MSc in Computational Fluid Dynamics

Atmospheric Dispersion

Objectives: To give an introduction to the theory of atmospheric dispersion and to describe the basic principles of atmospheric dispersion modelling.

Form of teaching: 12 lectures/tutorials

Form of assessment: 100% assignment

Syllabus:

1. Basic equations for transport of a scalar; source terms; turbulence; eddy diffusivity
2. Transport processes: pure diffusion from an instantaneous plane source in 3-dimensions; instantaneous line and point sources; pure advection of tracers; combined diffusion/advection and Taylor's mechanism
3. Introduction to the atmospheric boundary layer
4. Continuous point sources; modelling diffusivity
5. Dispersion in real environments: Pasquill stability classes; dispersion from a continuous line source
6. Effect of the ground; high chimneys
7. Deposition: dry deposition and wet deposition
8. Types of dispersion model: plume models; box models
9. Chemistry of atmospheric pollutants
10. Numerical schemes for pollutant transport equations

1. Scalar Transport in the Atmosphere

1.1 Basic Principles

Consider an element of air containing a concentration C of a passive pollutant (passive means that it doesn't react and is neutrally buoyant, i.e. it doesn't settle).

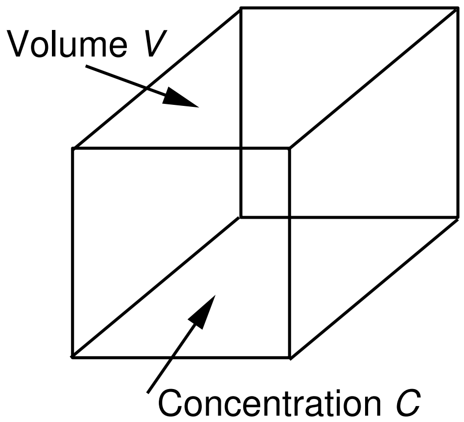

Figure 1. As an element of air is carried along by the flow it always contains the same air and therefore contains the same mass of pollutant.

If the flow is also incompressible, then the volume of the fluid element remains constant and so the concentration C remains constant. In mathematical terms

$$\frac{\mathrm{D}C}{\mathrm{D}t} = \frac{\partial C}{\partial t} + \mathbf{u}.\nabla C = \frac{\partial C}{\partial t} + u\frac{\partial C}{\partial x} + v\frac{\partial C}{\partial y} + w\frac{\partial C}{\partial z} = 0. \qquad (1)$$

It will be sufficient for our purposes to take the air to be incompressible so that

$$\nabla.\mathbf{u} = \frac{\partial u}{\partial x} + \frac{\partial v}{\partial y} + \frac{\partial w}{\partial z} = 0. \qquad (2)$$

Hence an alternative form of Eq. (1) is

$$\frac{\partial C}{\partial t} + \nabla.(\mathbf{u}C) = \frac{\partial C}{\partial t} + \frac{\partial}{\partial x}(uC) + \frac{\partial}{\partial y}(vC) + \frac{\partial}{\partial z}(wC) = 0. \qquad (3)$$

Suppose now that there is a source or sink of the pollutant within the element of air. This could be because the pollutant is created or destroyed by chemical reactions or because there is an outflow from, say, a chimney. The equation for C would then become

$$\frac{\mathrm{D}C}{\mathrm{D}t} = S(x, y, z, t), \qquad (4)$$

where S represents the source term (in $\mathrm{kgm^{-3}s^{-1}}$). Examples could be:

(i) $$S = -\alpha C \quad (\alpha \text{ constant}). \qquad (5)$$

This represents decay of C by, for example, chemical decomposition or radioactive decay.

(ii) $$S = S_0\delta(\mathbf{r} - \mathbf{r}_0) \quad (S_0 \text{ constant}), \qquad (6)$$

where $\delta(\mathbf{r} - \mathbf{r}_0)$ is a delta function at $\mathbf{r} = \mathbf{r}_0$. This represents a continuous point source (e.g. emission from a chimney).

(iii) $$S = S_0\delta(\mathbf{r} - \mathbf{r}_0)\delta(t - t_0) \quad (S_0 \text{ constant}). \qquad (7)$$

This represents an instantaneous point source occurring at time $t = t_0$ at $\mathbf{r} = \mathbf{r}_0$ (e.g. accidental release of a radioactive substance).

Another type of source/sink term is caused by diffusion. The pollutant may diffuse in or out of our element. The equation for C is then

$$\frac{\mathrm{D}C}{\mathrm{D}t} = D\left(\frac{\partial^2 C}{\partial x^2} + \frac{\partial^2 C}{\partial y^2} + \frac{\partial^2 C}{\partial z^2}\right) = D\nabla^2 C. \qquad (8)$$

D is the molecular diffusivity. D has dimensions $\mathrm{L^2T^{-1}}$. Typical values for pollutants in the atmosphere are $5\text{–}50\times10^{-6}\ \mathrm{m^2s^{-1}}$. We are usually concerned with dispersion on the scale of hundreds of metres to hundreds of kilometres. Consider $\mathrm{L} = 100$ m. Then the time-scale is

$$\mathrm{T} = \frac{\mathrm{L}^2}{D} = \frac{10^4}{50\times10^{-6}} = 2\times10^8 \text{ s}$$

which is infinite for all practical purposes. Hence *molecular diffusion is never directly relevant to atmospheric dispersion.*

1.2 Turbulence

Atmospheric flows are almost always turbulent. Turbulence occurs when the Reynolds number is high. It is characterised by eddy motions on a wide range of scales. When describing the dispersion of pollutants, we are usually interested in dispersion on scales much larger than many, if not all, of the eddies. In other words, we are interested in averages over length or time scales large compared to the turbulence.

In order to analyse dispersion in this way, we assume that it is possible to divide the flow into a "mean" flow which is slowly varying in time and a rapidly fluctuating, or "turbulent" part. We could perform this separation by defining an average as follows:

$$\text{Average of } \phi \; = \overline{\phi} = \frac{1}{T}\int_t^{t+T} \phi(x,y,z,t)\,\mathrm{d}t. \tag{9}$$

The average period T should be chosen to be long compared to the turbulence time-scales. Then we put

$$\phi = \overline{\phi} + \phi'. \tag{10}$$

ϕ' represents the turbulent part of ϕ. It follows (to a reasonable approximation at least) that

$$\overline{\phi'} = 0. \tag{11}$$

Let us perform this separation for all the variables in the concentration equation, Eq. (3).

$$\begin{aligned} C &= \overline{C} + C' \\ u &= \overline{u} + u' \\ v &= \overline{v} + v' \\ w &= \overline{w} + w' \end{aligned}$$

Therefore

$$\frac{\partial}{\partial t}(\overline{C}+C')+\frac{\partial}{\partial x}[(\overline{u}+u')(\overline{C}+C')]+\frac{\partial}{\partial y}[(\overline{v}+v')(\overline{C}+C')]+\frac{\partial}{\partial z}[(\overline{w}+w')(\overline{C}+C')] = 0.$$

We now average this equation. Consider, for example

$$\begin{aligned} \overline{(\overline{C}+C')(\overline{u}+u')} &= \overline{u}\overline{C} + \overline{\overline{u}C'} + \overline{u'\overline{C}} + \overline{u'C'} \\ &= \overline{u}\overline{C} + \overline{u'C'} \end{aligned}$$

since $\overline{u'} = \overline{C'} = 0$. Similar results hold for vC and wC, giving

$$\frac{\partial\overline{C}}{\partial t}+\frac{\partial}{\partial x}(\overline{u}\overline{C})+\frac{\partial}{\partial y}(\overline{v}\overline{C})+\frac{\partial}{\partial z}(\overline{w}\overline{C}) = -\frac{\partial}{\partial x}(\overline{u'C'})-\frac{\partial}{\partial y}(\overline{v'C'})-\frac{\partial}{\partial z}(\overline{w'C'}). \tag{12}$$

The right-hand side represents the average effect of turbulent eddies on the concentration. Molecular diffusion is caused by the random motion of molecules, whereas the effect here is caused by the random eddy motions. By *analogy* with the molecular scale, we assume that

$$\left.\begin{aligned} \overline{u'C'} &= -\,\varepsilon_x \frac{\partial \overline{C}}{\partial x} \\ \overline{v'C'} &= -\,\varepsilon_y \frac{\partial \overline{C}}{\partial y} \\ \overline{w'C'} &= -\,\varepsilon_z \frac{\partial \overline{C}}{\partial z} \end{aligned}\right\} \tag{13}$$

ε_x, ε_y and ε_z are analogous to the molecular diffusivity D. They must be measured experimentally. They differ from D in that

(i) ε_x, ε_y and ε_z need not be equal,

(ii) In general, ε_x, ε_y and ε_z are not constant,

(iii) $\varepsilon_x, \varepsilon_y, \varepsilon_z \gg D$.

