Chloroform Alert! University Students Exposed to Unhealthy Air

The Situation

AAA Chemical Inc. operates two chemical plants in the town of Bayou St. Edwards, home of Dixieland State University. New pollution monitoring equipment has shown elevated concentrations of chloroform in the air over the university. These concentrations are considered unhealthy and the student Engineering Society has formed a study group to review the problem. They have come up with a number of possible ways to reduce the pollution including relocating the plants, making the stacks taller, and adding air pollution control equipment to the plants. They will analyze the costs and compute the reduction in chloroform concentration that is expected from each possible solution. You are asked to help them with the project by completing Parts 1, 2, 3, and 4 below.

In Part 1, you will learn how to model chloroform concentrations in the atmosphere in the presence of diffusion and turbulence. In Part 2, you will add the effects of wind to the model. Part 3 shows how the model can be simplified in the case of steady state conditions (no change in chloroform emissions over time), and how the chloroform emissions from the two chemical production plants can be added together to calculate the combined effect of the two plants on air quality. In Part 4, you apply the simplified model to Dixieland University. You are asked to calculate concentrations of chloroform in the air over the university, and to choose between various engineering remedies.

1 Part 1: Diffusion and Turbulence via Discrete Approximation

Prevailing winds carry pollutants from several nearby smokestacks to the university campus. The students want to calculate the levels of chloroform over the campus produced by the smokestacks under various conditions.

The students began with a review of the literature on the dispersion of air pollutants from factory stacks. They learned that to find the chloroform levels, they must use the

priniciple of superposition. That is, they must first calculate the effects from each stack individually, and then add together the effects of all the smokestacks. In fact, they learned that even to find the effects of continuous emission from a single smokestack, superposition would be necessary. For this they would take an integral in time of so called fundamental solutions to the problem. So their overall strategy is to deal with dispersion in as simple a situation as possible, and then use superposition to build solutions for the more complex situation they face.

The students also learned that dispersion is governed by the effects of advection, diffusion, and turbulence. The effects of diffusion and turbulence can be represented as a **random walk.** A random walk is a mathematical model of a particle moving randomly, one step at a time, around $\mathbf{R}$ or $\mathbf{R}^n$. We will use the random walk model to do two things–first we will derive the partial differential equation (p.d.e.) for the concentration of molecules undergoing diffusion and turbulence. We will then find the fundamental solutions to the p.d.e. These are the concentrations resulting from an initial unit mass at a single point. In later parts we will modify our solutions to take account of the effects of advection, and see how to use superposition to find the concentrations corresponding to more complex situations.

We begin with a mass of particles located at discrete positions, able to move at discrete times, and subject to diffusion and turbulence. To simplify matters, we assume for now that the particle motion is taking place in one dimension. So consider a mass M_0 of particles distributed on a fine grid on the real numbers $\mathbf{R}$. Though the total mass M_0 is finite, we assume that the actual number of particles is virtually infinite, and that all particles have the same mass. Let

$$\ldots, -n\Delta x, -(n-1)\Delta x, \ldots, -\Delta x, 0, \Delta x, \ldots, n\Delta x, \ldots$$

denote the possible particle positions, where Δx is very small. At the same time, suppose that the particles can move only at times

$$t = 0, \Delta t, 2\Delta t, \ldots, n\Delta t, \ldots,$$

where Δt is also very small. For each $x = m\Delta x$ and $t = n\Delta t$ let $M(x,t)$ be the mass of particles located at position x at time t. Thus for each t the sum over x of $M(x,t)$ is M_0.

Now let $C(x,t)$ be the concentration of mass (mass per unit length) at point x at time t. In our discrete approximation $C(x,t) = M(x,t)/\Delta x$. When we obtain $C(x,t)$ for all x, t by passing to a limit as $\Delta x \to 0$, it will have the property that for each t, the mass in the interval $[a,b]$ at time t given by

$$\int_a^b C(x,t)dx \qquad (1.1).$$

Now we model the particle motion as a simple symmetric random walk. That is, at each time t each particle will move a distance Δx randomly either to the right or to the left. The direction of motion will be independent of all past motion, and equally likely to be right or left. (Thus it is impossible for the particle to remain at rest in our model. This assumption is not restrictive and keeps things simple.) Given these assumptions we have the equations

$$M(x, t + \Delta t) = \frac{1}{2}M(x - \Delta x, t) + \frac{1}{2}M(x + \Delta x, t)$$

$$C(x, t + \Delta t) = \frac{1}{2}C(x - \Delta x, t) + \frac{1}{2}C(x + \Delta x, t) \tag{1.2}$$

for every x, t in our grids.

Requirement 1. Use (1.2) to express $C(x, t + \Delta t) - C(x, t)$ as a linear combination of $C(x + \Delta x, t), C(x, t)$, and $C(x - \Delta x, t)$.

