from 0 to t, it is possible to express v_B as

$$v_B(t) = v_0 e^{-t/\tau} + \int_0^t \exp(\frac{t'-t}{\tau}) V(t') dt'.$$
 (103)

If $V = V_0$ is constant for t > 0, the solution becomes

$$v_B(t) = (v_0 - V_0)e^{-t/\tau} + V_0.$$
(104)

The effect of the initial value will die out with time constant τ , and if V varies slowly (that is, the time scale for variations in V is longer than τ), v_B will tend to follow V.

We want to formulate Eq. 102 for the velocity v as a function of both t and x. The car follows a path x(t), so that $v_B(t) = v(x(t), t)$. This requires what in mechanics is called the convective derivative,

$$\frac{dv_B}{dt} = \frac{d}{dt}v(x(t), t)
= \frac{\partial v}{\partial x}\frac{dx}{dt} + \frac{\partial v}{\partial t}
= \frac{\partial v}{\partial x}v + \frac{\partial v}{\partial t}.$$
(105)

Altogether, this gives two coupled equations for the motion

$$\frac{\partial \rho}{\partial t} + \frac{\partial (\rho v)}{\partial x} = 0,$$

$$\frac{\partial v}{\partial t} + v \frac{\partial v}{\partial x} = \frac{1}{\tau} \left(\left(v_k(\rho) - \kappa \frac{\partial \rho / \partial x}{\rho} \right) - v \right).$$
(106)

The equations are called a *hyperbolic system*, and we shall not go into the solution them in full detail, but we see immediately that the system has *equilibrium solutions*:

$$\rho = \rho_0,$$

$$v_0 = v_k(\rho_0).$$
(107)

The way of investigating whether the equilibria are stable or unstable is to write

$$\rho = \rho_0 + r,
v = v_0 + w,$$
(108)

where r(x,t) and w(x,t) are small perturbations. After some arithmetic, we arrive at the following system of equations, where we have inserted $c_0 = \frac{d}{d\rho}(v_k\rho)|_{\rho=\rho_0} = v'_k(\rho_0)\rho_0 + v_0$:

$$r_t + v_0 r_x + \rho_0 w_x = 0,$$

$$w_t + v_0 w_x = -\frac{1}{\tau} \left(w - \frac{c_0 - v_0}{\rho_0} r + \frac{\kappa}{\rho_0} r_x \right).$$
(109)

The equations may be combined into a single linear 2nd order equation containing only r:

$$r_t + c_0 r_x = \kappa r_{xx} - \tau \left(\frac{\partial}{\partial t} + v_0 \frac{\partial}{\partial x}\right)^2 r.$$
(110)

We may recognize the first part,

$$r_t + c_0 r_x = \kappa r_{xx},$$

as a linear convection/diffusion equation, which is known to have solutions quickly dying out with time. However, the last term, $-\tau \left(\frac{\partial}{\partial t} + v_0 \frac{\partial}{\partial x}\right)^2 r$, may create problems for us if it "dominates" over the diffusion term κr_{xx} . The standard method for studying such linear equations is to examine *Fourier components*:

$$r(x,t) = ae^{i(kx-\omega t)}.$$
(111)

The Fourier component is a travelling wave with wave number k and frequency ω . If this is inserted into the equation, we get a so-called *dispersion relation* linking k and ω :

$$\tau(\omega - v_0 k)^2 + i(\omega - c_0 k) - \kappa k^2 = 0.$$
(112)

Since the wave number $k = 2\pi/\lambda$, where λ is the wave length, k is a real number. On the other hand, the frequency will generally be complex. Moreover, since

$$ae^{i(kx-\omega t)} = ae^{(\operatorname{Im}\omega)t}e^{i(kx-(\operatorname{Re}\omega)t)},\tag{113}$$

we see that if the imaginary part of ω is greater than 0, the amplitude of the Fourier component will grow exponentially in time, while is decreases exponentially if $\operatorname{Im} \omega < 0$. It is possible to show that

$$\operatorname{Im} \sqrt{\frac{\kappa}{\tau}} < c_0 < v_0 + \sqrt{\frac{\kappa}{\tau}}.$$
(114)

This tells us that v_0 and c_0 can not be too different. For all Fourier components to die out we must have

$$|v_0 - c_0| < \sqrt{\frac{\kappa}{\tau}}.\tag{115}$$

If we introduce $v_k(\rho) = 1 - \rho$, we see that $v_0 = 1 - \rho_0$ and $c_0 = 1 - 2\rho_0$ (in dimensionless variables). Therefore, the perturbations above die out only when

$$\rho < \sqrt{\frac{\kappa}{\tau}}.\tag{116}$$

This result, which does not seem to be mentioned in Whitham, is interesting in the light of observations that have been reported. The traffic seems to follow a fundamental diagram from $\rho = 0$ and up to a certain ρ_c which is considerably less than ρ_{max} . For larger densities the well-defined behaviour breaks down, and J are significantly smaller than the fundamental diagram would indicate. It could therefore be interesting to know whether this is due to instabilities of the type we found here, but the problem is to find realistic numerical values to insert for τ and κ .

3.3 Individual Car Models

The theory in this section is mostly obtained from the book by Haberman, Sec. 64 [9].

Individual car models deal with individual cars on the road. With one lane, and no possibility of passing, we can assume that each car adjusts its own speed relative to the speed of the car ahead (assuming it is so close that the driver can see it). Let us denote the position of the vehicle No. n in the queue by $x_n(t)$.

$$\frac{d^2x_n}{dt^2} = -\lambda \left(\frac{dx_n}{dt} - \frac{dx_{n-1}}{dt}\right).$$
(117)

If car number n has higher speed than the vehicle in front (number n - 1), car number n will brake. Actually, there will be some delay in the reaction of drivers, so we should write

$$\frac{d^2x_n(t+T)}{dt^2} = -\lambda \left(\frac{dx_n(t)}{dt} - \frac{dx_{n-1}(t)}{dt}\right),\tag{118}$$

where T expresses the drivers' response time. The equation may be integrated once:

$$\frac{dx_n(t+T)}{dt} = -\lambda \left(x_n(t) - x_{n-1}(t) \right) + d_n.$$
(119)

In a uniform situation where all cars have the same speed and same distance, the density will be

$$\rho = \frac{1}{x_{n-1} - x_n}.$$
(120)

In that case, the cars' velocity is thus

$$v = \frac{dx_n}{dt} = -\frac{\lambda}{-\rho} + d. \tag{121}$$

The constant d is chosen so that v = 0 for $\rho = \rho_{\text{max}}$, and this leads to the following expression for v and the flux J:

$$v = \lambda \left(\frac{1}{\rho} - \frac{1}{\rho_{\max}}\right),\tag{122}$$

$$J = v\rho = \lambda\rho \left(\frac{1}{\rho} - \frac{1}{\rho_{\max}}\right).$$
(123)

The model is called the *California model*. The model is not very realistic for small densities since $v \to \infty$ when $\rho \to 0$. If there are very few cars on the road, where will be no car in sight most of the time, and then it is reasonable to move at maximum speed. A modified model would be to set

$$v = \min\left(v_{\max}, \lambda\left(\frac{1}{\rho} - \frac{1}{\rho_{\max}}\right)\right).$$
(124)

It is also possible to embed the drivers sensitivity for changes by assuming that λ varies with the distance to the car in front. We could for example assume that

$$\lambda = \frac{a}{x_{n-1} - x_n}$$

which means that the sensitivity disappears when the distance is great. The Eq. (117) then modifies to

$$\frac{d^2x_n}{dt^2} = -\frac{a}{x_{n-1} - x_n} \left(\frac{dx_n}{dt} - \frac{dx_{n-1}}{dt}\right),$$

which can still be integrated analytically to

$$\frac{dx_n(t+T)}{dt} = -a\ln|x_n(t) - x_{n-1}(t)| + d_n.$$
(125)

A similar argument to the above then yields

$$v = a \ln \frac{\rho_{\max}}{\rho},\tag{126}$$

$$J = \rho a \ln \frac{\rho_{\max}}{\rho}.$$
 (127)

This still causes $v \to \infty$ when $\rho \to 0$, but here $J \to 0$ for both $\rho = 0$ and $\rho = \rho_{\text{max}}$. The model is called the *Greenberg model*, and, according to [18], it fits the traffic in the Lincoln Tunnel from Manhattan to New Jersey when

$$a = 17.2 \text{ mph},$$

 $\rho_{\text{max}} = 228 \text{ cars/mile}.$ (128)

The model is still not entirely satisfactory, but the same idea could be taken further, e.g. assuming that

$$\lambda = \frac{\tilde{a}}{(x_{n-1} - x_n)^2}.$$
(129)

We then get a linear relationship between v and ρ . Measurements of flux as a function of density suggest a finite derivative at $\rho = 0$, in line with v going to a finite value when $\rho \to 0$.

3.3.1 Instabilities in a Queue

Driving in a queue, we may have experienced that it is uncomfortable to be behind drivers who keep an irregular speed, and this may also be analyzed with individual car models. With a finite reaction time, the equations are no longer pure differential equations, but what is denoted *Delay Equations*. Consider two cars and assume that the speed v_1 of the car in front vary periodically. It turns out to be convenient to work with complex solutions, but the result using physical real periodic solutions will be the same. We therefore assume that

$$v_1(t) = 1 + ae^{i\omega t},$$
 (130)

where the amplitude a is much smaller than 1. Assume that we have reached a stationary situation where the following car has a similar variation in the velocity,

$$v_2(t) = 1 + be^{i\omega t}.$$
 (131)

We put this into Eq. (119) and get

$$bi\omega e^{i\omega T} = -\lambda(b-a),\tag{132}$$

or

$$b = \frac{1}{1 + \frac{i\omega}{\lambda} e^{i\omega T}} a.$$
(133)

Thus

$$\frac{|b|}{|a|} = \left|\frac{1}{1 + \frac{i\omega}{\lambda}e^{i\omega T}}\right| = \frac{1}{\sqrt{\left(1 - 2\frac{\omega}{\lambda}\sin\omega T + \left(\frac{\omega}{\lambda}\right)^2\right)}}.$$
(134)

The amplitude of b will be greater than the amplitude of a if the denominator is less than 1 This occurs when

$$\sin(\omega T) > \frac{\omega}{2\lambda},\tag{135}$$

which can be expressed as

$$\frac{\sin\omega T}{\omega T} > \frac{1}{2\lambda T}.$$
(136)

Since $\sin x/x \leq 1$, there is no danger as long as $\lambda T < 1/2$, but if this is not the case, there are low frequencies where the amplitude for the second car is larger than for the car in front. With several cars in the line, a further magnification will occur for cars further back. Good drivers will notice this and try to dampen the fluctuations in the speed. A similar analysis could also be considered for a sudden braking of the first car.

4 CONSERVATION LAWS OF MECHANICS

It turns out that the physics of the continuum matter surrounding us, *i.e.* solid material, liquids and gases, can be described in a compact way using the framework above, and this is acknowledged in most recent books about continuum and fluid mechanics, for example [15].

However, the laws of physics are basically laws for a given collection of matter. For example, Newton's laws are laws for one or more "mass points". In the same way, a thermodynamic system, as we consider it when formulating the first law of thermodynamics, consists of a fixed collection of molecules. In continua like liquids and gases, where the material is moving, we are mostly interested in formulating the laws for a fixed region of space, that is, a *control volume*. The control volume will therefore contain different mass particles at different times.

In mechanics, a continuous medium in motion can be described in the *Eulerian* way by considering the velocity $\mathbf{v} = \mathbf{v}(\mathbf{x}, t)$ at each point \mathbf{x} , or we may use a *Lagrangian* description in which we follow the mass particles as time goes by, $\mathbf{x} = \mathbf{x}(t, \mathbf{a})$, $\mathbf{a} = \mathbf{x}(0, \mathbf{a})$.

A material region R(t) is a section of the medium which at any time contains the same mass particles. Mathematically, R(t) is defined as $R(t) = \{\mathbf{x}(t, \mathbf{a}); \mathbf{a} \in R(0)\}$, and a material region typically changes its shape and position as time passes, coinciding with the control volume at one instant of time, say at t = 0.

In this section we shall briefly review how the most important conservation laws of fluid mechanics may be derived by applying a simple result from vector analysis, namely *Reynolds' Transport Theorem*.

4.1 Reynolds Transport Theorem

From vector calculus we may know famous results such as the *Divergence Theorem* (also called Gauss' Theorem), and *Stokes' Theorem*. Reynolds Transport Theorem is another result in the same family. We introduce the theorem by first considering one-dimensional integrals.



Figure 16: Definition of the regions I, II and III.

If we need to take the derivative w.r.t. to t of H(t) defined by

$$H(t) = \int_{a(t)}^{b(t)} f(x,t) \, dx,$$
(137)

it is possible first to write

$$H(t) = F(b(t), t) - F(a(t), t),$$
(138)

where F is the anti-derivative of f with respect to the first argument, and then apply the Chain Rule,

$$\frac{dH}{dt}(0) = \left. \frac{d}{dt} \int_{a(0)}^{b(0)} f(x,t) \, dx \right|_{t=0} + f(b(0),0) \frac{\partial b}{\partial t}(0) - f(a(0),0) \frac{\partial a}{\partial t}(0) \,. \tag{139}$$

This result is useful to know, and we see that in addition to the expected first term, we have extra contributions because the integration interval changes with time.

Reynolds transport theorem is this identity when integrating over a moving region in space. We shall assume that the region we are looking at, R(t), is enclosed by a moving boundary, $\partial R(t)$. Furthermore, we assume that the points on the boundary are marked so that we can trace them as the time passes. In particular, all points on the boundary will, at any time, have a velocity $\mathbf{v}(\mathbf{x}(t))$, where $\mathbf{x}(t) \in \partial R(t)$.