Using Eq. (13),

$$\frac{\partial \overline{C}}{\partial t}+\frac{\partial}{\partial x}(\overline{u}\overline{C})+\frac{\partial}{\partial y}(\overline{v}\overline{C})+\frac{\partial}{\partial z}(\overline{w}\overline{C}) = \frac{\partial}{\partial x}\left(\varepsilon_x \frac{\partial \overline{C}}{\partial x}\right)+\frac{\partial}{\partial y}\left(\varepsilon_y \frac{\partial \overline{C}}{\partial y}\right)+\frac{\partial}{\partial z}\left(\varepsilon_z \frac{\partial \overline{C}}{\partial z}\right). \tag{14}$$

This equation is the basis of much of the modelling of atmospheric dispersion.

2. Transport Processes

2.1 Diffusion Without Shear

(i) Instantaneous plane source in 3-dimensions

Suppose that the initial distribution of C is dependent only on x and t and that u, v and w are constant. Then Eq. (14) reduces to

$$\frac{\partial C}{\partial t} + u\frac{\partial C}{\partial x} = \frac{\partial}{\partial x}\left(\varepsilon_x \frac{\partial C}{\partial x}\right). \tag{15}$$

We now transform to a frame of reference moving with the flow speed u:

$$X = x - ut.$$

Then Eq. (15) becomes

$$\frac{\partial C}{\partial t} = \frac{\partial}{\partial X}\left(\varepsilon_x \frac{\partial C}{\partial X}\right). \tag{16}$$

Suppose that ε_x is constant. Then the solution to Eq. (16) is

$$C(x,t) = \frac{Q}{2\sqrt{\pi\varepsilon_x t}}\exp\left(-\frac{X^2}{4\varepsilon_x t}\right). \tag{17}$$

It can be shown that

$$\lim_{t\to 0} C(x,t) = Q\delta(X) = Q\delta(x). \tag{18}$$

The solution (17) can be interpreted as an instantaneous release of an amount Q kgm^{-2} of pollutant at $t=0$ in the plane $X=x=0$. Eq. (17) is the Gaussian "puff" solution because it describes the release of a small "puff" of pollutant.

An important quantity is the mean square distance σ_x^2 which the pollutant has spread from $X=0$. This is given by

$$\sigma_x^2 = \frac{1}{Q}\int_{-\infty}^{\infty} CX^2\,\mathrm{d}X = 2\varepsilon_x t. \tag{19}$$

Therefore

$$C(x,t) = \frac{Q}{\sigma_x\sqrt{2\pi}}\exp\left(-\frac{X^2}{2\sigma_x^2}\right). \tag{20}$$

The pollutant therefore spreads at a rate proportional to $\sqrt{t}$.

(ii) Instantaneous line source in 3-dimensions

In this case we assume that $C=C(x,y,t)$ so that the equation for C is

$$\frac{\partial C}{\partial t} + u\frac{\partial C}{\partial x} + v\frac{\partial C}{\partial y} = \frac{\partial}{\partial x}\left(\varepsilon_x\frac{\partial C}{\partial x}\right) + \frac{\partial}{\partial y}\left(\varepsilon_y\frac{\partial C}{\partial y}\right).$$

As in the previous case we make the transformation $X=x-ut$ and also let $Y=y-vt$. Then

$$\frac{\partial C}{\partial t} = \frac{\partial}{\partial X}\left(\varepsilon_x\frac{\partial C}{\partial X}\right) + \frac{\partial}{\partial Y}\left(\varepsilon_y\frac{\partial C}{\partial Y}\right). \tag{21}$$

The solution is

$$C(X,Y,t) = \frac{Q}{4\pi t\sqrt{\varepsilon_x\varepsilon_y}}\exp\left[-\frac{1}{4t}\left(\frac{X^2}{\varepsilon_x} + \frac{Y^2}{\varepsilon_y}\right)\right].$$

It can be shown that $\sigma_x^2 = 2\varepsilon_x t$ and $\sigma_y^2 = 2\varepsilon_y t$. Hence

$$C(X,Y,t) = \frac{Q}{2\pi\sigma_x\sigma_y}\exp\left[-\frac{1}{2}\left(\frac{X^2}{\sigma_x^2} + \frac{Y^2}{\sigma_y^2}\right)\right]. \tag{22}$$

(iii) Instantaneous point source in 3-dimensions

This is the most general and practical case where $C=C(x,y,z,t)$. The equation for C is

$$\frac{\partial C}{\partial t}+u\frac{\partial C}{\partial x}+v\frac{\partial C}{\partial y}+w\frac{\partial C}{\partial z}=\frac{\partial}{\partial x}\left(\varepsilon_x\frac{\partial C}{\partial x}\right)+\frac{\partial}{\partial y}\left(\varepsilon_y\frac{\partial C}{\partial y}\right)+\frac{\partial}{\partial z}\left(\varepsilon_z\frac{\partial C}{\partial z}\right).$$

We could put $Z=z-wt$ in line with the cases of plane and line sources but it is difficult to think of real cases where there is a mean vertical velocity w so we keep $w=0$. The transsformed equation for C is then

$$\frac{\partial C}{\partial t}=\frac{\partial}{\partial X}\left(\varepsilon_x\frac{\partial C}{\partial X}\right)+\frac{\partial}{\partial Y}\left(\varepsilon_y\frac{\partial C}{\partial Y}\right)+\frac{\partial}{\partial z}\left(\varepsilon_z\frac{\partial C}{\partial z}\right). \tag{23}$$

The solution is

$$C(X,Y,z,t)=\frac{Q}{8(\pi t)^{3/2}\sqrt{\varepsilon_x\varepsilon_y\varepsilon_z}}\exp\left[-\frac{1}{4t}\left(\frac{X^2}{\varepsilon_x}+\frac{Y^2}{\varepsilon_y}+\frac{z^2}{\varepsilon_z}\right)\right].$$

In this case $\sigma_x^2=2\varepsilon_x t$, $\sigma_y^2=2\varepsilon_y t$ and $\sigma_z^2=2\varepsilon_z t$ so that

$$C(X,Y,z,t)=\frac{Q}{(2\pi)^{3/2}\sigma_x\sigma_y\sigma_z}\exp\left[-\frac{1}{2}\left(\frac{X^2}{\sigma_x^2}+\frac{Y^2}{\sigma_y^2}+\frac{z^2}{\sigma_z^2}\right)\right]. \tag{24}$$

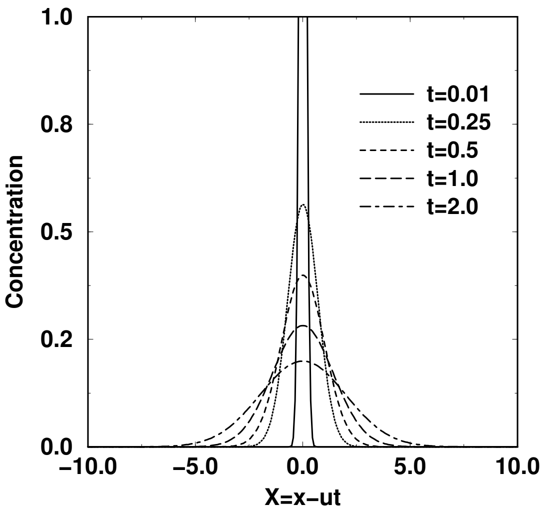

Figure 2. Concentration distributions at various times after pollutant release for the diffusion of an instantaneous plane source (Eq. (20)).

