Flow and Transport

1. The Transport Equation

We shall describe the transport of a dissolved chemical by water that is traveling with uniform velocity ν through a long thin tube G with uniform cross section S. (The very same discussion applies to the description of the transport of gas by air moving through a pipe.) We identify G with the open interval (a, b), and the velocity $\nu > 0$ is in the (rightward) positive direction of the x-axis. Since the tube is very thin, we can assume that the concentration of the chemical is constant across the cross section S at each point $x \in G$. Let $c(x, t)$ denote this concentration within the tube at a point $x \in G$ and at time $t > 0$.

The Conservation Law. The amount of chemical stored in the tube within a section $[x, x + h]$ of length $h > 0$ is given by

$$\int_x^{x+h} c(s, t)S \, ds,$$

The *flux* $q(x, t)$ at the point x is the mass flow rate of the chemical to the right per unit area, Equating the rate at which the chemical is stored within the section $[x, x + h]$ to the rate at which it flows into the section plus the rate at which the chemical is generated within this section, we arrive at

$$\frac{d}{dt} \int_x^{x+h} c(s, t)S \, ds = S\big(q(x, t) - q(x + h, t)\big) + \int_x^{x+h} F(s, t)S \, ds$$

where $F(x, t)$ represents the rate at which chemical is generated per unit volume. This *source* term is assumed to be a known function of space and time. We differentiate the integral on the left side and write the difference on the right side as an integral of a derivative to obtain

$$\int_x^{x+h} \frac{\partial c(s, t)}{\partial t} S \, ds = S \int_x^{x+h} \left(-\frac{\partial q(s, t)}{\partial x} + F(s, t) \right) ds.$$

Dividing this by Sh and letting $h \to 0$ yield the *conservation law*

(1) $$\frac{\partial c}{\partial t} + \frac{\partial q}{\partial x} = F(x,t).$$

The transport equation. The *flux* $q(x,t)$ at the point x is given by

(2) $$q(x,t) = \nu c(x,t).$$

This is the mass flow rate of the chemical due to *convection*, the direct transport by the moving water. Substituting this into the conservation law (1) yields the one–dimensional *transport equation*

(3) $$\frac{\partial c}{\partial t} + \nu \frac{\partial c}{\partial x} = F(x,t).$$

This is also known as the *first-order wave equation.* It is just the differential form of the conservation equation (1) combined with the constitutive equation (2) of convection. It is assumed here that the velocity ν is sufficiently large that we can ignore the comparatively smaller effects of diffusion, *i.e.*, the natural motion of the chemical from areas of high concentration to those of lower concentration. This will be a major topic later.

Initial and Boundary conditions. Since the transport equation is first–order in space and time, one may expect that in order to have a well–posed problem, one boundary condition and one initial condition should be specified. We shall see that this is true here. We want to find a solution of (3) which satisfies an *initial condition* of the form

$$c(x,0) = c_0(x), \quad a < x < b,$$

where $c_0(\cdot)$ is given. That is, we need to specify the *initial state* of the model. Furthermore we shall specify the value of the concentration at the left end point where the substance is entering the tube:

$$c(a,t) = c_a(t), \quad t > 0,$$

where $c_a(\cdot)$ is given. This type of *boundary condition* arises when the value of the concentration at the end point is known, usually from a direct measurement. Such a condition arises when one sets the boundary concentration to a prescribed value, for example, $c_a(t) = 0$ when only pure water with no chemical is entering the left end of the tube.

The Solution: introduction of characteristic curve. Consider the homogeneous transport equation

$$c = c(x, t): \quad c_t + \nu\, c_x = 0\,.$$

If we make a change of variable to the new coordinates ξ, τ which are defined implicitly by

$$x = \xi + \tau, \quad \nu\, t = \xi - \tau,$$

and use the chain rule,

$$\frac{\partial c}{\partial \xi} = \frac{\partial c}{\partial x}\frac{\partial x}{\partial \xi} + \frac{\partial c}{\partial t}\frac{\partial t}{\partial \xi}\,,$$