We now use your result in Requirement 1 to obtain a relation between $\partial C(x, t)/\partial t$ and $\partial^2 C(x, t)/\partial x^2$ for the case of particles continuously distributed along $\mathbf{R}$ moving at all positive times. To find such a relation it is possible to seek out in your equation approximating difference quotients for the derivatives we want, but we choose to use Taylor approximations and see what falls out. Of course the difference quotient approach properly executed will give us the same relationship.

Requirement 2. a) For small Δt, approximate $C(x, t + \Delta t) - C(x, t)$ by a first order polynomial in Δt. Use a first order Taylor expansion for C in the second variable with base point (x, t). Neglect the remainder term. Your answer should involve $\partial C(x, t)/\partial t$.

b) For small Δx, approximate the linear combination of $C(x + \Delta x, t), Cx, t)$ and $C(x - \Delta x, t)$ you got in Requirement 1 by a second order polynomial in Δx. Use a second order Taylor expansion for C in the first variable, again with base point (x, t). Neglect the remainder term. Your answer should involve $\partial^2 C(x, t)/\partial x^2$.

c) Set your answer in 2a equal to your answer in 2b. Now assume that $\Delta t = c(\Delta x)^2$. (We will see later, the standard deviation of the position in a random walk is proportional to the square root of the time elapsed–i.e. a typical x displacement is proportional to $\sqrt{t}$.) So divide the left hand side of your equation by Δt, and the right hand side by $c(\Delta x)^2$. Obtain an equation relating $\partial C(x, t)/\partial t$ and $\partial^2 C(x, t)/\partial x^2$.

If we set $k_1 = (2c)^{-1}$ in your equation, we now have the following **partial differential equation** for the concentration $C(x,t)$:

$$\frac{\partial C(x,t)}{\partial t} = k_1 \frac{\partial^2 C(x,t)}{\partial x^2} \qquad (1.3).$$

Here the constant k_1 is called the mass diffusivity; its value depends on the particular situation.

To determine the function $C(x,t)$ uniquely for all x,t we not only need to know that it satisfies (1.3) but we also need additional information on C. The usual requirement is specification of an initial distribution $C(x,0)$ for all x, but our situation is unusual. Rather than an initial distribution function for C over an interval of x, we must deal with an initial concentration of mass at a single point x_0 (the location of a smokestack). Can we specify an initial concentration function for this situation? Since we have positive unit mass at a single point and no initial mass elsewhere, our concentration function–the mass "density"–must be infinite at x_0 and zero elsewhere, and its integral over all x must yield the unit mass. Thus we must work with a "function" which is zero everywhere except a single point, where it is infinite, and its integral is 1. Such a "function" is called a **Dirac delta function**. A Dirac delta function is not really a function, but everyone agrees it is a very useful idea so everyone agrees to treat it as a function subject to the properties just set out. The standard notation for a Dirac delta function concentrated at x_0 is $\delta_{x_0}(x)$. Keep in mind its basic properties: $\delta_{x_0}(x) = 0$ for $x \neq x_0$, $\delta_{x_0}(x_0) = \infty$, and $\int_{-\infty}^{\infty} \delta_{x_0}(x)dx = 1$. For any function f we have $\int_{-\infty}^{\infty} f(x)\delta_{x_0}(x)dx = f(x_0)$.

The concentration $C_{x_0}(x,t)$ corresponding to an initial Dirac delta function is called a fundamental solution to our problem, because the concentration $C(x,t)$ corresponding to an arbitrary initial distribution $C(x,0) = f(x)$ can be built up from these fundamental solutions. In fact if $C_{x_0}(x,t)$ solves (1.3) for each x,t and $C_{x_0}(x,0) = \delta_{x_0}(x)$ for each x_0, x, then $C(x,t) = \int_{-\infty}^{\infty} f(u)C_u(x,t)du$ satisfies (1.3) and $C(x,0) = f(x)$ for all x. Here we assume we can differentiate under integrals.

We now derive the formula for the concentration corresponding to an initial point mass at $x = x_0$; i.e., for the fundamental solution corresponding to initial Dirac delta function δ_{x_0}. We denote the concentration we seek by $C_{x_0}(x,t)$. To work out the formula for $C_{x_0}(x,t)$ we return to the discrete grids we used above, and track the motion of a single particle beginning at x_0 at time $t = 0$. Its position at time $t = 0$ is fixed at x_0 but its position at any positive time $t = n\Delta t$ is random. To derive the probability distribution of its position at time t we introduce random variables $X_1, X_2, \ldots$. For each k the random variable $X_k = +1$ if the particle moves to the right at time $t = k\Delta t$ and $X_k = -1$ if the particle moves left at that time. The X_k's are independent and each X_k has distribution

$P(X_k = 1) = .5$ and $P(X_k = -1) = .5$ for each k. The random position $S(t)$ of our particle at time $t = n\Delta t$ can be written

$$S(t) = x_0 + \Sigma_{k=1}^{n} X_k \Delta x.$$

According to the Central Limit Theorem from probability theory, if n is large, the distribution of $S(t)$ is approximately normal. The mean of $S(t)$ is x_0 and the standard deviation of $S(t)$ is $\Delta x\sqrt{n}$.