2.2 Advection Without Diffusion in a Shear Flow

Suppose that we have a uni-directional shear flow:

$$\mathbf{u}=(u,0,0)=\left(\frac{Uz}{h},0,0\right) \tag{25}$$

and suppose that we are interested in the flow between $z=0$ and $z=h$.

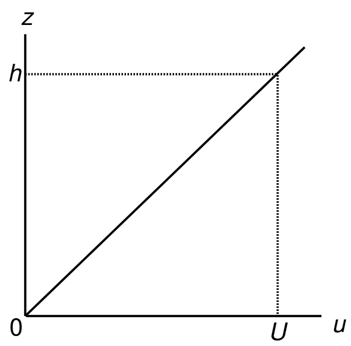

Figure 3. Shear flow $u = Uz/h$.

If we neglect diffusion, then the equation for C is

$$\frac{\partial C}{\partial t} + u\frac{\partial C}{\partial x} = 0. \tag{26}$$

If we again put $X = x - u(z)t$ Eq. (26) becomes

$$\frac{\partial C(X,t)}{\partial t} = 0 \tag{27}$$

and so $C = C(X)$, i.e. the concentration is independent of time moving with the local flow $u(z)$. Consider as in the previous section the case of an instantaneous plane source at $x = 0$, $t = 0$. Then at $t = 0$

$$C(X) = Q\delta(X).$$

This must be the solution for all time, because $\partial C/\partial t = 0$. Therefore

$$C = Q\delta(x - u(z)t) = Q\delta\left(x - \frac{Uz}{h}\right). \tag{28}$$

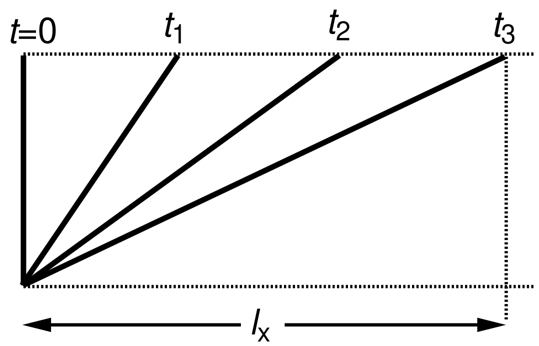

Figure 4. A line (or plane in 3-D) of pollutant initially lying on $x = 0$ is stretched and rotated by a shear flow $u = Uz/h$. At time t the x extent of the line of pollutant is denoted by l_x.

Consider the horizontal extent l_x of the pollutant. At time t it is clearly

$$l_x = Ut.$$

We can see that the pollutant spreads out at a rate proportional to t. This contrasts with the rate proportional to $\sqrt{t}$ for diffusion, so it would appear that advection is always more important than diffusion, except perhaps for a short time after release. However, we shall see in the next section that this is not the case.

2.3 Advection and Diffusion in a Shear Flow

When advection and diffusion occur simultaneously, the stretching of regions of high concentration, as occurs for pure advection, is less effective because transverse diffusion of the high concentration region is enhanced by the stretching caused by the shear. This is shown schematically in Fig. 5.

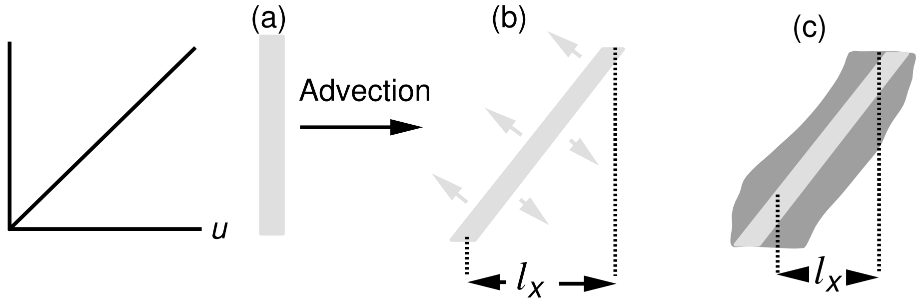

Figure 5. An initial slab (a) of pollutant is rotated and stretched by shear (b), leading to enhanced diffusion in the transverse direction (c). The spreading of the line of maximum concentration is clearly reduced by the diffusion.

The processes described here are known as Taylor's mechanism.

3. The Atmospheric Boundary Layer

3.1 Boundary Layer Equations

Let us write the Navier-Stokes equations as

$$\frac{\mathrm{D}\mathbf{u}}{\mathrm{D}t} = -\frac{1}{\rho}\nabla p - g\mathbf{k} + \nabla . \boldsymbol{\tau}$$

where $\boldsymbol{\tau}$ is the stress tensor. In laminar flows, $\boldsymbol{\tau}$ may be expressed in terms of the viscosity. In turbulent flows, molecular viscosity is not usually important because the Reynolds number is high. Instead, transport by turbulent eddies is more effective. Neglecting viscosity, we have for an incompressible flow

$$\frac{\partial u}{\partial t} + \frac{\partial}{\partial x}(u^2) + \frac{\partial}{\partial y}(uv) + \frac{\partial}{\partial z}(uw) = -\frac{1}{\rho}\frac{\partial p}{\partial x}, \tag{29}$$

$$\frac{\partial v}{\partial t} + \frac{\partial}{\partial x}(uv) + \frac{\partial}{\partial y}(v^2) + \frac{\partial}{\partial z}(vw) = -\frac{1}{\rho}\frac{\partial p}{\partial y}. \tag{30}$$

As for the case of turbulent transport of a tracer, we put

$$\left.\begin{aligned} u &= \overline{u} + u', \\ v &= \overline{v} + v', \\ w &= \overline{w} + w'. \end{aligned}\right\} \tag{31}$$

Substituting Eq. (31) into (29)–(30) and averaging

$$\frac{\partial \overline{u}}{\partial t} + \frac{\partial}{\partial x}(\overline{u}^2) + \frac{\partial}{\partial y}(\overline{uv}) + \frac{\partial}{\partial z}(\overline{uw}) = -\frac{1}{\rho}\frac{\partial \overline{p}}{\partial x} - \frac{\partial}{\partial x}(\overline{u'^2}) - \frac{\partial}{\partial y}(\overline{u'v'}) - \frac{\partial}{\partial z}(\overline{u'w'}),$$

$$\frac{\partial \overline{v}}{\partial t} + \frac{\partial}{\partial x}(\overline{uv}) + \frac{\partial}{\partial y}(\overline{v}^2) + \frac{\partial}{\partial z}(\overline{vw}) = -\frac{1}{\rho}\frac{\partial \overline{p}}{\partial y} - \frac{\partial}{\partial x}(\overline{u'v'}) - \frac{\partial}{\partial y}(\overline{v'^2}) - \frac{\partial}{\partial z}(\overline{v'w'}).$$

Close to the surface, variations in the vertical dominate horizontal variations so that we can neglect x and y derivatives. Furthermore, the mean flow is almost horizontal so that $w = 0$. Therefore

$$\frac{\partial \overline{u}}{\partial t} = -\frac{1}{\rho}\frac{\partial \overline{p}}{\partial x} - \frac{\partial}{\partial z}(\overline{u'w'}),$$

$$\frac{\partial \overline{v}}{\partial t} = -\frac{1}{\rho}\frac{\partial \overline{p}}{\partial y} - \frac{\partial}{\partial z}(\overline{v'w'}).$$

It turns out that on the scale of the whole boundary layer, we cannot neglect the effect of the rotation of the Earth. This effect is included by working in a frame of reference fixed relative to the surface of the Earth in the region of interest (this is of course a rotating, or non-inertial frame of reference). The frame of reference is rotating with angular speed $\Omega = 2\pi/(1 \text{ day})$. In the rotating frame of reference the equations of motion become

$$\frac{\partial \overline{u}}{\partial t} - 2\Omega\overline{v}\sin\phi = -\frac{1}{\rho}\frac{\partial \overline{p}}{\partial x} - \frac{\partial}{\partial z}(\overline{u'w'}), \tag{32}$$

$$\frac{\partial \overline{v}}{\partial t} + 2\Omega\overline{u}\sin\phi = -\frac{1}{\rho}\frac{\partial \overline{p}}{\partial y} - \frac{\partial}{\partial z}(\overline{v'w'}). \tag{33}$$

The extra terms which have been introduced are called the Coriolis force. ϕ is the latitude.