we find that the transport equation is equivalent to

$$c = c(\xi, \tau): \quad \frac{\partial c}{\partial \xi} = 0\,.$$

This shows that the solutions are given by

$$c(\xi, \tau) = f(\tau)\,,$$

so the general solution of the transport equation is of the form

$$c(x, t) = f(x - \nu\, t)$$

for some function $f(\cdot)$. Now let's choose this function so that $c(\cdot, \cdot)$ satisfies the initial and boundary conditions. The initial condition requires

$$c(x, 0) = f(x) = c_0(x), \quad x \geq a\,,$$

and the boundary condition likewise requires

$$c(a, t) = f(a - \nu\, t) = c_a(t), \quad t \geq 0\,,$$

so we must have $f(s) = c_a(\frac{a-s}{\nu})$, $s \leq a$. Thus, the solution of the initial-boundary-value problem is given by

$$c(x, t) = \begin{cases} c_0(x - \nu\, t), & x \geq \nu\, t \geq 0\,, \\ c_a(\frac{a - x + \nu\, t}{\nu}), & a \leq x \leq \nu\, t + a\,, \end{cases}$$

Note that the important fact behind these calculations is that the solution was constant along the curves where τ is constant, *i.e.*, along the curves where $x - \nu\, t$ is constant. It followed from this that the solution is a pure translation to the right with velocity ν, certainly no surprise in view of the origin of the transport equation. These special curves are the

characteristic curves for the transport equation, and they will arise in our discussions of first–order equations.

EXERCISE 1. *Suppose that $c_a(\cdot)$ and $c_0(\cdot)$ are continuous. Show that the solution of the initial-boundary-value problem is continuous if and only if $c_a(0^+) = c_0(a^+)$.*

EXERCISE 2. *Find the solution of the initial-value problem for the* non-homogeneous *transport equation (3) on the region $\{(x,t) : t \geq 0\}$ with the initial condition $c(x,0) = c_0(x)$ on $-\infty < x < +\infty$.*

2. The Porous Medium Equation

We shall describe the diffusion of fluid through the long thin tube G with uniform cross section S. As before, we identify G with the open interval (a,b), but here we assume that the tube contains a distribution of particles which impede the flow of the fluid. The fluid is constrained to flow in the complementary region of open channels and pores *not* occupied by the particles. This is the case for flow of fluids through soil or through any other such porous and permeable material.

The conservation law. Let $\rho(x,t)$ denote the *density* of the fluid within the tube at a point $x \in G$ and at time $t > 0$. The mass of fluid stored in the section $[x, x+h]$ of length $h > 0$ is given by

$$\int_x^{x+h} \phi(s)\rho(s,t)S \, ds,$$

where $\phi(x)$ is the *porosity* of the porous medium at x, *i.e.*, the volume fraction of the medium occupied by the fluid. The fluid *velocity* $\nu(x,t)$ at the point x is the flow rate to the right per unit area measured in volume of fluid per unit area per time. Equating the rate at which fluid is stored within the section to the rate at which fluid flows into the section plus the fluid source rate within this section, we arrive at the *fluid conservation* equation for the section $[x, x+h]$,

$$\frac{\partial}{\partial t} \int_x^{x+h} \phi(s)\rho(s,t)S \, ds =$$

$$S\big(\rho(x,t)\nu(x,t) - \rho(x+h,t)\nu(x+h,t)\big) + \int_x^{x+h} f(s,t)S \, ds \,,$$

where $f(x,t)$ represents the rate at which fluid is inserted per unit volume. This source term is assumed to be a known function of space and time. Dividing by Sh and letting $h \to 0$ yields the *fluid conservation* equation

$$(4) \qquad \phi(x)\frac{\partial \rho(x,t)}{\partial t} + \frac{\partial(\rho(x,t)\nu(x,t))}{\partial x} = f(x,t).$$