Requirement 3. Recall from probability theory that for random variables $X_1, \ldots, X_n$ the mean of the sum $X_1 + \ldots + X_n$ is the sum of the means of the X_i's, and if in addition the $X_1, \ldots, X_n$ are independent the variance of the sum is the sum of the variances. Use these facts to verify our claims about the mean and standard deviation of $S(t)$.

Requirement 4. Now assume that $\Delta t = (\Delta x)^2/(2k_1) = t/n$. What are the mean and variance of $S(t)$ in terms of t? Your answer should depend on t but not on Δx or n.

Since the distribution of $S(t)$ becomes normal as $n \to \infty$ and we know the mean and variance of $S(t)$ we can write down a limiting density for $S(t)$ as a function of x.

Requirement 5. Write down the formula for the limiting density of $S(t)$; that is, the normal density with mean x_0 and the standard deviation you found in Requirement 4.

If we now return to our assumptions that the number of mass particles is virtually infinite and the particles all have equal mass, and assume also that the total mass is 1, then the limiting density you wrote down in Requirement 5 is the mass density in x at time t. In other words, it is the desired solution $C_{x_0}(x, t)$.

Requirement 6. Verify that $C_{x_0}(x, t)$ satisfies equation (1.3).

The remaining point to check is that $C_{x_0}(x, 0)$ is a Dirac delta function at x_0. We point out $C_{x_0}(x, t)$ is a normal density with mean x_0 and standard deviation $\sqrt{2k_1 t}$. Hence $C_{x_0}(x, t)$ always integrates over all x to 1, and for t very close to zero, $C_{x_0}(x, t)$ is concentrated near x_0 and nearly infinite at x_0. So we believe that $C_{x_0}(x, 0)$ is a Dirac delta function at x_0. Finally, we ask you to take on faith that there can be only one positive solution to (1.3) whose initial distribution is the Dirac delta function at x_0.

2 Part 2: Advection via Discrete Approximation

In this section, we consider the effects of wind (advection) on our problem. For simplicity, we assume that the wind blows constantly in the same direction. Just as we used discrete approximations to investigate diffusion and turbulence we do the same for advection. Let us again consider the fine grid as in Part 1, but we neglect the effects of diffusion and turbulence and concentrate on advection for now. We assume that we have a wind whose velocity in the positive direction is c. We model this advective effect by the equations

$$M(x, t + \Delta t) = M(x - c\Delta t, t)$$

$$C(x, t + \Delta t) = C(x - c\Delta t, t) \qquad (2.1).$$

The right hand side of the first equation represents the mass with position $x - c\Delta t$ at the current time t. At time $t + \Delta t$ it will be the mass at position x, which mass is represented by the left hand side of the first equation. Hence the first equation; the second equation is simply the first equation divided by Δx.

Requirement 1. Use (2.1) to express $C(x, t + \Delta t) - C(x, t)$ as a linear combination of $C(x - c\Delta t, t)$ and $C(x, t)$.

Requirement 2. Use your result in Requirement 1 to obtain a relation between $\partial C(x, t)/\partial t$ and $\partial C(x, t)/\partial x$. As in Requirement 2 of Part 1 you should approximate both sides by Taylor polynomials for small Δt, and then divide through by Δt. This time you should use first order polynomials in Δt on both sides.

You should have obtained for $C(x, t)$ the equation

$$\frac{\partial C(x, t)}{\partial t} + c\frac{\partial C(x, t)}{\partial x} = 0 \qquad (2.2).$$

We need to put the effects of diffusion and turbulence and advection together. For the governing equation the standard assumption–the wisdom of the field, if you will–is that the two effects are additive; thus for the concentration $D(x, t)$ undergoing advection as well as diffusion and turbulence we arrive at

$$\frac{\partial D(x, t)}{\partial t} + c\frac{\partial D(x, t)}{\partial x} = k_1\frac{\partial^2 D(x, t)}{\partial x^2} \qquad (2.3).$$

A good guess for the fundamental solution of this equation is simply to take the fundamental solution we found in Part 1 and left it drift with velocity c: thus

$$D_{x_0}(x,t) = C_{x_0}(x - ct, t) \qquad (2.4).$$

Here C_{x_0} is the fundamental solutions from Part 1.