We may then formulate Reynolds transport theorem for the integral of a function $\varphi(\mathbf{x}, t)$ over the moving region R(t) as follows:

$$\left(\frac{d}{dt}\int_{R(t)}\varphi(\mathbf{x},t)dV\right)_{t=0} = \left(\frac{d}{dt}\int_{R(0)}\varphi(\mathbf{x},t)dV\right)_{t=0} + \int_{\partial R(0)}\varphi(\mathbf{x},0)\mathbf{v}\cdot\mathbf{n}d\sigma.$$
 (140)

The theorem requires that \mathbf{v} and φ are sufficiently nice functions, and that R(t) is a nice region, but we will not go into that here. The proof follows directly from the definition of the derivative. We assume R(0) and R(t) are as outlined in Fig. 16. Let $\Phi_i(t_0)$ denote the integral of φ over region "i" at time t, e.g.

$$\Phi_{III}(t) = \int_{\mathbf{III}} \varphi(\mathbf{x}, t) dV.$$
(141)

In general, the regions **I** in **II** are defined by the parts of $\partial R(0)$ where the velocity field points in and out of R(0), respectively. From the definition of the derivative and Fig. 16 we have

$$\left(\frac{d}{dt}\int_{R(t)}\varphi(\mathbf{x},t)dV\right)_{t=0} = \lim_{t\to 0}\frac{\Phi_{\mathbf{III}}(t) + \Phi_{\mathbf{II}}(t) - (\Phi_{\mathbf{I}}(0) + \Phi_{\mathbf{III}}(0))}{t}$$
$$= \lim_{t\to 0}\frac{\Phi_{\mathbf{I}\cup\mathbf{III}}(t) - \Phi_{\mathbf{I}\cup\mathbf{III}}(0)}{t} + \lim_{t\to 0}\frac{\Phi_{\mathbf{I}}(t)}{t} - \lim_{t\to 0}\frac{\Phi_{\mathbf{I}}(t)}{t}.$$
 (142)

The first limit value is just

$$\left(\frac{d}{dt}\int_{R(0)}\varphi(\mathbf{x},t)dV\right)_{t=0}.$$
(143)

For small t the parts I and II become thin shells such that we may use the volume elements $dV = \mathbf{v} \cdot \mathbf{n}td\sigma$ for region II, and $dV = -\mathbf{v} \cdot \mathbf{n}td\sigma$ for region I. In the limit $t \to 0$ we obtain

$$\lim_{t \to 0} \frac{\Phi_{\mathbf{II}}(t) - \Phi_{\mathbf{I}}(t)}{t} = \int_{\partial R(0)} \varphi(\mathbf{x}, t) \mathbf{v} \cdot \mathbf{n} d\sigma \bigg|_{t=0}.$$
 (144)

In many textbooks, one finds that the theorem is stated assuming

$$\frac{d}{dt} \int_{R(0)} \varphi(\mathbf{x}, t) dV = \int_{R(0)} \frac{\partial \varphi}{\partial t}(\mathbf{x}, t) dV.$$
(145)

This is quite unfortunate for our applications and a direct error if φ has discontinuities inside R(0) (recall the discussion in Sec. 2.5.4).

4.2 Mass Conservation

Mass conservation is a key principle in continuum mechanics. Here $\varphi = \rho$, i.e. the mass density of the medium. Without sources and sinks, the mass within a material region R(t)will be constant, since this is precisely the definition of a material region. Thus,

$$\frac{d}{dt} \int_{R(t)} \rho(\mathbf{x}, t) dV = 0, \qquad (146)$$

and, consequently, we get by applying the transport theorem

$$\frac{d}{dt} \int_{R(0)} \rho(\mathbf{x}, t) dV \bigg|_{t=0} + \int_{\partial R(0)} \rho(\mathbf{x}, 0) \mathbf{v}(\mathbf{x}, 0) \cdot \mathbf{n}(\mathbf{x}, 0) d\sigma = 0.$$
(147)

Since there is nothing particular with time t = 0, we can for any time and an arbitrary fixed control volume R write

$$\frac{d}{dt} \int_{R} \rho dV + \int_{\partial R} \rho \mathbf{v} \cdot \mathbf{n} d\sigma = 0.$$
(148)
This is the mass conservation law in *integral form* when we do not have sources or sinks within R. Any sources/sinks will enter the expression as

$$\frac{d}{dt} \int_{R} \rho dV + \int_{\partial R} \rho \mathbf{v} \cdot \mathbf{n} d\sigma = \int_{R} q dV.$$
(149)

and below this is discarded. Of course, we could see this immediately from the theory in Sec. 2.4, since mass is a material variable and the flux is $\rho \mathbf{v}$.

As discussed in Sec. 2.4 we can, when ρ and v are sufficiently smooth, differentiate under the integral sign and apply the Divergence Theorem:

$$\frac{d}{dt} \int_{R} \rho dV = \int_{R} \frac{\partial \rho}{\partial t} dV, \qquad (150)$$

$$\int_{\partial R} \rho \mathbf{v} \cdot \mathbf{n} d\sigma = \int_{R} \nabla \cdot (\rho \mathbf{v}) dV$$
(151)

so that

$$\int_{R} \left(\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \mathbf{v}) \right) dV = 0.$$
(152)

Holding for all R, this then leads to the differential formulation

$$\rho_t + \nabla \cdot (\rho \mathbf{v}) = 0. \tag{153}$$

The flow is called *stationary* if ρ and **v** are independent of time. Then $\int_R \rho dV$ will be constant and the mass conservation reduces to

$$\int_{\partial R} \rho \mathbf{v} \cdot \mathbf{n} d\sigma = 0. \tag{154}$$

Equation 154 can be directly used for calculations, as illustrated for the pipeline in Fig. 17. By letting R be as given in the figure, the conservation law when the flow is stationary is

$$\int_{A_1} \rho \mathbf{v} \cdot \mathbf{n} d\sigma + \int_{A_2} \rho \mathbf{v} \cdot \mathbf{n} d\sigma + \int_{A_3} \rho \mathbf{v} \cdot \mathbf{n} d\sigma = 0.$$
(155)

By assuming ρ is constant and defining the velocity over the cross section of the tubes,

$$v_i = \frac{1}{|A_i|} \int_{A_i} \mathbf{v} \cdot \mathbf{n} d\sigma, \tag{156}$$

we obtain

$$|A_1|\rho_1 v_1 + |A_2|\rho_2 v_2 + |A_3|\rho_3 v_3 = 0.$$
(157)

 $(|A_j|$ is the cross sectional area). As one understands, it is easy to generalize this to arbitrary networks and otherwise include sources and sinks.

We immediately deduce the following special cases of the differential formulation:

- Stationary flow (no time variation): $\nabla \cdot (\rho \mathbf{v}) = 0$
- Constant density (*incompressible flow*): $\nabla \cdot \mathbf{v} = 0$



Figure 17: Stationary flow in a network of pipes will obey the mass conservation.

4.3 Momentum Conservation

In mechanics, *momentum* (or *linear momentum*) is the product of a body's mass times its velocity. Besides mass conservation, the momentum conservation law is the most important.

For a continuum, the momentum density is defined as momentum per volume unit, $\mathbf{p} = \rho \mathbf{v}$, where ρ is the mass density and \mathbf{v} the velocity. The density is thus a threedimensional vector in space. Newton's Second Law, stating that force is equal to mass times acceleration, is a statement about a fixed collection of mass particles. Since a material region R(t) always contains the same mass particles, Newton's law applied to a material region R(t) is just

$$\frac{d}{dt} \int_{R(t)} \rho \mathbf{v} dV = \Sigma \mathbf{F}(t), \qquad (158)$$

where $\Sigma \mathbf{F}(t)$ is the sum of all forced acting on the material region. By applying Reynolds transport theorem at t = 0 we obtain

$$\left(\frac{d}{dt}\int\limits_{R(0)}\rho\mathbf{v}dV + \int\limits_{\partial R(0)}(\rho\mathbf{v})\left(\mathbf{v}\cdot\mathbf{n}\right)d\sigma\right)_{t=0} = \Sigma\mathbf{F}(0).$$
(159)

For a fixed control volume R, the conservation of momentum may therefore be expressed as

$$\frac{d}{dt} \int_{R} \rho \mathbf{v} dV + \int_{\partial R} (\rho \mathbf{v}) \left(\mathbf{v} \cdot \mathbf{n} \right) d\sigma = \Sigma \mathbf{F}.$$
(160)

The equation can be used to express the conservation of momentum in any direction: If **a**

is a fixed unit vector in space, the scaler product with Eq. 160 gives

$$\frac{d}{dt} \int_{R} \rho v_{a} dV + \int_{\partial R} (\rho v_{a}) \left(\mathbf{v} \cdot \mathbf{n} \right) d\sigma = \Sigma F_{a}, \tag{161}$$

where $v_a = \mathbf{a} \cdot \mathbf{v}$ and $F_a = \mathbf{a} \cdot \mathbf{F}$. For a Cartesian coordinate system in space, the three standard unit vectors give us three equations corresponding to the axes.

To get further, it is necessary to say something about forces acting on the mass in R. It is common to distinguish between mass forces (also called *body forces*) and surface forces. In general, it is possible to write

$$\mathbf{F}_B = \int\limits_R \mathbf{f}_B(\mathbf{x}, t) dV, \tag{162}$$

for mass forces and

$$\mathbf{F}_{S} = \int_{\partial R} \mathbf{f}_{S}(\sigma, t) d\sigma, \qquad (163)$$

for surface forces.

The most common mass force is gravity,

$$\mathbf{F}_g = \int\limits_R \rho \mathbf{g} dV. \tag{164}$$

In the geophysical fluid flow (such as oceans and atmosphere) the *Coriolis force* and the *centripetal acceleration* are important. These are forces that arise because our control volume is fixed on earth's surface and is thus rotating with the earth. The Coriolis force is given by

$$\mathbf{F}_{c} = \int_{R} \rho(-2\mathbf{\Omega} \times \mathbf{v}) dV, \tag{165}$$

where Ω is the angular velocity of the earth $(2\pi/24\text{hours} = 7.3 \times 10^{-5} \text{s}^{-1})$. The centripetal acceleration

$$\mathbf{F}_{s} = \int_{R} \rho(-\mathbf{\Omega} \times (\mathbf{\Omega} \times \mathbf{r})) dV, \qquad (166)$$

where \mathbf{r} is the position vector from the centre of the earth. Electromagnetic forces are other important examples of body forces.

The forces acting on the surface of R may be expressed in terms of the so-called *stress* tensor of the medium. Stress is the force per unit area. The force can act along a surface (*shear stress*) or orthogonal on the surface (*normal stress*). We refer to courses in mechanics for further discussion of the stress tensor. If we equip space with a Cartesian coordinate system, we may represent the stress tensor by a symmetric 3×3 matrix,

$$\mathbf{T} = \begin{bmatrix} t_{11} & t_{12} & t_{13} \\ t_{21} & t_{22} & t_{23} \\ t_{31} & t_{32} & t_{33} \end{bmatrix}.$$
 (167)

For a small surface element $d\sigma$ with normal vector **n** the force acting on $d\sigma$ is given by

$$d\mathbf{F} = \mathbf{T} \cdot \mathbf{n} d\sigma, \tag{168}$$

and the momentum conservation law in integral form may be written

$$\frac{d}{dt} \int_{R} \rho \mathbf{v} dV + \int_{\partial R} (\rho \mathbf{v}) \mathbf{v} \cdot \mathbf{n} d\sigma = \int_{R} \rho \mathbf{f}_{B} dV + \int_{\partial R} \mathbf{T} \cdot \mathbf{n} d\sigma.$$
(169)

If we are working with liquids, the stress tensor has contributions from pressure and viscosity forces. The pressure acts orthogonal on a small area element within the fluid and has the same value at a point no matter how the element is oriented. In addition, all common liquids are more or less viscous. Viscosity can be seen as a type of internal friction which provides resistance against deformations. For so-called *Newtonian fluids*, the shear stress in the x-direction for a flow with velocity u(y) parallel to the x-axis is given by

$$\tau = \mu \frac{\partial u}{\partial y},\tag{170}$$

where μ is called *dynamic viscosity*. It may be shown (See, *e.g.* [10]) from the mathematical properties of the stress tensor that the simplest expression consistent with Eq. 170 and giving the static pressure p when the fluid is at rest has to be of the form

$$t_{ij} = \left(-p - \frac{2}{3}\mu\nabla\cdot\mathbf{v}\right)\delta_{ij} + \mu\left(\frac{\partial v_i}{\partial x_j} + \frac{\partial v_j}{\partial x_i}\right), \ i, j = 1, 2, 3,$$
(171)

(indices refer to the standard Cartesian coordinate system). This expression leads to the quite famous equation for the momentum balance in a Newtonian fluid,

$$\frac{\partial}{\partial t}\rho\mathbf{v} + \nabla\cdot\left((\rho\mathbf{v})\mathbf{v}\right) = \rho\mathbf{f}_B - \nabla p + \mu\left(\nabla^2\mathbf{v} + \frac{1}{3}\nabla(\nabla\cdot\mathbf{v})\right),\tag{172}$$

called Navier-Stokes Equation(s). If the liquid is incompressible and the density is constant, the equation simplifies to

$$\frac{\partial}{\partial t}\mathbf{v} + \nabla \cdot \left((\mathbf{v})\mathbf{v} \right) = \mathbf{f}_B - \frac{1}{\rho}\nabla p + \frac{\mu}{\rho}\nabla^2 \mathbf{v}, \tag{173}$$

since $\nabla \cdot \mathbf{v} = 0$.