Darcy's law. Let $p(x,t)$ denote the *pressure* of the fluid in the pores. This is measured in force per unit area. A fundamental experimental observation in flow through porous media is that the fluid velocity $\nu(x,t)$ at the point x is proportional to the pressure gradient,

$$(5) \qquad \nu(x,t) = -\frac{k(x)}{\mu}\frac{\partial p(x,t)}{\partial x}.$$

The constant μ is the *viscosity* of the fluid, a measure of its resistance to *shear*, and this equation defines the *permeability* $k(x)$ of the porous medium at the point $x \in (a,b)$. It is a measure of the conductivity of the medium, *i.e.*, the inverse of resistance of the medium to internal flow. Since fluid flows in the direction of decreasing pressure, the minus sign is appropriate. In fact, if we write this in the form

$$\frac{\mu}{k(x)}\nu(x,t) = -\frac{\partial p(x,t)}{\partial x},$$

it is a balance of forces on the fluid as it flows through the medium, and the coefficient $\mu/k(x)$ is the *resistance* to flow. By substituting Darcy's law (5) into the energy conservation law (1), we obtain the one–dimensional *porous medium equation*

$$(6) \qquad \phi(x)\frac{\partial \rho}{\partial t} - \frac{\partial}{\partial x}\left(\rho\frac{k(x)}{\mu}\frac{\partial p}{\partial x}\right) = f(x,t).$$

It remains to specify the *state equation*, the relation between density ρ and pressure p for the particular fluid. If the fluid is *slightly compressible*, then we write $\rho = \rho_0 e^{c(p-p_0)}$ where the constant c is the compressibility of the fluid. In this case the chain rule shows that $\rho p_x = \frac{1}{c}\rho_x$, so we obtain the linear *diffusion equation* for fluid density

$$(7) \qquad c\phi(x)\frac{\partial \rho}{\partial t} - \frac{\partial}{\partial x}\left(\frac{k(x)}{\mu}\frac{\partial \rho}{\partial x}\right) = c\,f(x,t).$$

If the fluid is *incompressible, i.e.,* if $c = 0$, then the density is constant and we obtain the equation

$$(8) \qquad -\frac{\partial}{\partial x}\left(\rho_0\frac{k(x)}{\mu}\frac{\partial p}{\partial x}\right) = f(x,t).$$

Of course, either of these must be supplemented with appropriate initial and boundary conditions to get a well posed problem which determines the density and pressure along the length of the tube, and then these determine the Darcy velocity (5). This may be then used as data for the transport equation (3).

3. Dynamics of Chemical Adsorption

We consider next the effect of an *adsorbing medium* that is distributed throughout the length of the tube. This material occurs as a distribution of small particles or fibres, such as a porous medium. In equilibrium conditions, the concentration $a(x)$ of the chemical that is adsorbed onto the material at a point x is a specific function of the concentration $d(x)$ within the pores of the material. The quantities a and d are related by a given function

$$a = a(d)$$

called the *adsorption isotherm.* That is, $a(d)$ is the concentration of chemical adsorbed in the medium which is at the concentration d. In dynamic conditions, the concentration d in the medium can be different from the concentration c in the surrounding water. The relation of the adsorbed concentration $a(x,t)$ to the external water concentration $c(x,t)$ is given by

$$(9) \qquad \frac{\partial a(d)}{\partial t} = \beta(c - d)\,,$$

where $d(x,t)$ is the internal concentration of the chemical in the medium. The relation (9) is the equation of *kinetic adsorption,* and it describes the *dynamic* response of the adsorbed concentration to a changing concentration in the surrounding pores. The constant β is called the *kinetic coefficient* of the process.

The simplest form for the adsorption isotherm is the linear relationship $a(d) = \alpha\,d$ called the *Henry isotherm* in which the coefficient α is called the Henry coefficient. It is a reasonable assumption in regions for which

the variations of concentrations remain small. In this case, the kinetic adsorption equation then takes the form

$$\alpha \frac{\partial d}{\partial t} + \beta(d - c) = 0\,,$$

for which the solution is given explicitly by

$$d(t) = e^{-\frac{\beta}{\alpha}t} d(0) + \int_0^t \frac{\beta}{\alpha} e^{-\frac{\beta}{\alpha}(t-\tau)} c(\tau)\, d\tau\,.$$

Thus, the internal medium concentration d follows the true pore concentration exponentially with time constant $\frac{\beta}{\alpha}$. In particular, in the limiting case $\beta \to \infty$, we have instantaneous equilibrium and $d \equiv c$.

EXERCISE 3. *Note that the kernel appearing above is of the form $k(t - \tau)$, where the function $k(t) = \frac{\beta}{\alpha} e^{-\frac{\beta}{\alpha}(t)}$ satisfies*
  (1) $k(t) \geq 0$,
  (2) $\int_0^\infty k(t)\, dt = 1$.
Sketch $k(\cdot)$ for very large values of β.