As for the case of scalar transport, we assume that

$$\left.\begin{aligned} \overline{u'w'} &= -K\frac{\partial \overline{u}}{\partial z}, \\ \overline{v'w'} &= -K\frac{\partial \overline{v}}{\partial z}. \end{aligned}\right\} \tag{34}$$

K is called the *eddy viscosity.* We often write

$$\boldsymbol{\tau} = -\rho(\overline{u'w'}, \overline{v'w'}) = \rho K\left(\frac{\partial \overline{u}}{\partial z}, \frac{\partial \overline{v}}{\partial z}\right) \tag{35}$$

where $\boldsymbol{\tau}$ is the *turbulent stress.*

3.2 Constant Stress Layer — The Surface Layer

There is a thin region close to the surface where the stress $\boldsymbol{\tau}$ does not vary much from its surface value and so it can be assumed to be constant. This is called the *surface layer*. In the surface layer

$$\left.\begin{aligned}\tau_x &= -\rho K \frac{\mathrm{d}\overline{u}}{\mathrm{d}z}, \\ \tau_y &= -\rho K \frac{\mathrm{d}\overline{v}}{\mathrm{d}z}.\end{aligned}\right\} \tag{36}$$

Let the wind speed U be given by

$$U^2 = \overline{u}^2 + \overline{v}^2$$

and let

$$\tau^2 = \tau_x^2 + \tau_y^2$$

where τ is the magnitude of the surface stress. Because the direction of the stress does not vary with height in the surface layer it follows from Eq. (36) that

$$\tau = -\rho K \frac{\mathrm{d}U}{\mathrm{d}z}. \tag{37}$$

We usually write the constant stress τ as

$$\tau = -\rho u_*^2 \tag{38}$$

where u_* is a quantity called the *friction velocity*. We can use arguments from dimensional analysis to evaluate the eddy viscosity K. It turns out that the only scales available to us are u_* and the height z itself. In terms of these we have

$$K \propto u_* z.$$

Physically this indicates that at greater heights, larger turbulent eddies are acting to transport momentum. We put

$$K = k u_* z \tag{39}$$

where k is a constant called von Kármán's constant. It is usually taken as $k = 0.4$. From Eq. (37), (38) and (39)

$$\frac{\mathrm{d}U}{\mathrm{d}z} = \frac{u_*}{kz}. \tag{40}$$

Solving this for u we get

$$U = \frac{u_*}{k} \ln\left(\frac{z}{z_0}\right) \tag{41}$$

where z_0 is a constant. Note that as z decreases towards zero, U goes to zero at $z = z_0$. z_0 is called the *roughness length* and it is a measure of the size of the so-called roughness elements making up the surface. These roughness elements could be grains of sand, blades of grass, bushes, trees, etc.

Table 1. Roughness length for various surfaces

Ground Cover	z_0 (m)
Smooth water or ice	10^{-4}
Lawn	0.01
Long grass	0.05
Suburban housing	0.6
Forest, city centre	1–5

Eq. (41) usually applies up to a few tens of metres from the ground.

3.3 Effect of Stability

Under some circumstances (particularly at night when there is no cloud) the surface cools by radiation into space and the layer of air close to the surface becomes cold and dense.

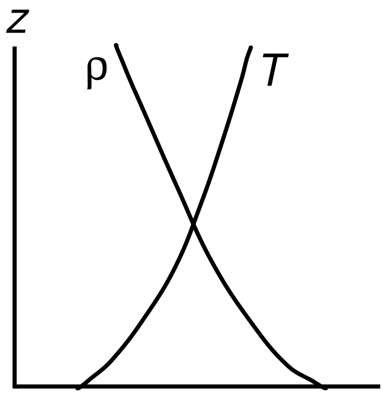

Figure 5. Temperature and density profiles close to the surface on a clear night. The air close to the surface is *stably stratified*.

This *stable stratification* inhibits vertical eddy motion. This can be thought of as reducing the size of the turbulent eddies so that $K = ku_*z$ no longer applies. Another way to think about the problem is that there is another length scale, in addition to z, introduced into the problem. This is

$$L = -\frac{\rho C_p u_*^3 \overline{T}}{kgH} \tag{42}$$

where C_p is the specific heat capacity at constant pressure, $\overline{T}$ is an average temperature (absolute) and H is the surface heat flux. For surface cooling, H is negative and so L is positive. L is called the Monin-Obukhov length. It is found experimentally that for stable stratification a reasonable approximation is

$$K = \frac{ku_*z}{1 + \alpha\frac{z}{L}}$$

so that

$$\frac{\mathrm{d}U}{\mathrm{d}z} = \frac{u_*}{kz}\left(1 + \alpha\frac{z}{L}\right) \tag{43}$$

where α is a constant. Typically, $\alpha \approx 5$. The solution of Eq. (43) is

$$U = \frac{u_*}{k}\left[\ln\left(\frac{z}{z_0}\right) + \alpha\frac{z}{L}\right]. \tag{44}$$

3.4 The Ekman Layer

On a scale deeper than the surface layer, we can, to a crude approximation, take $K =$ constant. For neutral stratification, $K \approx 10\ \mathrm{m^2s^{-1}}$. If the flow is steady, Eq. (32)–(34) become

$$-2\Omega\overline{v}\sin\phi = -\frac{1}{\rho}\frac{\partial\overline{p}}{\partial x} + K\frac{\partial^2\overline{u}}{\partial z^2},$$

$$+2\Omega\overline{u}\sin\phi = -\frac{1}{\rho}\frac{\partial\overline{p}}{\partial y} + K\frac{\partial^2\overline{v}}{\partial z^2}.$$

In the boundary layer we can assume that $\partial\overline{p}/\partial x$ and $\partial\overline{p}/\partial y$ are independent of height and are given by

$$\frac{\partial\overline{p}}{\partial x} = 2\Omega\rho v_g\sin\phi,$$
$$\frac{\partial\overline{p}}{\partial y} = -2\Omega\rho u_g\sin\phi$$

where u_g and v_g are called the *geostrophic wind* components. For our purposes, we can take them to be the wind above the boundary layer. Let $f = 2\Omega\sin\phi$ — the Coriolis parameter. Then

$$\left.\begin{aligned} K\frac{\partial^2\overline{u}}{\partial z^2} &= -f(\overline{v} - v_g), \\ K\frac{\partial^2\overline{v}}{\partial z^2} &= f(\overline{u} - u_g). \end{aligned}\right\} \tag{45}$$

These are the Ekman equations. The solutions are

$$\left.\begin{aligned} u &= u_g\left[1 - e^{-z/\delta}\cos\left(\frac{z}{\delta}\right)\right] - v_g e^{-z/\delta}\sin\left(\frac{z}{\delta}\right), \\ v &= v_g\left[1 - e^{-z/\delta}\cos\left(\frac{z}{\delta}\right)\right] + u_g e^{-z/\delta}\sin\left(\frac{z}{\delta}\right) \end{aligned}\right\} \tag{46}$$

where

$$\delta = 2\sqrt{\frac{K}{f}}.$$

δ is a measure of the thickness of the atmospheric boundary layer. In mid-latitudes, $f \approx 10^{-4}$ s^{-1} and we find that $\delta \approx 500$ m.

The Ekman solution (46) shows that the wind direction varies within the boundary layer and that the wind vectors form a spiral with increasing height (see Fig. 7).