4.4 Energy Conservation

The first law of thermodynamics says that for a system in thermodynamic equilibrium, the added heat will be used to perform work and change the system's the internal energy,

$$dQ = dW + dE. \tag{174}$$

The energy may be expressed as specific energy e (energy per unit mass) so that

$$E(t) = \int_{R(t)} e\rho dV.$$
(175)

Contrary to Q and W, the specific energy e is a material variable. Specific energy may, e.g. consist of *kinetic* and *inner* energy per mass unit,

$$e = \mathbf{v} \cdot \mathbf{v}/2 + u. \tag{176}$$

Work performed by the system may be of different kinds. If we consider the work per unit time (power), we have

(i) Work against the mass forces:

$$\frac{dW_B}{dt} = -\int\limits_R \mathbf{f}_B \cdot \mathbf{v} dV \tag{177}$$

(ii) Work against surface forces:

$$\frac{dW_S}{dt} = -\int\limits_{\partial R} \left(\mathbf{T} \cdot \mathbf{n} \right) \cdot \mathbf{v} d\sigma \tag{178}$$

(iii) Other work performed by the system (e.g. driving a turbine),

$$\frac{dW_t}{dt}.$$
(179)

From the first law and Reynolds transport theorem, the general energy conservation law becomes

$$\frac{d}{dt} \int_{R} e\rho dV + \int_{\partial R} e\rho \mathbf{v} \cdot \mathbf{n} d\sigma = \frac{dQ}{dt} - \frac{dW_t}{dt} + \int_{R} \mathbf{f}_B \cdot \mathbf{v} dV + \int_{\partial R} (\mathbf{T} \cdot \mathbf{n}) \cdot \mathbf{v} d\sigma.$$
(180)

In the same way as for mass conservation, we can also derive the differential formulation using the Divergence Theorem, provided that the smoothness conditions are fulfilled. Further information may be found in textbooks about continuum mechanics.

4.5 Comments and Examples

There are several other conservation laws than those presented here. In particular, the conservation law for *vorticity* $(\nabla \times \mathbf{v})$ is important for many applications in fluid mechanics.

Traditional mechanics and mathematics teaching is oriented towards differential equations, i.e. differential formulations. This is natural since there is a huge theory about the existence of solutions, and techniques such as separation of variables, integral transforms, Green functions, and perturbation methods for finding solutions.



Figure 18: How much force should we apply to keep a bent tube in position?

Nevertheless, modern textbooks of practical mechanics to a greater extent base their arguments on integral formulations. The integral formulations are independent of the choice of coordinate system and embodies the fundamental physical laws (which, after all, manage the real world) more directly than differential formulations. Integral formulations may be used for practical tasks and a control volume need not be just a small box!

Conservation laws also apply to situations where differential equations have shortcomings, such as for discontinuous variables. This is especially important for treating shock solutions.

While numerical models traditionally have been made from differential equations by replacing the derivatives with the finite difference approximations, one can also use the integral formulation directly by dividing the computational region into a pile of boxes. The equations for each box are then established based on the conservation laws. This guarantees that the numerical solutions are compatible with the conservation laws. Finite Element formulations and so-called weak solutions of differential equations are also related to the conservation laws in integral form.

Below we will look at three examples of how one can operate with conservation laws. The first example should be familiar to anyone with some background in fluid mechanics.

The second example deals with the phenomenon of shock, and is typical for that type of problems. The conservation laws provide conditions that help us to determine the properties of the shock. In aerodynamics shocks are associated with supersonic speeds, while the hydrodynamic shock in the example occurs at the very mundane speeds. This is also the case for the third, somewhat more challenging, example.

4.5.1 Forces on a Pipe Bend

We consider a tube bend with stationary horizontal flow, see Fig. 18. We know the pressure, the cross-sectional area, density and the speed at both the inlet and outlet. The problem is to find the forces F_x and F_y that we must apply in order to keep the bend in position. The velocities are vectors with directions indicated by arrows, and we assume that the velocity

magnitude and the pressure are constant over the cross sections $(A_1 \text{ and } A_2)$. Since the flow is stationary, the mass conservation requires

$$\rho_1 v_1 A_1 = \rho_2 v_2 A_2. \tag{181}$$

For the momentum balance we must first get an overview of the forces on R, which, in addition to the force needed to keep the bend in position, are composed of pressure forces:

$$(\Sigma F)_x = p_1 A_1 - F_x - p_2 A_2 \cos \alpha,$$

$$(\Sigma F)_y = -F_y + p_2 A_2 \sin \alpha.$$
(182)

Since conditions are stationary,

$$\frac{d}{dt} \int_{R} \rho \mathbf{v} dV = 0, \tag{183}$$

whereas

$$\int_{\partial R} \rho v_x \mathbf{v} \cdot \mathbf{n} d\sigma = \rho_1 v_1 (-v_1 A_1) + \rho_2 v_2 \cos \alpha (v_2 A_2),$$

$$\int_{\partial R} \rho v_y \mathbf{v} \cdot \mathbf{n} d\sigma = \rho_1 \cdot 0 \cdot (-v_1 A_1) + \rho_2 (-v_2 \sin \alpha) (v_2 A_2).$$
(184)

If this is inserted into the conservation law, we obtain

$$F_x = p_1 A_1 - p_2 A_2 \cos \alpha + \rho_1 v_1^2 A_1 - \rho_2 v_2^2 A_2 \cos \alpha,$$

$$F_y = p_2 A_2 \sin \alpha + \rho_2 v_2^2 A_2 \sin \alpha,$$
(185)

or, since $\rho_1 v_1 A_1 = \rho_2 v_2 A_2 = M$,

$$F_x = M(v_1 - v_2 \cos a) + p_1 A_1 - p_2 A_2 \cos \alpha, F_y = M v_2 \sin \alpha + p_2 A_2 \sin \alpha.$$
(186)

4.5.2 Flood Waves in Rivers

In this example we shall look at the simplest theory of flood waves and water jumps in rivers. Since the water level behind the water jump is higher than the level in front of the jump, people and livestock along the river can be swept away by the water, or suddenly find themselves in much deeper water than they appreciate. The reason for the jump could be torrential rain, sudden emission of water from a power station or a dam break.

To model what happens, we shall consider water flowing down a slope with a relatively small tilt angle α . The width of the flow across the inclined plane is B.

We assume that the velocity of the water is directed down the slope and has value v, is a function of position x and time t, and independent of z and y. This assumes that the flow is turbulent and that the water depth is not too large. In that case, the velocity is approximately constant over depth, but close to the bottom we will have a *boundary layer*



Figure 19: An idealized picture of a river.

where this assumption is not so good. Furthermore, we assume that the surface is defined by z = h(x, t). To model the flow, we use mass and momentum conservation. The situation is illustrated in Fig. 19.

Let us first see what mass conservation provides. The conservation law has the general form

$$\frac{d}{dt} \int_{R} \rho dV + \int_{\partial R} \mathbf{j} \cdot \mathbf{n} d\sigma = 0.$$
(187)

We assume that the density ρ is constant and use dV = Bh(x, t)dx. The amount j that flows past a point x per unit time has the form

$$j(x,t) = \rho v(x,t) \cdot (Bh(x,t)).$$
(188)

The flux vector (amount per surface and unit time) is thus as expected

$$\mathbf{j}(x,t) = \rho v\left(x,t\right) \hat{\imath}.\tag{189}$$

This may be inserted into Eq. 187 for a section of the river between x = a and x = b, while using $\mathbf{n} = -\hat{i}$ at x = a, and \hat{i} in x = b:

$$\frac{d}{dt} \int_{a}^{b} \rho Bh(x,t) dx + \left[\left(\rho v \right) \left(Bh \right) \right]_{a}^{b} =$$
(190)

$$\frac{d}{dt}\int_{a}^{b}\rho Bh(x,t)dx + \left[\rho v(b,t)\cdot Bh\left(b,t\right) - \rho v(a,t)\cdot Bh\left(a,t\right)\right] = 0.$$
(191)

Note that the flux orthogonal to the bottom and the surface is zero, and also in the ydirection, since we assume no flow in that direction. By letting $a \rightarrow b$, dividing by b - a in the usual way, and move the derivative inside the integral sign, we obtain the equation in differential form:

$$\frac{\partial h}{\partial t} + \frac{\partial}{\partial x} \left(vh \right) = 0. \tag{192}$$

Since this is an equation with two unknown functions, v and h, we can not solve the equation immediately.

The momentum balance will here give us something only for the x-direction, $p_x = \rho v$, and the conservation law takes the following form:

$$\frac{d}{dt} \int_{a}^{b} (\rho v) Bhdx + \left[(\rho v) v \cdot (Bh) \right]_{a}^{b} = \sum F_{x}.$$
(193)

It remains to specify the forces. Gravity acts directly on the water and, along the x-axis, this amounts to the force component proportional to $\sin \alpha$,

$$F_g = \int_a^b \rho g \sin \alpha B h(x, t) \, dx. \tag{194}$$

We then have the pressure forces. The pressure at the surface and the bottom does not contribute significantly to the x-component. However, we have a contribution from the end surfaces. Here we shall assume hydrostatic pressure, $p = \rho g (h - z)$, and sets $\cos \alpha \approx 1$ so that

$$dP = \rho g \left(h - z \right) \left(B dz \right). \tag{195}$$

The total pressure force on the surface at x = a is thus

$$P(a,t) = \int_{0}^{h} \rho g(h-z) B dz = \rho g B \frac{h^{2}(a,t)}{2}, \qquad (196)$$

and similarly at x = b, where the pressure force acts in the negative x-direction,

$$P(b,t) = -\rho g B \frac{h^2(b,t)}{2}.$$
(197)

The final force contribution is the friction force against the bottom. It turns out, partly based on dimensional analysis, that one can assume the friction force per area unit (*shear* stress in the x-direction) can be written

$$\tau = -\rho C_f \mathbf{v} \left| \mathbf{v} \right|. \tag{198}$$

The constant C_f is called the *Chézy-factor* and is empirically determined and depending of the roughness of the bottom. The total friction force is therefore found by integrating τ over the bottom surface:

$$F_f = -\int_a^b \rho C_f v^2 \left(B dx\right). \tag{199}$$

If we put all this together and divide by ρB , we get

$$\frac{d}{dt}\int_{a}^{b}vhdx + \left[\left(v\right)vh + \frac{g}{2}h^{2}\right]_{a}^{b} = \int_{a}^{b}\left(g\sin\alpha h - C_{f}v^{2}\right)dx.$$
(200)

It may be a bit tedious to establish the conservation law, but the principle is simple. The differential formulation follows in the same way as above:

$$\frac{\partial(hv)}{\partial t} + \frac{\partial}{\partial x} \left(v^2 h + \frac{g}{2} h^2 \right) = g \sin \alpha h - C_f v^2.$$
(201)

The equations 192 and 201 are often called the *shallow water equations*, or *Saint-Venant Equations*, and constitute what is called a hyperbolic system. There is a theory for hyperbolic systems of two equations that we shall not go into here, but in general the equations

can not be solved analytically. However, it is easy to see that the equations have the solution

$$h(x,t) = h_0,$$

 $v(x,t) = v_0,$ (202)

where

$$g\sin\alpha h_0 - C_f v_0^2 = 0. (203)$$

The last equation simply says that friction balances gravity. Linear stability analysis can tell whether the solution is stable, and this analysis, which is analogous to the one made for the instabilities in a traffic jam, may be found in the book by Whitham [18], p. 85–86.

In certain situations the flow is unstable, and more advanced analysis then leads to so-called *roll waves*. Roll waves may be observed on smooth sloping surfaces during heavy rain. Water flowing down a flat slope then has a tendency to create "waves" that are almost vertical in front and move slowly downward in relation to water velocity itself (see Fig. ??).

If we neglect the left side in Eq. 201, gravity always balances the friction. This is called the *kinematic theory* of flood waves. We obtain a relation between h and v,

$$v = \sqrt{\frac{g \sin \alpha}{C_f}} h^{1/2}, \tag{204}$$

and Eq. 192 becomes

$$\frac{\partial h}{\partial t} + \sqrt{\frac{g \sin \alpha}{C_f}} \frac{\partial}{\partial x} h^{3/2} = 0.$$
(205)

The kinematic velocity is

$$c(h) = \frac{d}{dh} \sqrt{\frac{g \sin \alpha}{C_f}} h^{3/2} = \frac{3}{2} \sqrt{\frac{g \sin \alpha}{C_f}} h^{1/2} = \frac{3}{2} v(h).$$
(206)

We leave to the reader to show that if the water level in the upper part of a river increases, in other words, if $\partial h/\partial x < 0$, it may develop a shock that in this case moves down the river like a wall. The phenomenon can occur during torrential rain or in rivers with regulated water flow, such as in rivers downstream from power plants. Note that the speed of the shock will be about 50% greater than the speed of the water flow!

On the figures 20 and 21, downloaded from the WEB-page of Dr. Hubert Chanson, Univ. of Queensland, Australia (http://www.uq.edu.au/~e2hchans/), we see examples of similar phenomena. These waves are called *tidal bores*, and occur as shock-solutions for the equations 192 and 201 in a flat river when the tide enters the river from its mouth. Fig. 20 is the most famous example of a tidal bore.

Figure 21 shows a somewhat different case. The picture is from the river Dorgonge in France. The river Seine had in the past a similar wave that could reach in some cases all the way to Paris, but this does not appear to be that prominent anymore.

The last image (Fig. 22) is copied from A. C. Fowler's photo gallery and shows *roll* waves on a road.



Figure 20: The tidal bore on Qiantang River near Hangzhou, China, also known as Hang chow or *Hangzou Bore*. The wave can be up to 9 feet tall and enters 2 times daily. It is most pronounced around the spring and autumn equinox (ⓒ Dr. H. Chanson).



Figure 21: Surfers on the tidal bore entering the Dordogne (© Dr. H. Chanson).



Figure 22: *Roll waves* on an asphalt road in the rain (Image copied from http://www.maths.ox.ac.uk/~fowler/pictures/gallery.html).

4.5.3 Research Project: The Circular Water Jump

Everyone who has run tapped water vertically into the kitchen sink, has observed that a circular water jump often forms some distance from where the jet hits the surface. If this does not sound familiar, one should before reading further make a simple experiment as in Fig. 23 The geometry of the problem is indicated in Fig. 24.

We assume radial symmetry and a constant density ρ . Furthermore, we assume that the water velocity is directed radially outward and is independent of z. Thus, both speed and depth are only functions of r and t. As for the pressure, we assume that this is given by the hydrostatic pressure, $p(r, t, z) = \rho g(h(r, t) - z)$ since any constant atmospheric pressure drops out. Frictional force per area unit at the bottom has the form $\mathbf{t}_C = -C_f \rho |\mathbf{v}| \mathbf{v}$ (where again C_f is the Chezy friction factor).