Transport with Adsorption. Consider again the transport of a chemical by water that is traveling with uniform velocity ν through a long thin tube G with uniform cross section S as before, but now the tube is filled with the adsorbing material. We let $c(x, t)$ be the concentration of chemical in the pores surounding the adsorbing material and $a(x, t)$ the concentration of chemical that is adsorbed onto the material. The chemical in the pores is carried by the water, but the adsorbed chemical is held stationary at the adsorption site. Thus, the flux is given exactly as before, but the total concentration of chemical at $x \in G$ is given by $c(x, t) + a(x, t)$, so the conservation law leads to the transport equation with adsorption,

$$(10) \qquad \frac{\partial}{\partial t}\big(c + a(d)\big) + \nu \frac{\partial c}{\partial x} = F(x, t).$$

In the case of *instantaneous* adsorption rates, $\beta \to \infty$, we have $c = d$ in the limit, and the adsorption equation becomes

$$(11) \qquad \frac{\partial}{\partial t}\big(c + a(c)\big) + \nu \frac{\partial c}{\partial x} = F.$$

This is a quasi-linear partial differential equation of first-order. More generally, the model of transport with kinetic adsorption leads to the system

$$\text{(12a)} \qquad \frac{\partial c}{\partial t} + \nu \frac{\partial c}{\partial x} + \beta(c - d) = F\,,$$

$$\text{(12b)} \qquad \frac{\partial a(d)}{\partial t} + \beta(d - c) = 0\,,$$

for the two unknown functions $c(x,t),\ d(x,t)$. The appropriate initial and boundary conditions for this system are

$$c(x,0) = c_0(x)\,, \quad d(x,0) = d_0\,, \qquad a < x < b\,,$$
$$c(a,t) = c_a(t)\,, \qquad t > 0\,.$$

Note that the condition on $d(x,0)$ is equivalent to specifying a corresponding condition on the adsorbed concentration, $a(x,0)$.

In the linear case of the *Henry isotherm*, we obtain the linear system of first–order partial differential equations

$$\text{(13a)} \qquad \frac{\partial c}{\partial t} + \nu \frac{\partial c}{\partial x} + \beta(c - d) = F\,,$$

$$\text{(13b)} \qquad \alpha \frac{\partial d}{\partial t} + \beta(d - c) = 0\,.$$

A Second–order Wave Equation. We continue with an additional assumption, namely, that the concentration of chemical in the pores is much less than the amount adsorbed in the material. This amounts to assuming that most of the available volume in the tube is occupied by the adsorbing material, and it means that $c << a$, and so we approximate $c + a \approx a$. Thus, we drop c from the sum $c + a$ in the conservation equation to obtain in the linear case

$$\text{(14a)} \qquad \nu \frac{\partial c}{\partial x} + \beta(c - d) = F\,,$$

$$\text{(14b)} \qquad \alpha \frac{\partial d}{\partial t} + \beta(d - c) = 0\,.$$

EXERCISE 4. *Eliminate d above to obtain a single equation of second order for the unknown c:*

$$\text{(15)} \qquad \frac{1}{\beta} c_{xt} + \frac{1}{\nu} c_t + \frac{1}{\alpha} c_x = \frac{1}{\nu\alpha} F + \frac{1}{\nu\beta} F_t\,.$$

What are the appropriate initial and boundary conditions for this equation?

EXERCISE 5. *Eliminate d from the system* (13) *to obtain a single equation of second order for the unknown c. What are the appropriate initial and boundary conditions for this equation?*

4. Longitudinal Vibrations

We describe the longitudinal vibrations in a long narrow cylindrical rod of cross section area S. The rod is located along the $x-$axis, and we identify it with the interval (a, b) in $\mathbb{R}$. The rod is assumed to stretch or contract in the horizontal direction, and we assume that the vertical plane cross-sections of the rod move only horizontally. Denote by $u(x, t)$ the *displacement* in the positive direction from the point $x \in [a, b]$ at the time $t > 0$. The corresponding *displacement rate* or *velocity* is denoted by $v(x, t) \equiv u_t(x, t)$.