Requirement 3. Verify that $D_{x_0}(x,t)$ solves (2.3). (Hint: Express the derivatives of D_{x_0} in terms of the derivatives of C_{x_0}, and use the fact that C_{x_0} satisfies (1.3).)

We now summarize your results from Parts 1 and 2: A concentration D of mass undergoing diffusion, turbulence and advection satisfies the equation (2.3). The solution D_{x_0} given by (2.4) is the concentration corresponding to an initial unit mass concentrated at x_0.

We will now extend, without proof, equations and solutions you obtained for one space dimension to the case of three space dimensions. From here on, we will denote all concentrations by C.

Let $C_{p_0}(p,t)$ be the concentration of mass at $p = (x,y,z)$ at time t corresponding to a unit mass concentrated at $p_0 = (x_0, y_0, z_0)$ at time $t = 0$. (In three dimensions concentration is mass per unit volume.) Assume a wind of constant velocity c in the positive x direction. Then we have the equation

$$\frac{\partial C}{\partial t} + c\frac{\partial C}{\partial x} = k_1\frac{\partial^2 C}{\partial x^2} + k_2\frac{\partial^2 C}{\partial y^2} + k_3\frac{\partial^2 C}{\partial z^2} \qquad (2.5).$$

The fundamental solution C_{p_0} is given by

$$C_{p_0}(p,t) = (4\pi t)^{-3/2}(k_1k_2k_3)^{-1/2}\exp\left(-\left(\frac{(x-x_0-ct)^2}{4k_1t} + \frac{(y-y_0)^2}{4k_2t} + \frac{(z-z_0)^2}{4k_3t}\right)\right) \qquad (2.6).$$

For the sequel, keep in mind that p and p_0 are position vectors in $\mathbf{R}^3$ and t is the time variable. In particular, in the context of differential equations including variables x, y, z, keep in mind that p is short for (x,y,z) and p_0 is short for (x_0, y_0, z_0).

3 Part 3: Superposition and Steady State

Having found the fundamental solutions to our diffusion-advection equation, we now want to put these together to deal with mass initially distributed over many locations, and also

with mass continuously generated over time, such as would arise from a smoke stack. One element that will be missing from our analysis is the effect of the ground–i.e., does the ground absorb or reflect the gas in question? However, our smoke stacks will be elevated, and in this case one can neglect the issues of absorption and reflection with little error, since the bulk of the movement takes place above ground.

To put together more general solutions from fundamental solutions, we make the key observation is that equation (2.5) is linear; thus if C_1 and C_2 both satisfy (2.5), then so does any linear combination of C_1 and C_2. In particular, if we begin at time $t = 0$ with masses $m_1, m_2, \ldots, m_k$ concentrated at the points $p_1, p_2, \ldots, p_k$ in $\mathbf{R}^3$ then the corresponding concentration C is given by

$$C(p,t) = \Sigma_{i=1}^{k} m_i C_{p_i}(p,t) \qquad (3.1).$$

Recall that the vector p as short for (x, y, z). If on the other hand we begin at time $t = 0$ with mass distributed over $\mathbf{R}^3$ according to the initial concentration $f(x, y, z)$, then the corresponding concentration C is

$$C(p,t) = \int f(u,v,w) C_{(u,v,w)}(p,t) dudvdw \qquad (3.2).$$

This process of taking linear combinations of fundamental solutions to a linear equation to obtain solutions corresponding to more complex initial conditions is called **superposition.**

Requirement 1. Give the solution to (2.5) corresponding to an initial distribution of 1 unit of mass at (0,0,1) and 2 units of mass at (0,2,1).

In our application we will need to consider not only mass generated at several points at the same time but also mass generated at the same point at different times. We handle this by superposition in the time variable. Let $C_{p_0}^{t_0}(p,t)$ denote the concentration at point p at time t corresponding to what was a unit mass at p_0 at time t_0. Then

$$C_{p_0}^{t_0}(p,t) = C_{p_0}(p, t - t_0) \qquad (3.3).$$

Requirement 2. Verify that $C_{p_0}^{t_0}$ satifies (2.5) for each p_0, t_0. (Hint: Relate the derivatives of $C_{p_0}^{t_0}$ to those of C_{p_0} and use the fact that C_{p_0} satisfies (2.5).) Let C denote the concentration corresponding to a unit of mass generated at p_0 at time $t = 0$ and another unit of mass generated at p_0 at time $t = 1$. Find C.