Let us set up the general conservation laws of mass and momentum for a control volume limited by r_1 and r_2 , $r_1 < r_2$, where r_1 is greater than the radius of the center jet. From the mass conservation law,

$$\frac{d}{dt} \int_{R} \rho dV + \int_{\partial R} \rho \left(\mathbf{v} \cdot \mathbf{n} \right) d\sigma = 0, \qquad (207)$$

we immediately get, using polar coordinates and dividing by $2\pi\rho$,

$$\frac{d}{dt} \int_{r=r_1}^{r_2} h(r,t)rdr + r_2h_2v_2 - r_1h_1v_1 = 0.$$
(208)



Figure 23: When a vertical water stream hits a horizontal surface, a circular jump in the flow forms some distance away from where the stream hits.



Figure 24: Vertical water jet hitting a horizontal plane.



Figure 25: Sector-shaped control volume for the momentum balance.

For the momentum balance it is necessary to choose a pie-shaped section as control volume and compute, e.g. the momentum balance in the x-direction, see Fig. 25.

Since the pressure on the bottom surface works vertically, it is sufficient to look at the pressure forces on the side walls. The pressure forces acting on a strip of width ds of the side wall is $dP = \rho g h^2(r, t) ds/2$, and by integrating around all side walls we obtain

$$P_x = \int_{\text{Sides}} -pn_x d\sigma = \rho g \sin \theta_0 \left(h^2(r_1, t)r_1 - h^2(r_2, t) + \int_{r=r_1}^{r_2} h^2(r, t)dr \right).$$
(209)

For the bottom friction we have, as for the flood waves,

$$C_x = -\int_{r=r_1}^{r_2} \int_{\theta=-\theta_0}^{\theta_0} C_f \rho v \cdot (v\cos\theta) r dr d\theta = -2C_f \rho \sin\theta_0 \int_{r=r_1}^{r_2} v^2(r,t) r dr.$$
(210)

The rest of the expressions is left to the reader, and we finally end with

$$\frac{d}{dt} \int_{r_1}^{r_2} vhr dr + \left[v^2 rh + \frac{r}{2} h^2 g \right]_{r_1}^{r_2} = \int_{r_1}^{r_2} \left(-C_f v^2 r + \frac{h^2}{2} g \right) dr.$$
(211)

Differential formulations of mass and momentum follow in the usual way:

$$\frac{\partial(rh)}{\partial t} + \frac{\partial(rhv)}{\partial r} = 0,$$

$$\frac{\partial(rhv)}{\partial t} + \frac{\partial}{\partial r}(rhv^2 + rh^2g/2) = -C_f v^2 r + \frac{h^2}{2}g.$$
 (212)



Figure 26: Formation of a circular water jump.

A suitable outflow will produce a stationary annular jump some distance from where the jet strikes, as indicated in Fig. 26. The water jump is actually a shock called a *hydraulic jump*. By assuming steady flow and letting $r_1 \rightarrow r_2 = R$ in the conservation laws, all the integrals of the conservation laws disappear, and we end up with the following classical shock conditions derived by J.-B. Belanger in 1838 [17]):

$$v_1 h_1 = v_2 h_2. (213)$$

$$v_1^2 h_1 + \frac{1}{2}h_1^2 g = v_2^2 h_2 + \frac{1}{2}h_2^2 g.$$
(214)

This is not sufficient to determine the position of the shock. We refer to the fluid mechanics text books for an discussion of the energy conservation in an ideal fluid under stationary conditions, leading to *Bernoulli's equation*, stating that the quantity

$$gz + \frac{v^2}{2} + \frac{p}{\rho} \tag{215}$$

is constant along streamlines. For a streamline on the surface (or at the bottom) this gives a third condition at the jump:

$$gh_1 + \frac{v_1^2}{2} = gh_2 + \frac{v_2^2}{2}.$$
(216)

In the theory of hyperbolic conservation laws, conditions such as the ones stated in the equations 213, 214 and 216 are called *Rankine-Hugoniot conditions*.

The equations 213, 214 and 216 have the obvious and not particularly exciting solution $h_1 = h_2$, $v_1 = v_2$, $h_L = 0$. However, if one requires that $h_1 \neq h_2$, the three equations do not have a solution. In reality, some of the energy is transformed to turbulence and eventually to heat at the shock. This requires the energy condition to include a certain energy loss at the jump:

$$gh_1 + \frac{v_1^2}{2} = gh_2 + \frac{v_2^2}{2} + gh_L.$$
(217)

The extra quantity gh_L on the right side is called *head loss* and is basically unknown.

If we only consider 213 and 214, it is possible to derive the equation

$$\left(\frac{h_2}{h_1}\right)^2 + \frac{h_2}{h_1} = 2\frac{v_1^2}{gh_1}.$$
(218)

The dimensionless combination

$$Fr = \frac{v}{\sqrt{gh}}.$$
(219)

occurring on the right hand side is called *Froude's Number*, and is an important number in hydrodynamics. The quadratic equation for h_2/h_1 has the solution

$$\frac{h_2}{h_1} = \frac{1}{2} \left(-1 \pm \sqrt{1 + 8Fr_1} \right)$$
(220)

For h_1 to be less that h_2 , it is necessary that $Fr_1 > 1$. The Froude number has an interesting physical interpretation. Water waves (longer than a few centimeters) have the propagation speed $c_p = \sqrt{gh}$ in shallow water. Thus, the Froude number is the ratio between v and c_p . A flow with a free surface where $v > c_p$ is called *supercritical flow*. If you are sitting in the flow, a disturbance in front of you cannot be warned by a surface wave before it happens to you. Thus, Fr is analogous to the *Mach number* in aerodynamics.

From the energy condition, we can find an expression for the relative energy loss in the shock expressed as the ratio h_L/h_1 :

$$\frac{h_L}{h_1} = \frac{h_1 - h_2 + v_1^2/2g - v_2^2/2g}{h_1},$$

= $1 - \frac{h_2}{h_1} + \frac{Fr^2}{2} - \frac{v_2^2}{2gh_1} = 1 - \frac{h_2}{h_1} + \frac{Fr^2}{2} \left(1 - \left(\frac{1}{h_2/h_1}\right)^2\right).$ (221)

where we finally may insert Eq. 220.

But what is the position of the water jump? A simplified analysis is found in [17], ignoring all other energy losses apart from at the shock. If the kinetic energy in the flow before the shock is much larger than potential energy, the velocity, according to Bernoulli's equation, will be approximately constant and equal to U_0 , i.e. the speed of the jet as it hits the plate. We then obtain from the mass and momentum, balance

$$q_0 = 2\pi R h_1 U_0 = 2\pi R H v_2,$$

$$U_0^2 h_1 + h_1^2 g/2 = v_2^2 H + H^2 g/2,$$
 (222)

which after a simple transformation gives

$$R = \frac{(U_0^2 - gH/2)q_0}{\pi gH^2 U_0}.$$
(223)

It is not unreasonable that U_0 enters in addition to q_0 , since both the added momentum and mass should be of importance for the position of the jump.

In September 1993, *Journal of Fluid Mechanics* presented a comprehensive analysis of the problem [3].

5 DIFFUSION AND CONVECTION

Whereas a material variable is a quantity passively transported along with the flowing medium, this is not always a reasonable assumption. On a small scale, the *molecular* diffusion mixes liquids and gases by the molecules tumbling around. This also applies if we add small particles of a liquid (mixture by *Brownian motion*). There are differences in the concentration that give rise to the mixing. If the medium is moving, we will also have a change because of transportation. Such transport is called *convection*.

Low viscosity fluids will often have speeds and length scales so that *turbulence* is developed. Turbulence is the chaotic movement where the flow develops vortices and thin layers that spin into each other and split up (smoke in the air visualizes this well). If we add a foreign substance to a medium, we observe that the mixing goes much faster when the flow is turbulent than it does if the mixture occurs by diffusion alone (this is why we use a spoon in the cup in order to mix milk and coffee!). Modeling by turbulent mixing is a classic problem. The simplest would then be trying to describe it as an enhanced diffusion, but there are also examples where such a description appears to be quite wrong. Turbulence in fluids can occur when the speed varies greatly from place to place (called the velocity shear in fluid mechanics). Otherwise, the turbulence may be caused by temperature and density differences (always observed when we boil water). In Chapter 6, we shall derive the conservation laws for turbulence from the conservation laws in Sec. 4

In addition to molecular diffusion and turbulence, diffusion-like spread has been shown to be very applicable in other contexts. Often, the offspring is a discrete phenomenon, modeled by stochastic random walk. Mathematically, one can then show that such discrete models in the limit with very many objects actually transform into diffusion models.

5.1 Conservation Laws with Diffusion

Diffusion is flux caused *concentration differences*. If the concentration is constant, there will be no net flux in any direction. To first order, the flux must be proportional to the change in concentration per unit length, in other words

$$\mathbf{j} = -\sigma \nabla \varphi, \tag{224}$$

where φ is the concentration and σ is called the *diffusion coefficient*. This expression is called *Fick's Law* for diffusion. Heat conduction obeys a similar law. If the specific heat is constant, the heat flux is $\mathbf{q} = -k\nabla T$, where T is the temperature and k is called the *heat conduction coefficient*. This expression is called *Fourier's Heat Conduction Law*.

Diffusion has a *smoothing* effect on the concentration gradients. If we start with a localized section R of a liquid with a different concentration of some substance, the largest concentration gradients occur along the edges of R. When we stir and develop turbulence, the batch of liquid is stretched and twisted so that an increasing proportion is located in areas with strong gradients. In this way, diffusion acts more strongly, and this is the mechanism behind what we call *forced mixing* or enhanced diffusion by turbulence.

Let us now consider a general situation where $c(\mathbf{x}, t)$ is the concentration of a substance in a liquid, and the vector field $\mathbf{j}(\mathbf{x}, t)$ denotes the corresponding flux. If the substance passively follows the flow, we have shown before that the flux is just $\mathbf{j}_c(\mathbf{x}, t) = c\mathbf{v}$. Even when the liquid is at rest, the material may be spread by a diffusion flux \mathbf{j}_d . We want to show that the total flux will be the sum of the fluxes, $\mathbf{j}(\mathbf{x}, t) = \mathbf{j}_d(\mathbf{x}, t) + \mathbf{j}_c(\mathbf{x}, t)$. Let R(t)be a material region of the liquid much smaller than the scale of variations in \mathbf{v} . For time intervals of the order of the diameter of R divided by $|\mathbf{v}|$, an observer traveling with R(t)set up

$$\frac{d}{dt} \int_{R(t)} c(\mathbf{x},t) \, dV \bigg|_{t=0} + \int_{\partial R(0)} j_d(\mathbf{x},0) \cdot \mathbf{n} d\sigma = \int_{R(0)} q(\mathbf{x},t) \, dV.$$
(225)

But Reynolds transport theorem applied to the first term gives

I

$$\frac{d}{dt} \int_{R(t)} c(\mathbf{x},t) \, dV \bigg|_{t=0} = \frac{d}{dt} \int_{R(0)} c(\mathbf{x},t) \, dV + \int_{\partial R(0)} c(x,0) \, \mathbf{v} \cdot \mathbf{n} d\sigma,$$
(226)

and altogether,

$$\frac{d}{dt} \int_{R} c dV + \int_{\partial R} (\mathbf{j}_d + c\mathbf{v}) \cdot \mathbf{n} d\sigma = \int_{R} q dV.$$
(227)

A general control region can be divided into arbitrary small parts where this formula holds. When all contributions are added, the area integrals over common borders cancel so that one ends up with the same formula for the whole region. This is thus the general diffusion conservation law, and the total flux is

$$\mathbf{j}(\mathbf{x},t) = \mathbf{j}_d(\mathbf{x},t) + \mathbf{j}_c(\mathbf{x},t).$$
(228)

If we apply the Divergence theorem as in Chapter 4, we find the differential form:

$$\frac{\partial c}{\partial t} + \nabla \cdot (\mathbf{j}_d + \mathbf{v}c) = q.$$
(229)

Inserting for $\mathbf{j}_d = -\sigma \nabla c$, we get a Convection/diffusion Equation:

$$\frac{\partial c}{\partial t} + \nabla \cdot (\mathbf{v}c) - \nabla \cdot (\sigma \nabla c) = q.$$
(230)

In general, both \mathbf{v} and σ may depend on c so that the equation is nonlinear. In the next section we will consider a simple mathematical model where this equation enters in a central way.

5.2 One-Dimensional Chemical Reactor

A simple chemical reactor consists of a tube (often filled with crushed glass or glass spheres) where a fluid is flowing with a constant mean velocity v. A certain substance is added to



Figure 27: Sketch of a simple one-dimensional chemical reactor. The fluid flows through a tube filled with crushed glass or glass spheres.

the fluid from a nozzle. The is mixed with a constant diffusion coefficient σ . In practice, σ is an *effective* diffusion coefficient due to the turbulent mixing in the flow around the glass), as illustrated in Fig. 27. The concentration of the substance (outside the source region) is described by a one-dimensional version of Eq. 230:

$$\frac{\partial c}{\partial t^*} + v \frac{\partial c}{\partial x^*} - \sigma \frac{\partial^2 c}{\partial x^{*2}} = 0.$$
(231)

Scaling x^* by the typical tube length L and a corresponding time scale T = L/v gives us

$$\frac{\partial c}{\partial t} + \frac{\partial c}{\partial x} - \varepsilon \frac{\partial^2 c}{\partial x^2} = 0, \qquad (232)$$

where $\varepsilon = \sigma/Lv$ is a dimensionless parameter, similar to the inverse Reynolds number. When ε is small, we have an equation with a small parameter in front of the highest derivative. This is the case when convection is dominating over diffusion. When $\varepsilon > 0$, the equation belongs to the *parabolic* class of PDEs, whereas it is *hyperbolic* when $\varepsilon = 0$. In this case, it is not just the order of the equation that changes, the type changes as well.