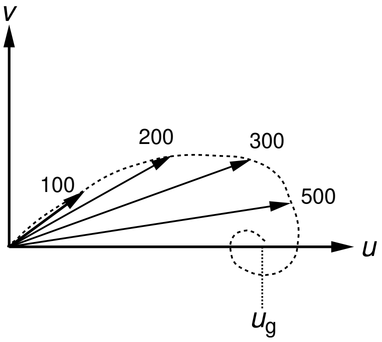

Figure 7. Wind vectors in the Ekman boundary layer. The heights of the wind vectors are shown in metres.

4. Continuous Point Sources of Pollutant

Consider a point source at $x = y = z = 0$ emitting pollutant continuously in time. The pollutant will be carried down stream by the wind and will disperse by turbulent diffusion. Suppose that the wind has speed u in the x direction. The situation is sketched in Fig. 8.

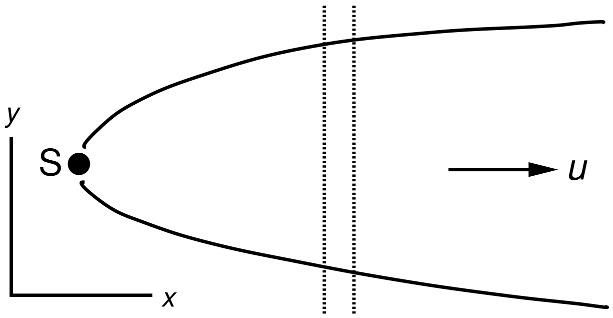

Figure 8. A plan view of a plume of pollutant from a continuous point source S.

Consider a slice of air 1 m thick moving in the x-direction, extending to infinity in the y and z directions and moving with the mean wind u. The time taken for the slice to pass a fixed point is $1/u$ seconds. If the source emits q kgs^{-1} of pollutant, then the amount in the slice is $Q = q/u$. The pollutant diffuses in the x, y and z directions. But since the source is continuous, about the same amount of pollutant diffuses into the sheet in the x-direction as diffuses out through the opposite side. Diffusion in the x-direction therefore has negligible effect. The diffusion problem reduces to that of 2-dimensional diffusion in the y, z plane but in a frame of reference moving in the x-direction with speed u. The 2-dimensional diffusion solution Eq. (22) therefore applies, but with $Q = q/u$. In other words

$$C(y, z, x) = \frac{q}{2\pi\sigma_y\sigma_z u}\exp\left(-\frac{y^2}{2\sigma_y^2} - \frac{z^2}{2\sigma_z^2}\right). \tag{47}$$

This is the *Gaussian plume equation* which is the basis of much dispersion modelling. Note that following the flow, $t = x/u$ so that we expect σ_y and σ_z to behave like

$$\sigma_y = \sqrt{2\varepsilon_y \frac{x}{u}}, \qquad \sigma_z = \sqrt{2\varepsilon_z \frac{x}{u}} \tag{48}$$

In fact this is not the case because ε_y and ε_z are not constant.

5. Dispersion in Real Environments

The Gaussian plume equation, Eq. (47) is derived from Eq. (22) and this in turn is only a true solution of the concentration equation, Eq. (21) if the eddy diffusivities are constant. This is generally not true. For example, in the neutrally stratified surface layer, the eddy viscosity K is given by $u_* kz$ and we can expect ε_z to behave similarly. In order to analyse real environments we have at least 3 possibilities:

(i) Estimate (for example using surface layer theory) or measure (usually indirectly by measuring wind fluctuations $\overline{v'^2}$ and $\overline{w'^2}$) ε_y, ε_z and then solve Eq. (21) numerically.

(ii) Assume that the solution (47) is still a reasonable approximation but that the variation of σ_y and σ_z with x is different to Eq. (48). Instead, we replace (48) by empirical relationships between σ_y, σ_z and x.

(iii) For some special cases, take ε_z to vary with z and solve the concentration equation analytically.

We now consider examples of (ii) and (iii).

5.1 Pasquill-Gifford Stability Classes

It is observed that in neutral stratification, Eq. (48) does not hold. Instead, measurements suggest that σ_y and σ_z are proportional to x^α for α in the range 0.75 to 1. This observation changes when the atmospheric stability changes. For example, when the air is very stable, vertical mixing is inhibited and σ_z grows only slowly with x. On the other hand, when there is strong solar heating of the surface, there may be strong convective activity with large vertical motions; then σ_z increases rapidly with x.

Based on measurements of atmospheric turbulence over flat plains, Pasquill and Gifford produced empirical results for the variation of σ_y and σ_z with x for six stability classes. These are shown in Table 2.

Class	Definition
A	Extremely unstable
B	Moderately unstable
C	Slightly unstable
D	Neutral
E	Slightly stable
F	Moderately stable

Table 2. Pasquill-Gifford stability classes

Guidelines are given for estimating the stability class from the wind speed, cloud cover and time of day. These are given in Table 3.

Table 3. Guidelines for determining Pasquill-Gifford stability classes

Surface wind speed (ms^{-1})	Day with insolation: Strong	Day with insolation: Moderate	Day with insolation: Slight	Night: Overcast or $\geq 4/8$ low low cloud	Night: $\leq 3/8$ cloud
2	A	A–B	B	–	–
2–3	A–B	B	C	E	F
3–5	B	B–C	C	D	E
5–6	C	C–D	D	D	D
6	C	D	D	D	D

Figs. 9 and 10 show the variation of σ_y and σ_z with x for the six stability classes. These variations may be approximated by

$$\sigma_y = ax^{0.894} \tag{49}$$

and

$$\sigma_z = cx^d + f \tag{50}$$

where the constants a, c, d and f depend on the stability class as shown in Table 4.

Table 4. Constants in empirical relationships for σ_y and σ_z							
		$x \leq 1$ km			$x \geq 1$ km		
Stability class	a	c	d	f	c	d	f
A	213	440.8	1.941	9.27	459.7	2.094	-9.6
B	156	106.6	1.149	3.3	108.2	1.098	2.0
C	104	61	0.911	0	61	0.911	0
D	68	33.2	0.725	-1.7	44.5	0.516	-13.0
E	50.5	22.8	0.678	-1.3	55.4	0.305	-34.0
F	34	14.35	0.740	0.35	62.6	0.180	-48.6

With these values of σ_y and σ_z, the concentration can be determined directly from Eq. (47). An example is shown in Fig. 11.

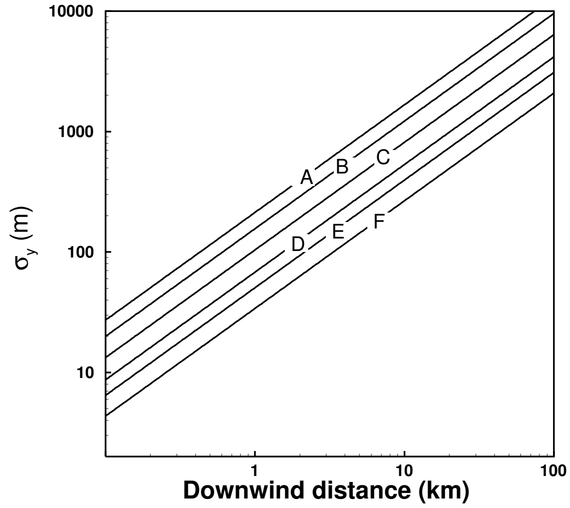

Figure 9. Variation of σ_y with downwind distance x for the six Pasquill-Gifford stability classes.