Requirement 3. a) Suppose that starting at time $t = A$ mass is continuously generated at $p = (0, 0, 0)$ according to a mass rate $dM/dt = Q(t)$. Find the concentration $C(x, t)$ by superposition in t. Your answer may be left in the form of an integral. (Hint: For each time s in the interval $[A, t]$ an initial mass $Q(s)ds$ is generated at $(0, 0, 0)$. Each unit of mass generated at $(0, 0, 0)$ at time s contributes $C^s_{(0,0,0)}(p, t)$ to the total concentration at (p, t).)

b) (optional) Assuming $Q(t) = Q_0$ is constant, show that your integral satisfies

$$\frac{\partial C}{\partial t} + c\frac{\partial C}{\partial x} = k_1\frac{\partial^2 C}{\partial x_1^2} + k_2\frac{\partial^2 C}{\partial x_2^2} + k_3\frac{\partial^2 C}{\partial x_3^2} + Q_0\delta_{(0,0,0)}(x) \qquad (3.4).$$

Here $Q_0\delta_{(0,0,0)}(x)$ is a "forcing term" corresponding to continuous generation of mass.

It is possible, given sufficient data on the pollution source, to calculate the concentration $C(x, y, z, t)$ by superposition, as outlined above. However, several simplifying assumptions will lead to easier calculations. The first simplifying assumptions are that the rate of emissions is a constant Q_0 and that we have a steady state–that is that the emissions have been going on for some time and the resulting concentrations do not vary with time.

Let us give some justification for this. If in your answer to Requirement 3a we let $A \to -\infty$ we get

$$C(p, t) = Q_0 \int_{-\infty}^{t} C_{(0,0,0)}(p, t - s)ds = Q_0 \int_0^{\infty} C_{(0,0,0)}(p, r)dr \qquad (3.5)$$

after the change of variable $r = t - s$. Notice that the last integral does not depend on t. Now to save space and effort let

$$L = k_1\frac{\partial^2}{\partial x^2} + k_2\frac{\partial^2}{\partial y^2} + k_3\frac{\partial^2}{\partial z^2} - c\frac{\partial}{\partial x}. \qquad (3.6)$$

Then accepting that we can differentiate under integrals we get, for $C(p, t)$ defined as in (3.5),

$$LC(p, t) = Q_0 \int_0^{\infty} LC_{(0,0,0)}(p, r)dr = Q_0 \int_0^{\infty} \frac{\partial C_{(0,0,0)}(p, r)}{\partial r}dr$$

since $C_{(0,0,0)}$ satisfies equation (2.5). But this last integral is equal to $-Q_0\delta_{(0,0,0)}$ since $C_{(0,0,0)}(p, t) \to 0$ as $t \to \infty$ and $C_{(0,0,0)}(p, 0) = \delta_{(0,0,0)}(p)$. Thus $C(p, t)$ as defined in (3.5) satisfies

$$c\frac{\partial C}{\partial x} = k_1\frac{\partial^2 C}{\partial x^2} + k_2\frac{\partial^2 C}{\partial y^2} + k_3\frac{\partial^2 C}{\partial z^2} + Q_0\delta_{(0,0,0)}(p) \qquad (3.7),$$

which is just equation (3.4) with the time derivative removed.

Further simplification is possible and customary. When the wind is appreciable, the advective effect in the x direction dominates the diffusion effect in that direction. Therefore we usually drop the $\partial^2 C/\partial x^2$ term out of (3.7) and divide through by c to get

$$\frac{\partial C}{\partial x} = k_2 \frac{\partial^2 C}{\partial y^2} + k_3 \frac{\partial^2 C}{\partial z^2} + \frac{Q_0}{c}\delta_{p_0}(p). \tag{3.8}$$

Except for the forcing term, this looks like equation (2.5) but with 2 space dimensions and with t replaced by x. Since the forcing term does not apply for positive x, we drop it from the equation and make it an initial condition $C(0, y, z) = (Q_0/c)\delta_{(y_0,z_0)}(y, z)$. Adjusting the solution (2.6) to meet our current needs we get a simplified approximate formula for the steady state solution:

$$C(x, y, z) = \frac{Q_0}{4\pi x\sqrt{k_2 k_3}} \exp\left(-\frac{c}{4x}\left(\frac{(y-y_0)^2}{k_2} + \frac{(z-z_0)^2}{k_3}\right)\right). \tag{3.9}$$

We have done a lot of simplifying and assuming. It is worthwhile to check up on this work numerically. It is helpful to rewrite (3.5) carefully. To keep things simple, let us take $p_0 = (0, 0, 0)$, let $s = ct$, and let $\gamma = k_1/c$. Then we can write (3.5) as

$$\int_0^\infty \frac{1}{\sqrt{4\pi\gamma s}} \exp(-\frac{(x-s)^2}{4\gamma s}) \frac{Q_0}{4\pi s\sqrt{k_2 k_3}} \exp(-\frac{c}{4s}(\frac{y^2}{k_2} + \frac{z^2}{k_3}))ds \qquad (3.10).$$

Thus in (3.5) we are integrating

$$\frac{Q_0}{4\pi s\sqrt{k_2 k_3}} \exp(-\frac{c}{4s}(\frac{y^2}{k_2} + \frac{z^2}{k_3})) \tag{3.11}$$

against

$$\frac{1}{\sqrt{4\pi\gamma s}} \exp(-\frac{(x-s)^2}{4\gamma s}) \tag{3.12}$$

for s ranging from 0 to ∞. We now relate (3.5) to (3.9).