Let us consider the solution of the initial value problem:

$$\frac{\partial c}{\partial t} + \frac{\partial c}{\partial x} - \varepsilon \frac{\partial^2 c}{\partial x^2} = 0, \ t > 0, \ -\infty < x < \infty,$$
$$c(x,0) = f(x)$$
(233)

For $\varepsilon = 0$ the equation is $c_t + c_x = 0$, and we have already seen in Sec. 2.5 that the solution is then simply

$$c(x,t) = f(x-t).$$
 (234)

The initial density profile moves unchanged to the right with speed 1 (speed v in the original variables). This is also reasonable from a purely physical reasoning.

When $\varepsilon > 0$, it is convenient to choose a coordinate system following the flow:

$$\begin{aligned} x' &= x - t, \\ t' &= \varepsilon t. \end{aligned} \tag{235}$$

Then

$$\frac{\partial c}{\partial t} = \frac{\partial c}{\partial t'} \frac{\partial t'}{\partial t} + \frac{\partial c}{\partial x'} \frac{\partial x'}{\partial t} = \varepsilon c_{t'} - c_{x'},$$

$$\frac{\partial c}{\partial x} = \frac{\partial c}{\partial t'} \frac{\partial t'}{\partial x} + \frac{\partial c}{\partial x'} \frac{\partial x'}{\partial x} = c_{x'},$$

$$\frac{\partial^2 c}{\partial x^2} = c_{x'x'}.$$
(236)

Thus,

$$c_t + c_x - \varepsilon c_{xx} = \varepsilon c_{t'} - c_{x'} + c_{x'} - \varepsilon c_{x'x'} = 0, \qquad (237)$$

or

$$c_{t'} = c_{x'x'},$$
 (238)

which is the classical parabolic equation. We leave to the reader to show that the function

$$c_f(x',t') = \frac{1}{\sqrt{4\pi t'}} \exp\left(-\frac{x'^2}{4t'}\right)$$
 (239)

is a solution for t' > 0. This is the so-called *fundamental solution*. From the formula

$$\int_{-\infty}^{\infty} e^{-x^2} dx = \sqrt{\pi},$$
(240)

we find that

$$\int_{-\infty}^{\infty} c_f(x',t')dx' = 1 \tag{241}$$

for all t' > 0. The fundamental solution is, in other words, a Gaussian distribution with variance increasing linearly with time. When $t' \to 0$, the solution approach a δ -function at the origin. Physically, this corresponds to a release of a unit quantity of the substance at the origin at time t' = 0.

If we return to original coordinates, we obtain

$$c_F(x,t) = \frac{1}{\sqrt{4\pi\varepsilon t}} \exp\left(-\frac{(x-t)^2}{4\varepsilon t}\right).$$
(242)

The solution is sketched in Fig. 28. It is easy to show that the general solution of the initial value problem c(x, 0) = f(x) can be expressed as a *convolution integral* with the fundamental solution:

$$c(x,t) = \int_{s=-\infty}^{\infty} f(s)c_F(x-s,t)ds.$$
(243)

A general feature of convolution says that the result is at least as nice as the nicest of the functions involved, and actually, the solution c(x, t) will be infinitely many times differentiable for t > 0 no matter how f looks. Fast variations are smoothed out more and more as the time goes on, and

$$\lim_{t \to \infty} c(x, t) = 0. \tag{244}$$



Figure 28: Time development of the fundamental solution shown for t = 0.1 up to 2, and $\varepsilon = 1$.

How fast smearing takes place depends on the size of ε . In this linear equation, the solution becomes smoother and smoother as time passes, but for more general non-linear convection/diffusion equations this does not need to be the case.

On its way towards the final stage, the solution of Eq. 243 passes what is called an *intermediate asymptotic* state. The concept was introduced in [1] and says (in the simplest case) that the solutions of differential equations asymptotically may approach simplified solutions as time passes, and before they reach their final stage.

Consider the diffusion equation

$$\frac{\partial c^*}{\partial t^*} = \kappa \frac{\partial^2 c^*}{\partial^2 x^*}, \ 0 < t^*, \ -\infty < x^* < \infty,$$
(245)

with initial condition $c^*(x^*, 0) = f(x^*)$, and where f is a function localized to the interval [-L, L] such that

$$\int_{-L}^{L} f(x^*) dx^* = Q_0, \qquad (246)$$

$$f(x^*) = 0 \text{ for } L \le |x^*|.$$
 (247)

For large times, $t = \mathcal{O}(T)$, the solution, due to diffusion, has a spatial extension $X = \mathcal{O}(\sqrt{\kappa T})$, where $X \gg L$ (However, mathematically the solution is non-vanishing on the whole interval $[-\infty, \infty]$ for all t > 0).

Let us scale the problem by T, X and Q_0/X :

$$t^* = Tt,$$

$$x^* = Xx = \sqrt{\kappa T}x,$$

$$c^* = \frac{Q_0}{X}c.$$
(248)

This gives

$$\frac{\partial c}{\partial t} = \frac{\partial^2 c}{\partial^2 x},\tag{249}$$

while the initial condition is now

$$f(x) = c(x,0) = \frac{X}{Q_0}c^*(xX,0) = \frac{X}{Q_0}f^*(Xx).$$
(250)

We see that f(x) = 0 for $|x| > \varepsilon = L/X \ll 1$, and

$$\int_{-\infty}^{\infty} f(x)dx = \frac{1}{Q_0} \int_{-\infty}^{\infty} f^*(Xx)Xdx = 1.$$
 (251)

The scaled problem becomes

$$c_t = c_{xx}, \ c(x,0) = f(x),$$
 (252)

$$\int_{-\infty}^{\infty} f(x)dx = 1, \ f(x) = 0 \text{ for } |x| > \varepsilon.$$
(253)

At t = O(1), the initial condition looks like a δ -function regardless of how irregular f is, and the actual solution must therefore be quite similar to the fundamental solution (The argument can be made mathematically precise by studying the convolution integral in Eq. 243). Fundamental solutions therefore have greater applicability than one might think:

For large times, the details of the initial conditions are blurred and we can use solutions derived from the simpler conditions.

Linear diffusion equations in one or several dimensions are thoroughly covered in all textbooks on partial differential equations.

5.3 A Nuclear Power Plant Accident

In this case study we show how one can use conservation principles and basic properties of the fundamental solution of the one-dimensional convection/diffusion equation to analyze a hypothetical release of radioactive material. The analysis is typical of how one will try to get a first rough overview of a relatively difficult modeling problem. The situation is of course fictional, and was an exam task at NTNU in 1986, just after the Chernobyl disaster.

From a nuclear power plant there is an uncontrolled release of radioactive cooling water to a river past the power plant. The radioactivity is mainly due to a certain short-lived isotope (Numerical values below are selected in order to produce reasonably simple numeric answers).

The special thing here is that the radioactive material breaks down. If we have a solution with a concentration c of radioactive material, the concentration decays exponentially with time,

$$c(t) = c(0) \exp(-t/t_0).$$
(254)

This could also be described by the differential equation

$$\frac{dc}{dt} = -\frac{c}{t_0} \tag{255}$$

where the time $t_0 \ln 2$ is the *half-life* for the isotope.

We assume that the river stream flows at a mean velocity U = 0.2m/s. In reality, the water velocity varies with the river topography, and the waters are mixed and spread both by turbulence and because the water velocity is not constant over the cross section of the river. In practice, it is common to model this by a so-called *eddy-diffusivity* (*eddy* = whirl) along the direction of the river, defined by a diffusion coefficient κ_E 6. The diffusion coefficient will have the same dimension as the molecular diffusions coefficient, but will be much larger. Here, we let κ_E be equal to $1\text{m}^2/\text{s}$, which is not a completely unreasonable value. We consider the river to be one-dimensional and assume that emissions come from from a stationary point-source.

When formulating the conservation law, the density of radioactive material c enters as amount per length unit of the river, while the flux will have two contributions, one from the diffusion and one from convection:

$$J(x,t) = c(x,t)U - \kappa \frac{\partial c}{\partial x}(x,t).$$
(256)

The decreasing radioactivity can be modeled as a sink with intensity $\frac{c}{t_0}$. The spill is a δ -function source in x = 0. The change of radioactive material within an interval $[x_1, x_2]$ of the river is thus described by the conservation law

$$\frac{d}{dt}\int_{x_1}^{x_2} c(x,t)\,dx + J(x_2,t) - J(x_1,t) = \int_{x_1}^{x_2} \left(-\frac{c(x,t)}{t_0} + q(t)\delta(x)\right)\,dx.$$
(257)

The differential form of the the equation will be

$$\frac{\partial c}{\partial t} + U\frac{\partial c}{\partial x} - \kappa \frac{\partial^2 c}{\partial x^2} = -\frac{c}{t_0} + q(t)\delta(x), \qquad (258)$$

which is a linear convection/diffusion equation with a source/sink term. Assume that the discharge has been going on with a constant amount q_0 per unit of time from time t = 0. The total amount of radioactive material in the river at any time can then be calculated from the conservation law by integrating from $x_1 = -\infty$ to $x_2 = \infty$:

$$\frac{dC}{dt} = -\frac{C}{t_0} + q_0,$$

$$C(t) = \int_{-\infty}^{\infty} c(x, t) dx.$$
(259)

Note that the flux terms disappear since $\lim_{x\to\infty} J(x,t) = \lim_{x\to-\infty} J(x,t) = 0$. The solution for C(t) under the assumption that C(0) = 0 follows immediately:

$$C(t) = q_0 t_0 \left(1 - \exp(-t/t_0)\right).$$
(260)

As $t \to \infty$, the total amount converges to $q_0 t_0$.

Consider now a situation where a constant discharge q_0 lasts for $t_1 = 30$ minutes. We are seeking an approximate solution for c(x, t) at two different times: (i) immediately after the spill is over, and (ii) after $t_2 = 10^6 \text{s} \approx 11.5$ days.

After the 30 minutes are over, there is a total amount

$$C_0 = t_0 q_0 \left(1 - e^{-t_1/t_0} \right) \approx t_1 q_0 \tag{261}$$

in the water (note that $t_1 \ll t_0$). Convection (i.e. the motion of water masses with mean speed U) has led to a spreading of material over a length $L = Ut_1 = 360$ m. How much diffusion has affected the solution is estimated by the length scale for diffusion,

$$\sigma_1 = \sqrt{2\kappa t_1} = 60 \mathrm{m}. \tag{262}$$

This is significantly less than L. Since there is no appreciable radioactive decay during this short period, the concentration, c_0 , is nearly constant from x = 0 to x = L, and mass balance gives $c_0L = q_0t_1$. Thus,

$$c(x,t_1) \approx \begin{cases} c_0 = q_0/U, & 0 \le x \le L\\ 0, & \text{otherwise.} \end{cases}$$
(263)

Actually, the solution should be a little "rounded" on both ends, but we have a good approximation when neglecting both radioactive decay and turbulent diffusion.

After 10^6 s the dispersion and decay can no longer be neglected. The length scale for the diffusion is now

$$\sigma_2 = \sqrt{2\kappa t_2} \approx 1400 \mathrm{m},\tag{264}$$

which is significantly larger than the original length L of the discharge. The total amount of radioactive material is given by

$$\int_{-\infty}^{\infty} c(x, t_2) \, dx = \left[q_0 t_1 (1 - e^{-t_1/t_0}] \, e^{-(t_2 - t_1)/t_0} \approx q_0 t_1 \exp(-t_2/t_0) \right] \tag{265}$$

Relative to the amount just after the end of the discharge, the remaining amount is about $\exp(-t_2/t_0) \approx 0.8 \cdot 10^{-12}$ less.

Since $t_1 = 30$ minutes is much less than $t_2 = 10^6$ s, and $L/\sigma_2 \approx 0.25$, we can, with high accuracy, assume that all emissions of radioactive material occurred at time zero. It is then possible to exploit the fundamental solution to the convection/diffusion equation stated in Eq. 242 giving the solution of a unit discharge at t = 0 and x = 0. The full solution becomes, approximately,

$$c(x, t_2) \approx [q_0 t_1 \exp(-t_2/t_0)] \frac{1}{\sqrt{4\pi\kappa t_2}} e^{-(x-Ut_2)^2/(4\kappa t_2)},$$
 (266)

where the first part denotes the total remaining radioactive material and $Ut_2 = 200$ km.

It is actually easy to write down the solution for an arbitrary time-variable discharge q(t) from a point-source. Since we can assume that the emissions at different times do not affect each other, it is possible to consider emissions as a series of point-discharges, and then sum up the corresponding solutions. In the same way as above, the solution of a discharge over time duration $d\tau$ at a time $\tau < t$

$$dc(x,t) = [q(\tau)d\tau \exp(-(t-\tau)/t_0)] F(x,t-\tau).$$
(267)

The distribution of radioactive material at time t is then given by the integral

$$c(x,t) = \int_{-\infty}^{t} dc(x,t) = \int_{-\infty}^{t} \left[q(\tau) d\tau \exp(-(t-\tau)/t_0) \right] F(x,t-\tau) d\tau.$$
(268)

In practice, the radioactive emissions often include several different isotopes. Decomposition of one isotope could also lead to other radioactive isotopes. This will lead to connections between the conservation laws for the individual isotopes, but the link is limited to the source-terms. Moreover, the modeling of the river will naturally also be made considerably more advanced. In particular, turbulent mixing is described by models that relate the strength of the diffusion of the amount of turbulent kinetic energy. The modeling will first calculate the flow and turbulence level in the water using a hydrodynamic turbulence model. Then run a *transport model* calculating the distribution of the radioactive material on the basis of the hydrodynamic solution.

Today, the authorities require that such models are developed and tested *before* an accident occurs (the models can actually be tested by controlled release of radioactive isotopes).

5.4 Similarity Solutions

So far we have always been able to scale the variables in our equations, but for some "academic" problems there are no natural scales to use. The fundamental solution to the linear diffusion equation one such simple example. It is impossible to find reasonable time and space scales for this problem by just looking at the equation and the definition domain, $-\infty < x < \infty$ and 0 < t. In this case it turned out not to be necessary. However, if there are no scales to use, we must combine the variables in order to obtain dimensionless equations.

We will not go into further detail on the theory of similarity solutions, where in particular, the Norwegian mathematician Sophus Lie has provided important contributions ([12], [1], [16]). However, we will, based on dimensional analysis, illustrate the method by means of an example from heat conduction. The idea of this section comes from [5].