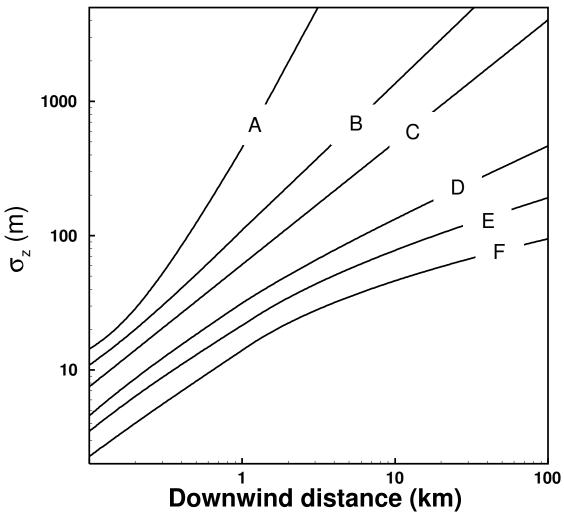

Figure 10. Variation of σ_z with downwind distance x for the six Pasquill-Gifford stability classes.

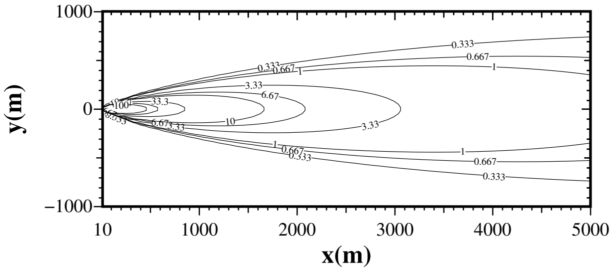

Figure 11. The solution to the Gaussian plume equation (47) with σ_y and σ_z given by the Pasquill-Gifford recommendations for stability class C. Contours of concentration are shown at $z = 0$ for a wind speed of 10 ms^{-1}.

5.2 Dispersion from a Continuous Line Source

A major application here is to the dispersion of emissions from motor vehicles travelling along a road on a cross-wind. If the wind is in the x-direction, perpendicular to the road, and y is along the road, then we do not expect the concentration of pollutant to depend on y. Just as described in §4, we can neglect diffusion in the windward direction, so that the concentration equation for a steady concentration distribution is

$$u\frac{\partial C}{\partial x} = \frac{\partial}{\partial z}\left(\varepsilon_z \frac{\partial C}{\partial z}\right). \tag{51}$$

For neutral stability, it is reasonable to assume that ε_z is equal to the eddy viscosity in the neutral surface layer, so that

$$\varepsilon_z = k u_* z. \tag{52}$$

Therefore

$$u\frac{\partial C}{\partial x} = \frac{\partial}{\partial z}\left(k u_* z \frac{\partial C}{\partial z}\right). \tag{53}$$

We need also to describe the height variation of the wind, u. It would seem to be consistent with the assumptions on ε_z to take a logarithmic velocity profile but unfortunately we cannot then solve Eq. (53) analytically. Instead, a commonly made assumption is that

$$\frac{u}{u_1} = \left(\frac{z}{z_1}\right)^p \tag{54}$$

where u_1 is the wind speed at a fixed height z_1. This can only be *approximately* equal to the logarithmic profile (41) over a relatively small height range. To get a reasonable correspondence, note that from Eq. (54)

$$\frac{1}{u}\frac{\mathrm{d}u}{\mathrm{d}z} = \frac{p}{z}$$

and therefore

$$\frac{\mathrm{d}u}{\mathrm{d}z} = \frac{pu}{z}.$$

If we now substitute from Eq. (40) and (41) into the left and right sides of the above equation, we get

$$\frac{u_*}{kz} = \frac{p}{z} \ln\left(\frac{z}{z_0}\right)$$

and hence

$$p = \frac{1}{\ln\left(\frac{z}{z_0}\right)}. \tag{55}$$

Of course p should be a constant and so in Eq. (55) we take an average value of z over the range of interest. The precise value of p should really depend not only on the height range of interest but also on the atmospheric stability. Generally, values in the range 0.1–0.4 are used, but for high stability they may be even larger. Typical values are given in Table 5.

Table 5. Exponent in Power Law Wind Profile

Surface/stability	p
Neutral/smooth	0.14
Neutral/rough	0.3
Moderately unstable	0.1
Extremely unstable	0
Stable	0.2–1

Using Eq. (54), Eq. (53) becomes

$$u_1 \left(\frac{z}{z_1}\right)^p \frac{\partial C}{\partial x} = \frac{\partial}{\partial z}\left(k u_* z \frac{\partial C}{\partial z}\right) \tag{56}$$

and the solution is

$$C(x, z) = \frac{q}{(p+1) u_* k x} \exp\left(-\frac{z_1^{-p} u_1 z^{p+1}}{(p+1)^2 u_* k x}\right). \tag{57}$$

Note that the concentration at the ground decreases with x like $1/x$, unlike the one-dimensional diffusion solution with constant diffusivity which suggests decay like $1/\sqrt{x}$. Note also that the decay rate is larger for smaller p, i.e. for unstable air flow. Eq. (57) has been shown to agree quite well with observations.

6. Gaussian Plumes from High Chimneys

The Gaussian plume equation (47) assumed that the source was at $x = y = z = 0$. We can easily change this so that the source is from a chimney of height h

by replacing Eq. (47) by

$$C(x,y,z) = \frac{q}{2\pi\sigma_y\sigma_z u}\exp\left(-\frac{y^2}{2\sigma_y^2} - \frac{(z-h)^2}{2\sigma_z^2}\right). \tag{58}$$

However, this equation tells us that diffusion takes place not only for $z > 0$ (above the ground) but also for $z < 0$ (below the ground). The simplest assumption available to correct this is to assume that any pollutant which reaches the ground is reflected back. Thus the pollutant which, according to Eq. (58) should be below the ground actually appears above the ground. This is exactly equivalent to allowing Eq. (58) to apply unmodified but then introducing another source at $z = -h$ (i.e. the image of the true source in the ground). We then replace Eq. (58) by

$$C(x,y,z) = \frac{q}{2\pi\sigma_y\sigma_z u}\left[\exp\left(-\frac{y^2}{2\sigma_y^2} - \frac{(z-h)^2}{2\sigma_z^2}\right) + \exp\left(-\frac{y^2}{2\sigma_y^2} - \frac{(z+h)^2}{2\sigma_z^2}\right)\right] \tag{59}$$

and use Eq. (59) for $z > 0$ only. The concentration at ground level is

$$C(x,y) = \frac{q}{\pi\sigma_y\sigma_z u}\exp\left(-\frac{y^2}{2\sigma_y^2} - \frac{h^2}{2\sigma_z^2}\right). \tag{60}$$

Fig. 12 shows the concentration at ground level downwind of two chimneys (one 25 m high and the other 50 m high) emitting the same amount of pollutant. It is clear that for the higher chimney the maximum concentration is both lower and further down wind.

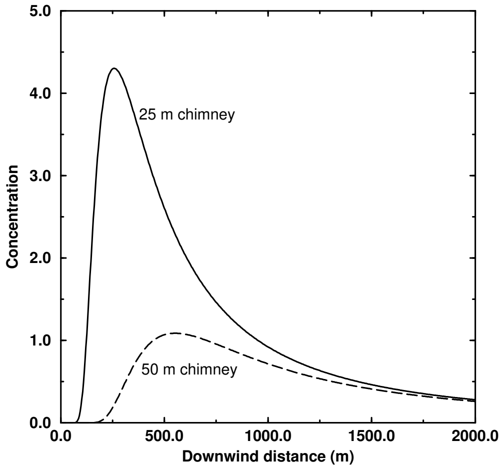

Figure 12. The ground level concentration of pollutant down wind of two chimneys emitting equal amounts of pollutant. Pasquill stability class C is assumed.

If we consider the Pasquill-Gifford stability class C (slightly unstable) then $\sigma_y \approx 100x^{0.9}$ and $\sigma_z \approx 60x^{0.9}$. The maximum ground level concentration according to Eq. (60) can then be shown to be at $\sigma_z = h/\sqrt{2}$ and its value is

$$C_{\max} \approx \frac{q}{0.83\,\pi e u h^2} \approx \frac{0.15q}{h^2}. \tag{61}$$

Note that the maximum concentration decreases as the square of the chimney height — so tall chimneys are a good idea.