Requirement 4. (optional)

a) Use a scientific calculator or computer package to convince yourself that the integral of (3.12) in s from 0 to ∞ is 1, no matter what x or γ are.

b) Convince your self with a graphics calculator or computer graphics package that as $\gamma \to 0$, the function in (3.12) becomes a Dirac delta function concentrated at $s = x$.

c) Substitute $s = x$ in 3.11. You should get (3.8).

The upshot of Requirement 4 is

(i) (3.5) is an average over s of the two dimensional Gaussian densities in the variables y, z given by (3.11);

(ii) As $k_1/c \to 0$, the mixing function (3.12) becomes concentrated at $s = x$;

(iii) For $s = x$ (3.10) becomes (3.9).

Therefore for small k_1/c (3.5) is well approximated by (3.9).

For your requirements in Part 4, you will be asked to carry out various calculations using (3.9). In those situations $\gamma = k_1/c$ is not so small. However x is quite large in those cases, and this also has an impact. It limits the effective range of the variable s in (3.12) to an interval around x whose length is a relatively small fraction of x, and (3.11) is relatively constant over that range. So we can hope that in this case also that (3.5) is well approximated by (3.9).

However, rather than ask you to chase through analytic verifications of all these claims, we simply suggest that you compare some answers you will get in Part 4 by the simplified approximate formula (3.9) to the answers you would get from the superposition formula (3.5). This will be part (b) of Requirement 1 in Part 4.

4 Part 4:

Having derived–with your assistance–the equations for calculating the concentration of chloroform in the air due to a stack discharge, the students then collected data on the two plants. They found the following information:

Plant 1:

- $Q_0 = 100$ grams/second
- stack height: $z = 25$ meters
- Distance from Student Union (parallel to the predominant wind direction): $x = 4000$ meters
- Distance from Student Union (perpendicular to the predominant wind direction): $y = 300$ meters

Plant 2:

- $Q_0 = 50$ grams/second
- stack height: 10 meters
- Distance from Student Union (parallel to the predominant wind direction):$x = 1100$ meters
- Distance from Student Union (perpendicular to the predominant wind direction): $y = 45$ meters

Students in the Environmental Engineering Department have conducted atmospheric diffusion experiments and determined that appropriate values for k_2 and k_3 are 0.45 m^2/s and 0.32 m^2/s, respectively. Also, wind velocities in the area are typically 0.5 m/s.

Requirement 1. a) Predict the chloroform concentrations in the ambient air over the Student Center due to the emissions from these plants under the prevailing wind conditio ns.

b) Consider the two smokestacks introduced in Part 4. For each smokestack use a graphing calculator or computer package to determine intervals where the corresponding integrand in (3.5) is concentrated. Then use numerical integration from a calculator or computer package to evaluate (3.5) for each smokestack. Assume $k_1 = 0.45$. Your answers should be fairly close to those you obtained in part a).

Requirement 2. Suppose an atmospheric inversion occurs and a mass of stagnant air settles over the area for several days. In this case, wind velocities drop to approximately 0.05 m/s. Find the resulting chloroform concentrations. Compare these to the concentrations found with the usually prevailing wind conditions. Under which conditions is the air quality healthier?

Requirement 3. The students have proposed several methods for reducing chloroform concentrations in the ambient air over the campus:

1. increase each stack's height by 8 meters.
2. add pollution control equipment such as air scrubbers to the stacks to reduce the mass rate by 35 grams/second.
3. shut down production at Plant 2 and transfer all operations to Plant 1.

4. move Dixieland State University to Hawaii so students and faculty can escape the chloroform without interrupting chemical plant operations.

Determine the effect that each of these options would have on ambient air concentrations of chloroform at the Student Center. Discuss the options (including the chemical plants as presently constructed) from the point of view of ambient air quality, cost (estimated), and feasibility. Provide a recommendation as to how the chloroform emissions should be reduced.

Requirement 4. When the students take their recommendations to AAA Chemical Inc., company managers reply that cost considerations should be evaluated more scientifically. The managers supply the students with the following data.