Two infinite materials with different but constant temperatures are brought into contact at time t = 0, as shown in Fig. 29. We assume that heat is transported smoothly through the contact surface, and we assume one-dimensional heat conduction. The problem is to determine the temperature development in the material as time goes on. Since we assume infinite extent, and we consider the time from 0 to ∞ , there is no length or time scale. In practice, the materials will have finite extent, L, and after some time T, the temperature at the ends begin to change. As long as we limit ourselves to times that are significantly smaller than T, we should be able to use the solution valid for an infinite extent of the material.

Heat transfer and storage of a material is (in its simplest form) determined by three material constants: mass density, ρ , $[\rho] = \text{kgm}^{-3}$, specific heat capacity, c, $[c] = \text{Jkg}^{-1}\text{K}^{-1}$, and the heat conduction coefficient, k, $[k] = \text{Js}^{-1} \text{m}^{-1}\text{K}^{-1}$.



Figure 29: The temperature in the blocks for t = 0 and after a some time in contact.

We introduce a dimensionless temperature τ by writing

$$T = T_1 + (T_2 - T_1)\tau,$$

and quite general we expect

$$\tau = \tau(x, t, \rho_1, c_1, k_1, \rho_2, c_2, k_2).$$
(269)

where the indices indicate material 1 and 2. If we know the heat conduction equation, we know that ρ , c and k in the material combines into a heat diffusion coefficient $\kappa = k/c\rho$, while the heat fluxes are generally of the form $-k\nabla T$. The heat flux should be continuous across the border between the materials. This means that we must be able to simplify Eq. 269 to

$$\tau = \tau(x, t, \kappa_1, \kappa_2, k_1, k_2). \tag{270}$$

The dimension matrix for these six variables has rank 3 (check!), and we have therefore also three dimensionless combinations, for example,

$$\eta = \frac{x}{\sqrt{\kappa_1 t}},$$

$$a = \frac{k_1}{k_2},$$

$$b = \frac{\kappa_1}{\kappa_2}.$$
(271)

Thus, we have found that the solution of the problem must be written in the form

$$\tau(x,t) = \tau_0(\eta, a, b) = \tau_0\left(\frac{x}{\sqrt{\kappa_1 t}}, \frac{k_1}{k_2}, \frac{\kappa_1}{\kappa_2}\right).$$
(272)

As expected, the solution depends, on combination of x and t, and already here we make a surprising observation:

$$\tau(0,t) = \tau_0(0,a,b) \tag{273}$$

is constant and independent of time for t > 0! Unfortunately, dimensional analysis can not give us the exact expression for $\tau(0,t)$, but the expression for τ has reduced the problem from a partial to an ordinary diff.-equation. The heat conduction equation in material 1 now takes the form

$$\frac{\partial \tau}{\partial t} = \kappa_1 \frac{\partial^2 \tau}{\partial x^2},\tag{274}$$

and by using $\frac{\partial \tau}{\partial t} = \frac{d\tau_0}{d\eta} \frac{\partial \eta}{\partial t}$ etc., we find

$$\frac{d^2\tau_0}{d\eta^2} + \frac{1}{2}\eta \frac{d\tau_0}{d\eta} = 0,$$
(275)

and similarly for material 2,

$$\frac{d^2\tau_0}{d\eta^2} + \frac{1}{2}b\eta \frac{d\tau_0}{d\eta} = 0.$$
 (276)

Equation 276 has general solution

$$\tau_0 = A_2 + B_2 \operatorname{erf}\left(\frac{\sqrt{b}}{2}\eta\right),\tag{277}$$

whereas we for material 1 get

$$\tau_0 = A_1 + B_1 \operatorname{erf}\left(\frac{1}{2}\eta\right).$$
(278)

We have 4 constants from the integration, but since $\tau_0(\eta) \to 0$ when $\eta \to -\infty$, and $\tau_0(\eta) \to 1$ when $\eta \to \infty$, only two remain:

$$\tau_0 = A \left(1 + \operatorname{erf}\left(\frac{1}{2}\eta\right) \right), \ \eta < 0,$$

$$\tau_0 = 1 + B \left(\operatorname{erf}\left(\frac{\sqrt{b}}{2}\eta\right) - 1 \right), \ \eta > 0.$$
 (279)

The solution found requires that t > 0, and then τ_0 is continuous at $\eta = 0$. This gives

$$A = 1 - B. \tag{280}$$

Finally, we use that the flux must be continuous across the contact surface,

$$k_1 \frac{\partial T}{\partial x}\Big|_{0-} = k_2 \frac{\partial T}{\partial x}\Big|_{0+}.$$
(281)

After introducing τ and η , this gives

$$a \left. \frac{d\tau_0}{d\eta} \right|_{0-} = \left. \frac{d\tau_0}{d\eta} \right|_{0+},\tag{282}$$

or

$$aA\frac{1}{2} = B\frac{\sqrt{b}}{2},\tag{283}$$

	$\rho [\mathrm{kgm}^{-3}]$	c[J/kgK]	k[W/mK]	$T[^{\circ}C]$	$w [m^2 Ks^{.5}]$
Foot	1000	4000	0.6	37	1550
Hot coal	150	800	0.04	600	70

Table 2: Approximate values of density, specific heat and heat conduction coefficient for the human foot and burning coal

and finally,

$$A = \frac{\sqrt{b}}{\sqrt{b} + a}, \ B = \frac{a}{\sqrt{b} + a}.$$
(284)

We get a surprisingly simple expression for the temperature of the interface:

$$T(0,t) = T_1 + (T_2 - T_1)A = \frac{T_1w_1 + T_2w_2}{w_1 + w_2}, \quad w_i = \sqrt{\rho_i c_i k_i}.$$
 (285)

Now we could stop here, but the expression explains why, in winter, it feels much colder to touch a piece of metal than a piece of wood. In summer, we may get burned by a piece of metal in the sun, whereas touching a piece of wood with the same temperature is without any risk. The explanation is as follows. Your finger will have a temperature T_f and a certain w_f . Although wood and metal have the same temperature T_0 , $w_{wood} < w_f$, while $w_f \ll w_{metal}$. This means that $T(0,t) \approx T_f$ when we touch the tree, while $T(0,t) \approx T_0$ when we touch the metal.

This reasoning can actually be taken even further. Some literature search has revealed the values in Table 2.

These values gives a contact temperature T_k between a human foot and glowing coal given by

$$T_k = \frac{37^{\circ}\mathrm{C} \times 1550 + 600^{\circ}\mathrm{C} \times 70}{1550 + 70} \approx 62^{\circ}\mathrm{C}.$$
 (286)

By no means deterring! Such an explanation of why it is possible to walk on hot coals is of course rejected by a compact majority on the Internet. Some years ago, Swedish physics professor visited NTNU and let students try this astonishing experiment. He waited until the top of the coal was burned out so that it screened somewhat for exposure to the heat radiation from below. As far as I know, no one was hurt by walking over the bed.

One might wonder for how long time one could trust the similarity solution. If we assume that the outer layer of the skin (*epidermis*) is about L = 0.5mm, it is possible to estimate the time by setting $\eta = 1$, or

$$t = \frac{L^2}{\kappa} = \frac{\left(10^{-3}/2\right)^2 \times 1000 \times 4000}{0.6} s = 1.7s.$$
 (287)

It is not worth stopping!

The temperature for this particular example is shown for 0(1)5 seconds on Fig. 30. As one can see, our estimate is realistic, but the temperature increase has reached far less than 2mm into the foot even after 5 seconds.



Figure 30: The temperature profile across the contact for a situation with the foot to the left and hot coals to the right shown for 0(1)5 seconds. Note that both the temperature and flux are continuous at x = 0 when t > 0.

5.5 Non-linear Diffusion

While models leading to linear diffusion equations are relatively simple to analyze, new and unexpected things when the diffusion coefficient depends on the dependent variable and the equation becomes nonlinear.

Gas flowing isothermally in a porous medium is a simple example that leads to a nonlinear diffusion equation. A porous medium, such as sandstone, have small pores that gas can flow in. *Porosity*, ϕ , is the volume fraction of pores so that $0 < \phi < 1$. *Darcy's Law* says that the volume flow (m³ / (m² s) is given by

$$\mathbf{q} = -\frac{K}{\mu} \nabla p \tag{288}$$

where K is a constant of proportionality called the *permeability*. Furthermore, μ is the dynamic viscosity of the gas and p the pressure. We shall assume that the state equation for the gas has the form $p = a\rho^{\gamma}$, where $\gamma > 0$. The conservation law for the gas will then be

$$\frac{d}{dt} \int_{R} \phi \rho dV + \int_{\partial R} \rho \mathbf{q} \cdot \mathbf{n} d\sigma = 0, \qquad (289)$$

which gives us the differential formulation

$$\phi \frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \mathbf{q}) = 0.$$
(290)

If we insert the state equation in the expression for \mathbf{q} , we obtain

$$\mathbf{q} = -\frac{K}{\mu}\nabla p = -\frac{Ka\gamma}{\mu}\rho^{\gamma-1}\nabla\rho,\tag{291}$$

and therefore

$$\frac{\partial \rho}{\partial t} = \nabla \cdot \left(\frac{Ka\gamma}{\mu\phi} \rho^{\gamma} \nabla \rho \right).$$
(292)



Figure 31: Sketch of the solution for $\kappa(\rho) = \rho$.

As we see, we have got a diffusion equation with a diffusion coefficient which is proportional to ρ^{γ} . In particular, we see that diffusion coefficient approaches 0 when the density tends to 0 (when γ is greater than 0). There is a lot of theory for non-linear diffusion equations although it is no longer possible to apply the superposition principle for solutions. Even for such equations there are similarity solutions. For equations

$$\frac{\partial \rho}{\partial t} = \frac{\partial}{\partial x} \left(\kappa(\rho) \frac{\partial \rho}{\partial x} \right) \tag{293}$$

one may look at solutions on the form $\rho(x,t) = g(s)$, $s = x/t^{1/2}$. If we insert this, we obtain an ordinary differential equation for g:

$$\kappa(g)g'' + \kappa'(g)g'^2 + \frac{s}{2}g' = 0.$$
(294)

For $\kappa(g) = 1$ the equation is reduced to g'' + sg'/2 = 0 with the well-known solution

$$g(s) = A \int_{-\infty}^{s} e^{-\xi^2/4} d\xi + B.$$
 (295)

If $\kappa(\rho) = \rho$, we obtain a solution that is sketched in Fig 31. The solution is 0 at a finite value of s, and therefore, $x_{\max} = s_{\max}\sqrt{t} \propto \sqrt{t}$. For this diffusion equation the solution spreads out at a final speed! See [4] for a more detailed analysis of diffusion.

Another class of solutions are the so-called *Barenblatt solutions* for $\kappa = \kappa_0 \left(\rho/\rho_0\right)^m$:

$$\rho(x,t) = \rho_0 \left(\frac{t_0}{t}\right)^{1/(m+2)} \left(1 - \left(\frac{x}{x_1}\right)^2\right)^{1/m}, \ t > 0, \ |x| \le x_1 = x_0 \left(\frac{t}{t_0}\right)^{1/(m+2)}$$
(296)

 $(t_0 \text{ and } x_0 \text{ may be expressed by } \kappa_0 \text{ and } Q = \int_{x=-\infty}^{\infty} c(x,0) dx$). Contrary to the standard fundamental solution corresponding to the limit $m \to 0$, the Barenblatt solutions for m > 0 have finite extension on the x-axis. Examples of Barenblatt solutions for a selection of m-values are shown on Fig. 32.

Also for these equations there are theorems saying that solutions of random, but localized initial conditions approach the Barenblatt solutions when the time increases. The solutions are described in [8], but not in [1].



Figure 32: Barenblatt solutions shown for four different values of m. The solutions are scaled according to their maximum.



Figure 33: An observed signal consisting of rapid fluctuations and a more slowly varying mean.

6 MODELLING OF TURBULENCE

The theory of turbulence is a very good example of how we can make use of stochastic considerations in mathematical modeling. We abandon to describe the phenomenon in a deterministic way below a certain level, saying that faster variations are *stochastic* or *random*. When a complete description is out of reach, we try instead to model the evolution of the mean values, as illustrated on Fig. 33.

We shall illustrate this technique by showing how one obtains equations for turbulence in the very simplest case, namely for an incompressible, viscous fluid without any influence of external forces.

To derive the equations we need the continuity equation and Navier-Stokes equation that was derived in Sec. 4. We start by the following four differential equations

$$\nabla \cdot \mathbf{v} = 0, \tag{297}$$

$$\frac{\partial}{\partial t}\mathbf{v} + \nabla \cdot ((\mathbf{v})\mathbf{v}) = -\frac{1}{\rho}\nabla p + \frac{\mu}{\rho}\nabla^2 \mathbf{v}$$
(298)

In turbulence theory a full solution of equations 297 and 298 is out of reach. The velocity

and the pressure are however seen as random variables and written

$$\mathbf{v} = E(\mathbf{v}) + (\mathbf{v} - E(\mathbf{v})),$$

$$p = E(p) + (p - E(p)).$$
(299)

Expectation values vary over space and time scales given by the dimensions of the phenomenon we see. These scales are called the *macroscopic scales*. "Small-scale variations" or the so-called *fluctuations* take place at the *microscopic scales*. In turbulence theory assumes that these scales are well separated, but in some situations that does not not need to be the case.

Unfortunately, the practice of turbulence theory is the opposite of the one used in statistics and probability theory: Deterministic variables are denoted by capital letters and random variables with lower case letters. In order not to confuse readers with a background in mechanics, we shall stick to this practice. Thus we use V for E(v), and v - E(v) by v:

$$\mathbf{v} := \mathbf{V} + \mathbf{v},$$

$$p := P + p. \tag{300}$$

Here **V** and *P* are deterministic functions of the macroscopic variables **x** and *t*, while **v** and *p* are stochastic variables with expectations 0, $\mathsf{E}(\mathbf{v}) = 0$, $\mathsf{E}(p) = 0$. Often it is assumed that **v** and *p* are Gaussian variables, and in general, the parameters in the probability distributions of **v** and *p* will depend on **x** and *t*.