7. Deposition

For some pollutants, what matters is not only the concentration in the air but also the amount which settles on the ground. For example, dust particles from a quarry may cause a nuisance down wind. Sulphuric acid which is created from power station emissions causes acidification of soil and can be harmful to plants and animals (e.g. destruction of forests and fish in lakes by acid rain). Methods for calculating the rate of deposition are needed. We will not go into details here. However, some important factors are:

(i) *Settling rate of particles.* This is strongly dependent on the particle size and hence a knowledge of particle size distributions is important.

(ii) *Dry deposition by diffusion.* The flux of a pollutant with concentration C $\mathrm{kgm^{-3}}$ through the ground is

$$F = -\varepsilon_z \frac{\partial C}{\partial z}. \quad \mathrm{kgm^{-2}s^{-1}}.$$

Note that in the image model for plumes reflecting from the ground, $\partial C/\partial z = 0$ at the ground (by symmetry) and hence the deposition rate is zero.

(iii) *Wet deposition.* Important processes are washout (collection of pollutant by rain drops as they fall) and rainout (collection of pollutants by cloud droplets which subsequently form rain drops). Knowledge of precipitation rates is clearly essential.

8. Types of Atmospheric Dispersion Models

8.1 Gaussian Plume Models

These use an equation such as (24), (47) or (57) to predict the concentration of pollutant emitted by a short-lived or continuous point or line source. They are particularly useful for studying the effects of a single source. They are less well adapted to problems involving many sources (e.g. a whole city) or problems where chemical reactions of pollutants are important.

8.2 Single Box Models

These models define a box enclosing the region of interest and for that box consider

$$\begin{pmatrix}\text{Accumulation}\\ \text{rate}\end{pmatrix} = \begin{pmatrix}\text{All flow}\\ \text{rates in}\end{pmatrix} - \begin{pmatrix}\text{All flow}\\ \text{rates out}\end{pmatrix} + \begin{pmatrix}\text{Creation}\\ \text{rate}\end{pmatrix} - \begin{pmatrix}\text{Destruction}\\ \text{rate}\end{pmatrix}.$$

This is particularly suitable for a model of a polluted city. It is well-adapted to the inclusion of chemical reactions and many different pollutants but it is of no use for predicting local concentrations of pollutants.

8.3 Multi-Box Models

These are similar to single box models except that the fluxes of pollutant into each box are derived from the fluxes out of the adjacent box (see Fig. 13).

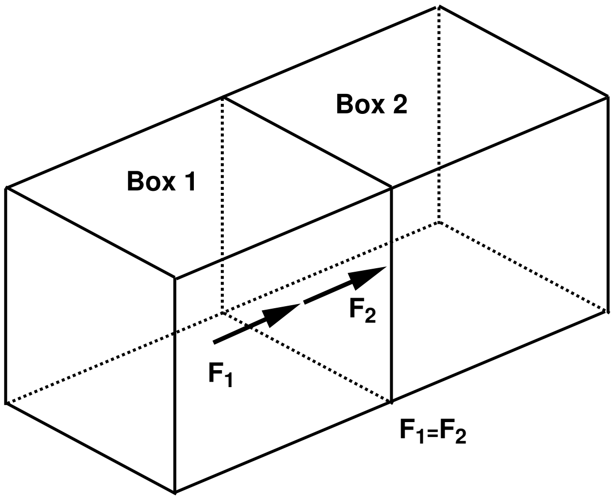

Figure 13. Two boxes of a multi-box pollutant transport model showing the matching of fluxes across inter-box boundaries. The flux F_1 of pollutant out of Box 1 is equal to the flux F_2 of pollutant into Box 2.

8.4 Numerical Solution of the Concentration Equation

This is the most general approach but is usually the most expensive (see §10 for more details).

9. Chemical Reaction of Atmospheric Pollutants

As noted in §1, pollutants may react with each other or with the air to form new chemicals. Some of the more important reactions for pollution studies are now described.

9.1 Nitrogen Oxides and Ozone

The oxides of nitrogen NO (nitric oxide) and NO_2 are produced during combustion. There are two sources:

(i) From nitrogen in the air in contact with flames at a few thousand K.
(ii) From nitrogen present within the fuel.

The dominant reaction producing nitrogen oxides (NO_x) is

$$N_2 + O_2 \longrightarrow 2NO.$$

NO is a colourless and odourless gas. It reacts with oxygen in the air over a few hours to produce nitrogen dioxide:

$$2NO + O_2 \longrightarrow 2NO_2.$$

NO_2 is a brown gas which is a respiratory irritant. Some of the NO_2 reacts with water vapour to form nitric acid:

$$3NO_2 + H_2O \longrightarrow 2HNO_3 + NO.$$

Another important reaction of NO_2 is a photochemical reaction producing ozone, O_3:

$$NO_2 + h\nu \longrightarrow O + NO,$$

$$O + O_2 + M \longrightarrow O_3 + M$$

where $h\nu$ represents a photon of sunlight and M is any air molecule (usually N_2 or O_2). Ozone is the main contributor to photochemical smog and is a strong respiratory irritant.

9.2 Oxides of Sulphur

All fuels (e.g. oil, coal, gas, wood) contain sulphur. When these are burnt the sulphur is mostly released as sulphur dioxide (SO_2):

$$S + O_2 \longrightarrow SO_2.$$

A sequence of reactions in the atmosphere then produces sulphuric acid:

$$SO_2 + OH + M \longrightarrow HSO_3 + M,$$

$$HSO_3 + O_2 \longrightarrow SO_3 + HO_2,$$
$$SO_3 + H_2O \longrightarrow H_2SO_4.$$

The sulphuric acid condenses onto existing particles or condenses to form new particles. These are often captured by rain drops and fall to the ground as acid rain.

SO_2 can be removed from emissions by reaction with limestone ($CaCO_3$) to form gypsum ($CaSO_4$):

$$2CaCO_3 + 2SO_2 + O_2 \longrightarrow 2CaSO_4 + 2CO_2.$$

9.3 Oxides of Carbon

Carbon dioxide (CO_2) is a naturally occurring gas in the atmosphere. It is absorbed by plants during photosynthesis and is therefore an essential component of the biosphere. The amount of carbon dioxide is increasing in the atmosphere because

(i) It is produced during the burning of all fuels
(ii) As tropical forests are cut down for timber, there are fewer trees to absorb the CO_2.

The proportion of CO_2 in the atmosphere has increased by about 25% since the Industrial Revolution.

The air is quite transparent in incoming solar radiation. This heats the surface of the Earth which in turn emits radiation at much longer wavelengths. This long-wave radiation is strongly absorbed by CO_2. Thus, increasing the proportion of CO_2 has the potential to increase the temperature of the atmosphere and oceans (global warming). It is thought that doubling the amount of CO_2 over the next century would result in a temperature rise of 0.5–5°C. There are great uncertainties, particularly connected with the response of the biosphere and absorption of CO_2 by the oceans. The main consequences of global warming would be

(i) changes in climate patterns (with desertification in places)
(ii) rising sea levels due to melting of land ice and thermal expansion of the sea.

Burning of fossil fuels also produces carbon monoxide (CO). This is very poisonous. It is produced in equilibrium with CO_2:

$$2CO_2 \longrightarrow 2CO + O_2.$$

At high temperatures the equilibrium moves more to the right in the above equation.

9.4 CFCs

CFCs (chloro-fluoro-carbons) are compounds containing chlorine, fluorine and carbon. They are very inert, non-toxic, non-inflammable, invisible and odourless. They have been used as refrigerants and as propellants in aerosol cans. The problem with CFCs is that when they reach the stratosphere (10–50 km) they can release chlorine which reacts to destroy naturally occurring ozone. For example

$$\begin{aligned} CFCl_3 + h\nu &\longrightarrow CFCl_2 + Cl, \\ Cl + O_3 &\longrightarrow ClO + O_2, \\ ClO + O &\longrightarrow Cl + O_2. \end{aligned}$$

Stratospheric ozone is responsible for absorbing much of the ultra-violet part of the incident solar radiation. Loss of ozone results in increased UV radiation reaching the surface. This is harmful to humans and animals and possibly to plants. CFCs are rapidly being replaced by other chemicals as a result of international agreements. However, their residence time in the atmosphere is tens to hundreds of years, so the effects of 20^{th} century CFC production will continue for a considerable time.