- Cost of increasing stack height: \$30,000 fixed cost plus \$5,000 per meter (to a maximum stack height of 40 meters)
- Cost of pollution control equipment per plant : Cost $= 10,000 + 2,000r^2$, where r is the number of grams/second reduced (to a minimum emission of 2 grams/second at each plant) and Cost is in dollars.
- Shut down and transfer operations at either plant: \$2,000,000.
- Relocate Dixieland State University: \$500 million to rebuild the university in Hawaii, offset by \$200 million in sale of Bayou StĖdwards property and \$100 million in present worth value of the larger student population eager to attend college in Hawaii.

a) Calculate the cost of building each stack to a 40 meter height. What is the resulting ambient concentration at the Student Center under prevailing wind conditions?

b) Calculate the cost of reducing emissions at each plant to 2 grams/second. What is the resultant ambient chloroform concentration at the Student Center under prevailing wind conditions?

c) Compute the costs of each of the options in Requirement 3. Is your recommendation from Requirement 3 more expensive than the other options? Would you change your initial recommendation based on these costs? Write a paragraph comparing the cost and effectiveness of each option.

Requirement 5. a.)The cost of transferring the chemical plant operations to a single plant is \$2,000,000. By how much would emissions at each plant be reduced if \$1,000,000

is spent on pollution control equipment at each plant? What would the resulting ambient concentrations at the Student Center be?

b.)What is the optimal allocation of the $2,000,000 for pollution control equipment between the two plants? You should base your answer on the allocation which provides the lowest ambient chloroform concentration at the Student Center.

5 Solutions

Part 1 Requirement 1.

$$C(x,t+\Delta t)-C(x,t)=\frac{1}{2}C(x+\Delta x,t)-C(x,t)+\frac{1}{2}C(x-\Delta x,t) \qquad (S1.1).$$

Requirement 2. Using a first degree Taylor expansion in variable t, the left hand side of (S1.1) can be approximated by $\partial C(x,t)\Delta t$. Using second degree Taylor expansions in the variable x, the right hand side of (S1.1) can be approximated by

$$\frac{1}{2}\left(C(x,t)+\frac{\partial C(x,t)}{\partial x}\Delta x+\frac{\partial^2 C(x,t)}{\partial x^2}\frac{\Delta x^2}{2}\right)-C(x,t)+\frac{1}{2}\left(C(x,t)-\frac{\partial C(x,t)}{\partial x}\Delta x+\frac{\partial^2 C(x,t)}{\partial x^2}\frac{\Delta x^2}{2}\right).$$

Simplifying the right hand Taylor expansion, assuming $\Delta t = c(\Delta x^2)$ and then dividing through by Δt we get

$$\frac{\partial C(x,t)}{\partial t}=\frac{1}{2c}\left(\frac{\partial^2 C(x,t)}{\partial x^2}\right). \qquad (S1.2)$$

Requirement 3. $E(S(t)) = x_0 + \Sigma_{k=1}^{n} E(X_k)\Delta x = x_0$ since $E(X_k) = 0$ for each k. Also the variance $V(S(t)) = \Sigma_{k=1}^{n} V(\Delta x X_k) = n(\Delta x)^2$. So the standard deviation of $S(t)$ is $\Delta x\sqrt{n}$.

Requirement 4. $E(S(t)) = x_0$ and $V(S(t)) = n(\Delta x)^2 = 2k_1 t$.

Requirement 5. $C_{x_0}(x,t) = (4\pi k_1 t)^{-1/2}\exp(-(x-x_0)^2/4k_1 t)$.

Requirement 6.

$$\frac{\partial C_{x_0}(x,t)}{\partial t}=(4\pi k_1)^{-1/2}\left(-\frac{1}{2t^{3/2}}+\frac{(x-x_0)^2}{4k_1 t^{5/2}}\right)\exp(-\frac{(x-x_0)^2}{4k_1 t}) \qquad (S1.3).$$

But

$$\frac{\partial^2 C_{x_0}(x,t)}{\partial x^2}=(2\pi k_1 t)^{-1/2}\left(-\frac{1}{2k_1 t}+\frac{(x-x_0)^2}{4(k_1 t)^2}\right)\exp(-\frac{(x-x_0)^2}{4k_1 t}) \qquad (S1.4).$$

It follows immediately that C_{x_0} satisfies (1.3).

Part 2

Requirement 1. $C(x,t+\Delta t)-C(x,t) = C(x-c\Delta t,t)-C(x,t)$.

Requirement 2. Approximating the left hand side of the equation in Requirement 1 by a first order Taylor polynomial in the variable t and the right hand side of that

equation by a first order Taylor polynomial in the variable x we get $(\partial C(x,t)/\partial t)\Delta t = -c(\partial C(x,t)/\partial x)\Delta t$. Dividing through by Δt we get

$$\frac{\partial C(x,t)}{\partial t} + c\frac{\partial C(x,t)}{\partial x} = 0 \qquad (S2.1).$$

Requirement 3. The key here is to use our results from Part 1, and not repeat all the differentiation. From the defining equation (2.4) we get $\partial D_{x_0}(x,t)/\partial t = -c\partial C_{x_0}(x-ct,t)/\partial x + \partial C_{x_0}(x-ct,t)/\partial t$. Also from (2.4) $\partial D_{x_0}(x,t)/\partial x = \partial C_{x_0}(x-ct,t)/\partial x$ and $\partial^2 D_{x_0}(x,t)\partial x^2 = \partial^2 C_{x_0}(x-ct,t)/\partial x^2$. Putting all these together and using (2.2) we get that D_{x_0} satisfies (2.3).