We now introduce Eq. 300 into Eq. 297 and apply the expectation operator, which we assume commutes with the differentiation:

$$0 = E\left(\nabla \cdot (\mathbf{V} + \mathbf{v})\right) = \nabla \cdot \mathbf{V} + \nabla \cdot E\mathbf{v} = \nabla \cdot \mathbf{V}.$$
(301)

Thus we see that \mathbf{V} also satisfies the Eq. 297

$$\nabla \cdot \mathbf{V} = 0 \tag{302}$$

and even $\nabla \cdot \mathbf{v} = 0$.

If Eq. 298 is treated in the same way, we obtain for component "j"

$$\rho\left(\frac{\partial V_j}{\partial t} + \nabla \cdot (V_j \mathbf{V}) + \nabla \cdot E\left(v_j \mathbf{v}\right)\right) = -\frac{\partial P}{\partial x_j} + \nabla \cdot (\mu \nabla V_j).$$
(303)

It is usual here to insert the tensor $\mathbf{T} = -\rho E(\mathbf{v}\mathbf{v}')$, that is, $T_{ij} = -\rho E(v_i v_j)$. This tensor is called the Reynolds stress tensor. The momentum equation for the macroscopic variables is then

$$\rho(\mathbf{V}_t + \nabla \cdot ((\mathbf{V})\mathbf{V}) = -\nabla P + \nabla \cdot (\mu \nabla \mathbf{V} + \mathbf{T}).$$
(304)

Eq. 304 differs from Eq. 302 by an extra force term, $\nabla \cdot \mathbf{T}$, whereas Eq. 302 is essentially the same as Eq. 297.

By subtracting Eq. 304 from 298 and inserting $\mathbf{V} + \mathbf{v}$ etc., we obtain an equation for \mathbf{v} . If we then take the scalar product with \mathbf{v} and apply the expectation operator, the result is a transport equation for *turbulent energy per unit volume*,

$$e = \rho \frac{1}{2} E(\mathbf{v} \cdot \mathbf{v}). \tag{305}$$

The fundamental question now is how to express the Reynolds stresses by means of macroscopic variables. This is the main problem in turbulence theory. The oldest attempt was made by Boussinesq as early as 1877. He defined **T** as a function of $\partial V_i/\partial x_j$ in the same way as the stress tensor for a Newtonian fluid. Thus we can write equation

$$\rho(\mathbf{V}_t + \mathbf{V} \cdot \nabla \mathbf{V}) = -\nabla P + \nabla \cdot ((\mu + \mu_T) \nabla \mathbf{V}), \qquad (306)$$

and the conservation laws of mass and momentum have exactly the same form as before. The constant μ_T , with the dimension of viscosity, represents an additional "viscosity" due to turbulence, called *eddy viscosity*. It has been shown that this model matches free turbulent flow well, where μ_T can be 10 to 1000 times greater than μ . Since it is easy to apply, this has led to an extensive use as an adjustment factor in numerical computations. More advanced models relate μ_T to the local turbulent energy.

If a liquid contains a substance that is mixed with the liquid by turbulent diffusion, we will, in addition to Eq. 297 and 298 have a convection/diffusion equation for the concentration c of the substance (the "substance" may well be heat content):

$$\frac{\partial c}{\partial t} + \mathbf{v} \cdot \nabla c = \nabla \cdot (\kappa \nabla c), \tag{307}$$

where κ is the diffusion coefficient.

In the same way as for **V** and *P* it is possible to write the concentration Ec + (c - Ec) := C + c, and if this is inserted into the equation, we have

$$\frac{\partial(C+c)}{\partial t} + (\mathbf{V} + \mathbf{v}) \cdot \nabla(C+c) = \nabla \cdot (\kappa \nabla(C+c)).$$
(308)

When we then apply the expectation operator and apply $\nabla \cdot \mathbf{v} = 0$, we obtain

$$E(\mathbf{v} \cdot \nabla c) = E(\nabla \cdot (\mathbf{v}c)) - E(c\nabla \cdot \mathbf{v}) = \nabla \cdot E(\mathbf{v}c), \qquad (309)$$

and

$$\frac{\partial C}{\partial t} + \mathbf{V} \cdot \nabla C = \nabla \cdot \left(\kappa \nabla C - E(\mathbf{v}c)\right). \tag{310}$$

The vector $\mathbf{q}_T = E(\mathbf{v}c)$ is called the turbulent flux. As for the Reynolds stresses, it is difficult to relate this flux to macroscopic variables. The simplest way is of course again to assume that $\mathbf{q}_T = -\kappa_T \nabla C$, as this gives the same equation as before with a new diffusion constant $\kappa + \kappa_T$.

7 PROBLEMS

7.1 Simple Problems

Note: No solutions are provided for the simple problems.

Problem 1

(a)

- How is *density* defined?
- How is *flux* defined?
- What is a *point source*, and how can it be described?
- What is a *distributed source*, and how can it be expressed when the flux is known?

(b) What is the flux for a substance that passively follows a fluid velocity field $\mathbf{v}(\mathbf{x},t)$? Show that the dimension of the expression is consistent with the definition of flux.

(c) How do we derive the differential form the integral form of the general conservation law?

Problem 2

A hemisphere with radius r has center at the origin, and is bounded by $0 \le z$. The flux field **j** is defined in the space as

$$\mathbf{j}(\mathbf{x},t) = (y\sin z)\,\hat{\imath}_x + xz^3\hat{\imath}_y + z\hat{\imath}_z,\tag{311}$$

where $\{\hat{i}_x, \hat{i}_y, \hat{i}_z\}$ are the unit vectors along the coordinate axes. Calculate the flow of material through the curved part of the surface of the hemisphere, i.e. $|\mathbf{x}| = r, z > 0$. *Hint:* The solution is simple.

Problem 3

A chemical dissolved in a liquid spreads by molecular diffusion, modeled by means of the flux

$$\mathbf{j} = -\kappa \nabla \varphi, \tag{312}$$

where φ is the concentration of the substance (kg/m³), κ is a constant, and ∇ the gradient. What is the unit of κ ? The substance decays over time, and during the time from 0 to t, the concentration (if nothing else happens) has decreased as

$$\varphi\left(\mathbf{x},t\right) = \varphi_0 e^{-t/t_0}.\tag{313}$$

This represents a distributed sink, but how can this be described as a function $q(\mathbf{x},t)$?

Use the general conservation law to derive the differential equation

$$\frac{\partial \varphi}{\partial t} = \kappa \nabla^2 \varphi - \frac{\varphi}{t_0}.$$
(314)

Problem 4

Find the solution surface, z = f(x, y), to the quasi-linear first order partial differential equation

$$\frac{\partial z}{\partial x} + y \frac{\partial z}{\partial y} - 2 = 0 \tag{315}$$

so that the space curve defined by

$$\begin{aligned} x &= t, \\ y &= 1, \\ z &= t, \end{aligned}$$
 (316)

 $t \in \mathbb{R}$ is in the surface.

Hint: Follow the recipe in the Appendix of the note step-by-step.

Problem 5

How is the flux of a substance defined if it diffuses and is simultaneously transported by a moving fluid? State the conservation law both in integral and differential form.

Problem 6

(a) Define the fundamental solution $c_f(x,t)$ of the equation

$$\frac{\partial c}{\partial t} = \kappa \frac{\partial^2 c}{\partial x^2}, \ x \in \mathbb{R}, \ t \ge 0.$$
(317)

where c(x,t) is the concentration of a substance and κ is a positive constant (what is κ called?).

The fundamental solution represents a unit discharge in the point x = 0 at time t = 0.

(b) Show that the total amount, $\int_{-\infty}^{\infty} c(x,t) dx$, remains equal to 1 for all t > 0. It is reasonable to consider c(x,t) as a probability density on \mathbb{R} . What is in this case the *mean value*, η , and *standard deviation*, σ ?

(c) In statistics $\pm 3 \times \sigma$ is often said to be the typical extension of a distribution. What is the $[-3\sigma, 3\sigma]$ -interval here?

(d) The equation

$$\frac{\partial c}{\partial t} + v \frac{\partial c}{\partial x} = \kappa \frac{\partial^2 c}{\partial x^2},\tag{318}$$

where v is a positive constant, represents a situation where what we are considering is moving to the right with constant speed v. What is the fundamental solution in this case?

(e) Show that if the distribution at $t = t_0$ is $c(x, t_0) = h(x)$, the general solution of Eq. 1 for $t > t_0$ may be written

$$c(x,t) = h * c_f(\cdot, t - t_0)(x,t) = \int_{-\infty}^{\infty} h(s) c_f(x - s, t - t_0) ds.$$
(319)

(f) Use the expression in (e) (or a smarter way, based on the uniqueness of solutions) to find the solution for t = 3 when the solution of t = 1 is

$$h(x) = c_f(x, 1).$$
 (320)

Can you derive a general property of convolutions of the fundamental solutions based on this?

(g) Which condition on the diffusive flux \mathbf{j}_d must hold at x_0 if there is a dense wall there, so that all diffusion occurs to the right of the wall $(x \ge x_0)$.

(h) Show (or argue) that if x_0 in (g) is larger than 0, it is possible to write the solution for a unit emission at x = 0 for t = 0 as

$$c(x,t) = c_f(x,t) + c_f(x - 2x_0,t), \ x \ge x_0, t > 0.$$
(321)

Problem 7

(a) Determine the fundamental solutions for

$$\frac{\partial c}{\partial t} = \kappa \left(\frac{\partial^2 c}{\partial x^2} + \frac{\partial^2 c}{\partial y^2} \right), \ (x, y) \in \mathbb{R}^2, \ t \ge 0,$$
(322)

$$\frac{\partial c}{\partial t} = \kappa \left(\frac{\partial^2 c}{\partial x^2} + \frac{\partial^2 c}{\partial y^2} + \frac{\partial^2 c}{\partial z^2} \right), \ (x, y, z) \in \mathbb{R}^3, \ t \ge 0,$$
(323)

As long as we are interested in solutions defined on \mathbb{R}^n , we may use the fundamental solution to express more general solutions. The two-dimensional equation 322 may, *e.g.* describe the extent of an oil spill on the surface of the sea.

(b) Determine how a unit emission at t = 0 from an off shore oil platform situated at x = 0 will evolve if it in addition is a constant current in the sea. A variable emission over a period of time can be approximated as a number of small spills occurring at constant time intervals. State an expression for the solution in this case. The extent of the oil slick could be defined as the area where the oil film is thicker than a certain thickness, e.g. 5 molecular diameters. *Challenge*: Program and visualize this slick using Matlab or Octave.

7.2 Modeling Problems

Note: Solution outlines and comments are found in Sec. 7.3.

7.2.1 The Student 10km Race

Many years ago, the students' sport club at NTNU arranged the *Student 10km Race* at the old Trondhjem Stadion. The arrangement was terribly crowded with more than 1000 participants, all starting (or trying to start) at the same time. This spectacular event, often in rain and on a terribly dirty track is the origin of the following problem.

Consider an ordinary race-track with length L = 400m. We assume that the mean running speed v^* decreases linearly with the density ρ^* , so that $v^* = v^*_{\text{max}}$ for $\rho^* = 0$ students/m, and is $v^* = 0$ m/s when $\rho^* = \rho^*_{\text{max}}$. We also consider the track to be onedimensional and 0-shaped.

(a) State the conservation law for students (assuming no late entries or drop-outs) under these conditions, introduce dimensionless variables, and show that the differential
formulation for the students' density may be written as

$$\rho_t + (1 - 2\rho)\,\rho_x = 0,\tag{324}$$

where $0 \le \rho \le 1$ and $\rho(x, t)$ is a 2π -periodic function of x.

(b) Find (in implicit form) the exact solution of Eq. 324 when

$$\rho(x,0) = \rho_0 + \varepsilon \cos(x), \quad (0 < \rho_0, \ 0 < \varepsilon < \rho_0). \tag{325}$$

Sketch the characteristics for the solution in the xt-plane and show that, as a solution of the integral conservation law, it breaks down and forms a shock in the density after some time.

(c) When will the shock start, and what happens to the shock when $t \to \infty$?

(*Hint*: Start by determining the crossing points for characteristics starting at $3\pi/2 - \theta$ and $3\pi/2 + \theta$, when θ varies from 0 to π . Try to prove that the crossing points lie on a straight line segment, and that there are no crossings elsewhere. Finally, check that the line segment is a shock and that the corresponding solution indeed satisfies the integral conservation law.

7.2.2 Two Phase Porous Media Flow

Oil is found in porous rocks. Often the porous rock is trapped between layers of solid impermeable rock, called an *oil reservoir*, and when we pump oil out, ground water enters. In so-called *enhanced oil recovery*, water is actively pumped into the reservoir and the oil is forced out. The simultaneous flow of oil and water is complex, and in order to study this in detail, small samples of rock are taken from the reservoir and investigated in the laboratory. The following model is essential in these investigations.

A long thin cylinder of porous sandstone with constant cross section A is situated along the x-axis. The pores occupy a constant fraction Φ of the volume ($0 < \Phi < 1$), and are initially filled with oil. We assume that the oil has constant density and measure the amount of oil by its volume. The sides of the cylinder are closed, but by applying a pressure at one end, it is possible to press oil or water through the stone.

In order to find an expression for the flux of oil in the x-direction, $j \, [m^3/(m^2s)]$, we assume it only depends of the viscosity, $\mu \, [kg/ms]$, the permeability (inverse flow resistance) of the stone, $K \, [m^2]$, and the pressure gradient, $\partial p / \partial x$.

(a) Show that dimensional analysis gives

$$j = -k\frac{K}{\mu}\frac{\partial p}{\partial x},\tag{326}$$

where k is a dimensionless constant.

Assume that the pores of the cylinder in addition to oil also contains water. All pores are either filled with water or oil, so that a volume V of rock contains a volume $S_o \Phi V$ of oil and $S_w \Phi V$ of water, where $S_o + S_w = 1$. We assume that water and oil have the same pressure and that the corresponding fluxes may be written as

$$j_i = -k_i \left(S_i\right) \frac{K}{\mu_i} \frac{\partial p}{\partial x}, \ i = o, w.$$
(327)

The parameter $k_i(S_i)$ is called the relative permeability.