Let $\sigma(x, t)$ denote the local *stress*, the force per unit area with which the part of the rod to the right of the point x acts on the part to the left of x. Since force is positive to the right, the stress is positive in conditions of *tension*. For a section of the rod, $x_1 < x < x_2$, the total (rightward) force acting on that section due to the remainder of the rod is given by

$$\big(\sigma(x_2, t) - \sigma(x_1, t)\big)S \,.$$

If the density of the rod at x is given by $\rho_0 > 0$, the momentum of this section is just

$$\int_{x_1}^{x_2} \rho_0\, u_t(x, t)\, S\, dx \,.$$

If we let $F(x, t)$ denote any external applied force per unit of volume in the positive $x-$direction, then we obtain from Newton's second law that

$$\frac{d}{dt} \int_{x_1}^{x_2} \rho_0\, u_t(x, t)\, S\, dx = \big(\sigma(x_2, t) - \sigma(x_1, t)\big)S + \int_{x_1}^{x_2} F(x, t)\, S\, dx$$

for any such $x_1 < x_2$. For a sufficiently smooth displacement $u(x, t)$, we obtain the *conservation of momentum* equation

$$(16) \qquad \rho_0\, u_{tt}(x, t) - \sigma_x(x, t) = F(x, t)\,, \qquad a < x < b,\ t > 0 \,.$$

The *stress* $\sigma(x, t)$ is determined by the type of material of which the rod is composed and the amount by which the neighboring region is stretched or compressed, i.e., on the *elongation* or *strain*, $\varepsilon(x, t)$. In order to define this, first note that a section $[x, x + h]$ of the rod is deformed by the

displacement to the new position $[x + u(x), (x + h) + u(x + h)]$. The *elongation* is the limiting increment of the change in the length due to the deformation as given by

$$\lim_{h \to 0} \frac{[u(x+h) + (x+h)] - [u(x) + x] - h}{h} = \frac{d\,u(x)}{dx} \, ,$$

so the strain is given by $\varepsilon(x,t) \equiv u_x(x,t)$.

The relation between the stress and strain is a *constitutive law*, usually determined by experiment, and it depends on the type of material. In the simplest case, with small displacements, we find by experiment that $\sigma(x,t)$ is proportional to $\varepsilon(x,t)$, i.e., that there is a constant k called *Young's modulus* for which

$$(17) \qquad\qquad\qquad \sigma(x,t) = k\,\varepsilon(x,t) \, .$$

The constant k is a property of the material, and in this case we say the material is purely *elastic*. The partial differential equation for the longitudinal vibrations of the rod is obtained by substituting (17) into (16) to obtain

$$(18) \qquad \rho_0\,u_{tt} - ku_{xx} = F(x,t) \, , \qquad a < x < b, \ t > 0 \, .$$

This is the *second-order wave equation.*

A rate-dependent component of the stress-strain relationship arises when the force generated by the elongation depends not only on the magnitude of the strain but also on the speed at which it is changed, i.e., on the *strain rate* $\varepsilon_t(x,t) = v_x(x,t)$. The simplest such case is that of a *visco-elastic* material defined by the linear constitutive equation

$$\sigma(x,t) = k\,\varepsilon(x,t) + \mu\,\varepsilon_t(x,t) \, ,$$

in which the material constant μ is the *viscosity* or internal friction of the material. In terms of displacement, this has the form

$$(19) \qquad\qquad\qquad \sigma(x,t) = ku_x(x,t) + \mu u_{xt}(x,t) \, .$$

The partial differential equation for the longitudinal vibrations of the visco-elastic rod is obtained by substituting (19) into (16) to obtain

$$(20) \qquad \rho_0\,u_{tt} - \mu u_{xxt} - ku_{xx} = F(x,t) \, , \qquad a < x < b, \ t > 0 \, .$$

For $\mu > 0$ this is the *viscous wave equation.* In order to see the character of this equation, note that the highest order terms are of the form

$$\rho_0 \, v_t - \mu v_{xx}$$

for the velocity $v = u_t$, so this equation can be expected to be similar to the diffusion equation. For this reason, (20) is also called the *strongly-damped wave equation.*