Part 3.

Requirement 1. $C_{(0,0,1)} + 2C_{(0,2,1)}$.

Requirement 2. Each derivative of $C_{p_0}^{t_0}$ involved in this equation is the corresponding derivative of C_{p_0} evaluated at $(p, t-t_0)$. Since C_{p_0} satisfies (2.5) so does $C_{p_0}^{t_0}$. For the conditions given here, $C = C_{p_0}^0 + C_{p_0}^1$.

Requirement 3. a) $C(x,t) = \int_A^t Q(s)C_{(0,0,0)}^s(p,t)ds$.

b) For convenience define L as in equation (3.6). Then accepting that we can differentiate under integrals we get

$$\frac{\partial C}{\partial t} = Q_0 C_{(0,0,0)}^t(p,t) + Q_0\int_A^t \frac{\partial C^s}{\partial t(p,t)}ds$$

$$= Q_0 C_{(0,0,0)}(p,0) + \int_A^t LC_{(0,0,0)}^s(p,t)ds = Q_0 C_{(0,0,0)}(p,0) + LC.$$

Requirement 4. a) It is possible to show that this integral is 1, as Victor Moll has shown us. However plugging in various values of x and γ will also convince us of this.

b) Use a standard graphing calculator such as the TI-82 and adjusting the window.

c) obvious

Part 4.

Requirement 1. a) Plant 1: 9.52×10^{-6} grams/m^3. Plant 2: 5.52×10^{-3} grams/m^3. Total ambient air concentration: 5.52×10^{-3} grams/m^3.

b) Plant 1: (3.5) integrand concentrated in r on [7500,8500]; $C = 9.6 \times 10^{-6}$. Plant 2: (3.5) integrand concentrated in r on [1900,2500]; $C = .0055$.

Requirement 2. Plant 1: 2.79×10^{-3} grams/m^3. Plant 2: 9.02×10^{-3} grams/m^3. Total ambient air concentration: 12.81×10^{-3} grams/m^3.

Requirement 3. Option 1: Plant 1: 9.10×10^{-6} grams/m^3 Plant 2: 5.09×10^{-3} grams/m^3. Total ambient air concentration: 5.09×10^{-3} grams/m^3. **Option 2**: Plant 1:

6.19×10^{-6} grams/m^3 Plant 2: 1.66×10^{-3} grams/m^3. Total ambient air concentration: 1.66×10^{-3} grams/m^3. **Option 3**: Combined plant at Plant 1 location: 1.42×10^{-5} grams/m^3. **Option 4** 27.07×10^{-3}. **Option 4**: 0 grams/m^3, assuming no chloroform-emitting plants in Hawaii within transport distance of the University.
Costs and Feasibility: Option 1: High cost option. Must add height to existing structure. Makes little difference in ambient concentrations. Option 2: lower capital costs but will increase operating and maintenance costs. Very feasible – the common practice, in fact. Best for the overall environment since total emissions are reduced. Options 3 & 4: may actually be less expensive to operate in the long run since operations are centralized. May be infeasible if the company had a good reason to separate the plants to begin with. Does not reduce the total amount emitted but if all operations are moved to plant 1, the concentration at the Student Center is greater reduced. Option 5: costs are very high and the project, while tempting, is probably infeasible. Existing project: the default choice. Obviously feasible, presumably the preferred choice from a cost perspective.

Requirement 4. a.) \$105,000 for Plant 1, \$180,000 for Plant 2. Concentration due to Plant 1:8.65×10^{-6}grams/m^3. Concentration due to Plant 2: 3.23×10^{-3} grams/m^3. b.)\$19.21 million for Plant 1, \$4.62 million for Plant 2. Concentration due to Plant 1: 1.90×10^{-7} grams/m^3. Concentration due to Plant 2 : 2.21×10^{-4} grams/m^3. c.) Option 1: \$70,000 at each plant. Option 2: \$246,00 0 at each plant. Option 3: \$2,000,000. Option 5: \$2,000,000. Option 5:\$200 million.

Requirement 5. a.)22.25 grams/sec. Concentration due to Plant 1: 7.38×10^{-6}grams/m^3. Concentration due to Plant 2: 3.03×10^{-3}grams/m^3. b.) Optimal allocation would be to use the entire \$2,000,000 to reduce emissions at Plant 2.