(b) Establish the conservation laws for oil and water for the part of the cylinder between x = a and x = b. Show that if we apply a pressure gradient such that

$$q = j_o + j_w = \text{constant},\tag{328}$$

then we have, for $S \equiv S_w$, the following hyperbolic equation for S:

$$\Phi \frac{\partial S}{\partial t} + \frac{\partial}{\partial x} f(S) = 0,$$

$$f(S) = \frac{qk_v(S)/\mu_v}{k_o(1-S)/\mu_o + k_v(S)/\mu_v}.$$
(329)

(c) Assume that $\mu_o = \mu_w$, $k_o(1-S) = 1 - S^2$ and $k_w(S) = S^2$. Solve the equation (329) for t > 0 for a cylinder of length L when

$$S(x,0) = 1 - x/L, \ 0 \le x \le L,$$

$$S(0,t) = 1, \ 0 \le t.$$
(330)

7.2.3 Reduced Speed Limit

In this problem we are considering the *standard model* for the traffic of cars along a one-way road.

(a) Describe the basis of the standard model. State the hyperbolic equation the model leads to (when no cars are assumed to enter or leave the road). When will the car density develop shocks?

(b) Between x = 0 and x = 1 there is now a reduction in the speed limit such that the maximal speed reduces to 1/2, while the maximum density remains the same. We assume that a similar linear relation between the car velocity and the density also applies for this part of the road.

Which condition on the flux of cars has to hold at x = 0 and x = 1? Find the solution $\rho(x, t)$ for t > 0 and all x when

$$\rho(x,0) = \begin{cases} 1/2, & x < 1, \\ 0, & x > 1. \end{cases}$$
(331)

Hint: The density ρ between 0 and 1 remains constant for all $t \ge 0$.

7.2.4 Traffic Lights at a Pedestrian Crossing

In this problem we study the traffic along a one way street, and without cars entering or exiting in the first part. All variables are scaled so that the car density ρ is between 0 and 1, and car velocity v is equal $1 - \rho$.

(a) Show how to find an expression for the shock velocity U of a jump in car density, and derive that in this case, $U = 1 - \rho_1 - \rho_2$, where ρ_1 and ρ_2 are the densities on each side of the shock.

For t < 0, there is a constant car density $\rho = 1/2$ on the street. Between t = 0 and t = 1 the cars face a *red* light at a pedestrian crossing at x = 0. For t > 1, the light is again *green*.

(b) Determine the solution $\rho(x, t)$ for $t \ge 0$.

(*Hint*: Make a sketch of the situation in an x/t-diagram. Show that the solution for ρ has to be found in five different domains, of which the values in four of them are obvious. In order to determine the domains it is necessary to determine their exact borders).

At another place on the street, a second one way street of the same type as the first merges with the first street.

(c) Which condition must hold at the junction? Assume that the flux on the first street towards the junction is constant, $j_1 = 1/8$, and the corresponding car density is less than 1/2. Describe the development of car density on the streets when the density ρ_2 on the second street increases from 0 to 1. The drivers on the first street have the right of way, but are flexible and let cars enter from the second street if this is possible. In particular, look at what happens when the flux on the second street reaches 1/8.

7.2.5 A Water Cleaning System

A part of a water cleaning system is modelled as a tube of length L along the x^* -axis, where polluted water flows with constant velocity V. The tube also contains absorbers that remove the pollution. The concentration of pollutant in the water is c^* , measured as amount per length unit of pipe. Similarly, the amount of absorbed pollutant per length unit of pipe is denoted ρ^* . The maximum value of ρ^* is A. Some of the absorbed pollutant will over time re-enter the water stream. The absorption and re-entering is modelled by the equation

$$\frac{\partial \rho^*}{\partial t^*} = k_1 \left(A - \rho^* \right) c^* - k_2 \rho^*.$$
(332)

(a) State the integral conservation law for the pollutant and show that this leads to the differential form

$$\frac{\partial}{\partial t^*} \left(c^* + \rho^* \right) + \frac{\partial}{\partial x^*} \left(V c^* \right) = 0.$$
(333)

Based on the integral law, establish that a discontinuity in the concentrations, moving with velocity U^* , has to fulfil

$$U^* = \frac{c_2^* - c_1^*}{(c_2^* + \rho_2^*) - (c_1^* + \rho_1^*)} V,$$
(334)

where (c_1^*, ρ_1^*) and (c_2^*, ρ_2^*) are the concentrations on each side of the discontinuity.

(b) Introduce suitable scales and show that the differential equations may be written

$$\frac{\partial}{\partial t}\left(c+\rho\right) + \frac{\partial c}{\partial x} = 0,\tag{335}$$

$$\varepsilon \frac{\partial \rho}{\partial t} = (1 - \rho) c - \beta \rho.$$
(336)

Explain the meaning of ε and β (*Hint*: Use the same scale for ρ^* and c^*).

Assume that the tube is infinitely long in both directions and consider analytic solutions of equations 335 and 336 in the form of "fronts", travelling with velocity U, that is,

$$c(x,t) = C(x - Ut), \qquad (337)$$

$$\rho(x,t) = R(x - Ut). \qquad (338)$$

With $\eta = x - Ut$, we limit ourselves to the special case where $C(\eta)$ and $R(\eta)$ satisfy

$$\lim_{\eta \to -\infty} C\left(\eta\right) = 1,\tag{339}$$

$$\lim_{\eta \to \infty} C\left(\eta\right) = 0,\tag{340}$$

$$\lim_{\eta \to -\infty} R\left(\eta\right) = \frac{1}{1+\beta},\tag{341}$$

$$\lim_{\eta \to \infty} R\left(\eta\right) = 0. \tag{342}$$

(c) Insert 337 and 338 into Eq. 335, integrate once, and use the behaviour at $-\infty$ and ∞ to determine U and a simple relation between C and R. Use this information and Eq. 336 to determine $C(\eta)$ and $R(\eta)$. How is the behaviour of the solution when $\varepsilon \to 0$? (*Hint*: The equation

$$\frac{dy}{d\zeta} = y\left(-1 + \frac{y}{M}\right) \tag{343}$$

has a solution

$$y\left(\zeta\right) = M \frac{1}{1 + \exp\zeta} \tag{344}$$

for 0 < y < M).

(d) Assume $\varepsilon = 0$ in Eq. 336 so that the system (335 and 336) simplifies to

$$\rho = \frac{c}{c+\beta}, \ \frac{\partial Q(c)}{\partial t} + \frac{\partial c}{\partial x} = 0, \tag{345}$$

$$Q(c) = c + \frac{c}{c+\beta}, \ -\infty < x < \infty, \ t \ge 0.$$
 (346)

Consider the initial condition

$$c(x,0) = \begin{cases} 1, & x < 0, \\ 0, & x > 0. \end{cases}$$
(347)

Show that the corresponding solution of Eq. 345 develops a shock. Determine the shock velocity from the expression in point (a) and compare to the result in (c).

7.2.6 River Contamination

Discharge of contaminants into a river will be transported with the flow (*convection*) and spread due to turbulence mixing and varying water velocity (*diffusion*). Consider a one-dimensional river with mean flow U and the diffusion coefficient κ .

(a) Derive the expression for the flux of contaminants under these simple conditions, and find a length scale of the extent of an instantaneous point discharge after this has been carried a length L down the river by means of the current. At the point x = 0 there is a continuous discharge of a substance A so that the concentration in the river becomes a(x,t). The substance A is converted into substance B with constant rate μ . Thus, for a water sample from the river we would have

$$\frac{da}{dt} = -\mu a. \tag{348}$$

The substance B decays with rate λ , and for the same water sample, the concentration b(x,t) of B fulfils

$$\frac{db}{dt} = +\mu a - \lambda b.$$

(b) State the conservation laws for A and B on the integral and differential form.

(c) The discharge at x = 0 takes place at a constant rate q_0 (amount per time unit). Neglect diffusion and decide how far down the river the concentration of the substance A is at its highest when we assume that $\lambda = \mu$.

Hint: The differential equation $\frac{dy}{dt} + ky = e^{-kt}$ has the general solution $y(t) = C_1 e^{-kt} + te^{-kt}$.

7.2.7 Lake Sedimentation

A river flows into a lake. The river brings sand and clay so that the lake is filled up over time. We shall formulate and analyze a simple one-dimensional model for how the lake is filled, and assume that it reaches from x = 0 to $+\infty$ and has a constant depth h at t = 0. Conditions across (in the y-direction) are assumed to be constant.

The amount of sand and clay which settle on the bottom per time and area unit is q(x,t). We write the depth $z = b(x,t), x \ge 0, t \ge 0$, and assume $b(x,t) \le 0$. If the bottom tilts (is not horizontal), the particles on the bottom will continue to move, and it has been found that the mass flux is proportional to the slope, that is, the volume flux may be written

$$j = -k\frac{\partial b}{\partial x}.\tag{349}$$

(a) Write the conservation equation in integral form for a part of the bottom, $x_0 \le x \le x_1$, and show that the differential form is identical to the heat diffusion equation,

$$\frac{\partial b}{\partial t} = k \frac{\partial^2 b}{\partial x^2} + q. \tag{350}$$

(b) Assume that all sand and clay enter at x = 0 (i.e. q = 0 for x > 0), and that the amount entering is always sufficient for Eq. 350 to hold for t > 0. Argue that the solution to Eq. 350 will be a similarity solution in this case, and find b(x,t) for $x \ge 0$ and t > 0. (*Hint:*The equation

$$\frac{d^2y}{d\eta^2} + \frac{\eta}{2}\frac{dy}{d\eta} = 0 \tag{351}$$

has the general solution $A + B \operatorname{erf}(\eta/2)$, where $\operatorname{erf}(x) = \frac{2}{\sqrt{\pi}} \int_0^x \exp(-s^2) \, ds$).

(c) A more realistic scenario is that the shore, s(t), moves forward into the lake over time. Assume that a constant volume of sand and clay enter the basin per time unit, q_0 , and that all sand and clay enter at the shore.

The solution will then have a stationary shape and may be written by means of a function b_0 so that

$$b(x,t) = \begin{cases} 0 & x \le s(t) = Ut + x_0 \\ b_0(x - Ut - x_0) & x > Ut + x_0 \end{cases}$$
(352)

Determine the velocity U and the solution in this case.

7.2.8 The Insect Swarm

Flying insects sometimes form dense swarms where the insects are attracted to each other. On the other hand, the swarm has a certain extension, which implies that there is also something preventing the insects from coming too close to each other. This modeling study tries to explain this as a balance between the attraction towards the swarm and a random motion modelled as a diffusion.

The model is for simplicity one-dimensional, where the insects are assumed to stay in a straight tube (For more information, see: P. Grindrod: *Patterns and Waves*, Claredon Press, Oxford, 1991, pp. 188–189).

An insect swarm with density $\rho(x^*, t^*)$ is situated in a long tube parallel to the x^* -axis. In the swarm random flight (diffusion) contributes to spreading the insects, while the insects in the swarm are also attracted towards the center of the swarm. This latter effect can be modeled as a mean drift velocity w,

$$w(x^*, t^*) = -K\left(\int_{-\infty}^{x^*} \rho(s^*, t^*) \ ds^* - \int_{x^*}^{\infty} \rho(s^*, t^*) \ ds^*\right).$$
(353)

We shall assume that the total amount of insects,

$$M = \int_{-\infty}^{\infty} \rho(x^*, t^*) \, dx^*, \tag{354}$$

remains constant.

(a) Explain why the model for w is not unreasonable, and state the conservation law for insects in integral form.

(b) Introduce the cumulative distribution of insects,

$$v^*(x^*, t^*) = \int_{-\infty}^{x^*} \rho(s^*, t^*) \, ds^*, \tag{355}$$

and show from the conservation law that v^* satisfies the equation

$$\frac{\partial v^*}{\partial t^*} = \sigma \frac{\partial^2 v^*}{\partial x^{*2}} - K(M - 2v^*) \frac{\partial v^*}{\partial x^*}$$
(356)

where σ is the diffusion coefficient. We assume that σ and K are constant.

(c) For a swarm with a diameter L there are two characteristic time scales,

$$T_K = \frac{L}{KM}$$
 and $T_D = \frac{L^2}{\sigma}$ (357)

What do these scales signify? Scale the equation for v^* when $x^* = \mathcal{O}(L)$, $t^* = \mathcal{O}(T_K)$ and $T_D \gg T_K$, and show that it can be stated as

$$\frac{\partial v}{\partial t} = \varepsilon \frac{\partial^2 v}{\partial x^2} - (1 - 2v) \frac{\partial v}{\partial x}.$$
(358)

What is the interpretation of ε ?

(d) Determine $\rho^*(x^*, t^*)$ when

$$\rho^*(x^*, 0) = \begin{cases} \frac{M}{2L}, & |x^*| < L\\ 0, & \text{otherwise} \end{cases},$$
(359)

when we ignore the effect of diffusion. How do you expect, in rough terms, that the exact solution looks when diffusion is included?

(e) To examine the solution in (d) after a long time, it is reasonable to consider a length scale $L' = \sigma/(KM)$ and a time scale $T \gg T_K$ and T_D . Show that with this scaling the equation for v is independent of t to leading order. Verify that the leading order equation has a solution

$$\rho^*(x^*, t^*) = A \frac{1}{\cosh^2(Bx^*)}$$
(360)

and determine A and B for a solution with the initial distribution as in (\mathbf{d}) .

Hint: Use that $\frac{d}{dx} \tanh(x) = \cosh^{-2}(x)$, and try a v with the correct behaviour when $x \to -\infty$ and $x \to \infty$.

7.3 Solution Outline for the Modeling Problems

7.3.1 The Student 10km Race

(a) The derivation is the standard one with the flux given by

$$j^*(\rho^*) = \rho^* v_{\max} \left(1 - \rho^* / \rho_{\max} \right).$$
(361)