10. Numerical Schemes

We will consider some finite difference numerical schemes for the solution of the advection-diffusion equation with source term $S(C,t)$:

$$\frac{\partial C}{\partial t}+\frac{\partial}{\partial x}(uC)+\frac{\partial}{\partial y}(vC)+\frac{\partial}{\partial z}(wC) = \frac{\partial}{\partial x}\left(\varepsilon_x\frac{\partial C}{\partial x}\right)+\frac{\partial}{\partial y}\left(\varepsilon_y\frac{\partial C}{\partial y}\right)+\frac{\partial}{\partial z}\left(\varepsilon_z\frac{\partial C}{\partial z}\right)+S(C,t). \tag{62}$$

10.1 Source Terms

The equation

$$\frac{\partial C}{\partial t} = S(C,t) \tag{63}$$

can be approximated by

$$C^{n+1} = C^n + \Delta t S(C^n, t^n) \tag{64}$$

where C^n denotes C evaluated at time $t^n = n\Delta t$. Eq. (64) is not usually practical because stability is only achieved with severe restrictions on the time step. Eq. (64) is an *explicit* scheme. The corresponding implicit scheme is

$$C^{n+1} = C^n + \Delta t S(C^{n+1}, t^{n+1}). \tag{65}$$

This is unconditionally stable but if S is a nonlinear function, Eq. (65) requires solution of a system of nonlinear equations. Semi-implicit schemes are possible, such as

$$C^{n+1} = C^n + \Delta t[\xi S(C^{n+1}, t^{n+1}) + (1-\xi)S(C^n, t^n)]. \tag{66}$$

If S is a linear function, then the scheme (66) with $\xi = 0.5$ is unconditionally stable and is furthermore second order accurate in time, unlike (64) and (65) which are only first order accurate.

10.2 Advection Terms

Consider the simplified advection equation

$$\frac{\partial C}{\partial t} + u\frac{\partial C}{\partial x} = 0 \tag{67}$$

where u is assumed to be constant. The simplest scheme is

$$\frac{C_i^{n+1} - C_i^n}{\Delta t} = -u\frac{C_{i+1}^n - C_{i-1}^n}{2\Delta x} \tag{68}$$

where C_i^n denotes C evaluated at x_i and where $x_{i+1} - x_i = \Delta x$. Eq. (68) is unconditionally unstable and therefore useless. The Lax scheme is a modification of (68) in which C_i^n is replaced by $\frac{1}{2}(C_{i+1}^n + C_{i-1}^n)$:

$$\frac{C_i^{n+1} - \frac{1}{2}(C_{i+1}^n + C_{i-1}^n)}{\Delta t} = -u\frac{C_{i+1}^n - C_{i-1}^n}{2\Delta x}. \tag{69}$$

This scheme is stable if the Courant-Friedrichs-Lewy (CFL) condition

$$\frac{|u|\Delta t}{\Delta x} \leq 1 \tag{70}$$

is satisfied. However, it is only first order accurate in time. Another problem is that it is possible for C to become negative. This problem is overcome in so-called upwind schemes:

$$\frac{C_i^{n+1} - C_i^n}{\Delta t} = \left.\begin{array}{ll} -u\dfrac{C_i^n - C_{i-1}^n}{\Delta x} & \text{for } u > 0 \\ -u\dfrac{C_{i+1}^n - C_i^n}{\Delta x} & \text{for } u < 0. \end{array}\right\} \tag{71}$$

This is stable if the CFL condition is satisfied but is only first order accurate in space. Use of the upwind scheme is equivalent to the introduction of a large artificial diffusion. A scheme which is explicit, second order accurate in space and time and is stable if the CFL condition is satisfied is the two-step Lax-

Wendroff scheme:

$$\left.\begin{aligned} C_i^{n+1} &= C_i^n - \frac{u\Delta t}{\Delta x}\left(C_{i+1/2}^{n+1/2} - C_{i-1/2}^{n+1/2}\right) \\ C_{i+1/2}^{n+1/2} &= \frac{1}{2}\left(C_{i+1}^n + C_i^n\right) - \frac{u\Delta t}{\Delta x}\left(C_{i+1}^n - C_i^n\right). \end{aligned}\right\} \tag{72}$$

This scheme does however still allow negative values of C.

10.3 Diffusion Terms

Consider the simple, one-dimensional diffusion equation

$$\frac{\partial C}{\partial t} = \frac{\partial}{\partial x}\left(\varepsilon \frac{\partial C}{\partial x}\right). \tag{73}$$

For simplicity we will assume that the diffusivity ε is constant. An explicit scheme which is first order accurate in time and second order accurate in space is

$$\frac{C_i^{n+1} - C_i^n}{\Delta t} = \frac{\varepsilon}{(\Delta x)^2}[C_{i+1}^n - 2C_i^n + C_{i-1}^n]. \tag{74}$$

This is stable if

$$\frac{2\varepsilon\Delta t}{(\Delta x)^2} \leq 1. \tag{75}$$

This usually requires a vast number of time steps for the effects of diffusion to become noticeable. The fully implicit scheme

$$\frac{C_i^{n+1} - C_i^n}{\Delta t} = \frac{\varepsilon}{(\Delta x)^2}[C_{i+1}^{n+1} - 2C_i^{n+1} + C_{i-1}^{n+1}]. \tag{76}$$

is unconditionally stable but it is necessary to solve a tridiagonal system of equations at each time step. If the average of Eq. (74) and (76) is taken we get the Crank-Nicholson scheme which is unconditionally stable and second order accurate in space and time.

If ε is not constant, the above schemes can easily be generalised. For example, we can write

$$\begin{aligned} \frac{\partial}{\partial x}\left(\varepsilon\frac{\partial C}{\partial x}\right) &= \frac{1}{(\Delta x)^2}\left[\varepsilon_{i+1/2}(C_{i+1} - C_i) - \varepsilon_{i-1/2}(C_i - C_{i-1})\right] \\ &= D_x. \end{aligned} \tag{77}$$

10.4 Operator Splitting

For multi-dimensional problems or problems in which there is advection *and* diffusion, many of the above methods can still be used if an operator splitting approach is used. For example, consider the one-dimensional advection-diffusion equation:

$$\frac{\partial C}{\partial t} + u\frac{\partial C}{\partial x} = \frac{\partial}{\partial x}\left(\varepsilon\frac{\partial C}{\partial x}\right). \tag{78}$$

Now consider

$$\left.\begin{aligned}\frac{\partial C_1}{\partial t} &= -u\frac{\partial C}{\partial x},\\ \frac{\partial C_2}{\partial t} &= \frac{\partial}{\partial x}\left(\varepsilon\frac{\partial C}{\partial x}\right),\\ C &= C_1 + C_2.\end{aligned}\right\} \tag{79}$$

By adding the first two equations in (79) we get Eq. (78) but we can step forward these two equations separately, thus using the techniques available for the solution of simpler equations.

As another example, consider the three-dimensional diffusion equation:

$$\frac{\partial C}{\partial t} = \frac{\partial}{\partial x}\left(\varepsilon_x\frac{\partial C}{\partial x}\right) + \frac{\partial}{\partial y}\left(\varepsilon_y\frac{\partial C}{\partial y}\right) + \frac{\partial}{\partial z}\left(\varepsilon_z\frac{\partial C}{\partial z}\right). \tag{80}$$

Using the notation in Eq. (77), we can solve

$$\left.\begin{aligned}\frac{C_i^{n+1/3} - C_i^n}{\frac{1}{3}\Delta t} &= D_x^{n+1/3} + D_y^n + D_z^n,\\ \frac{C_i^{n+2/3} - C_i^{n+1/3}}{\frac{1}{3}\Delta t} &= D_x^{n+1/3} + D_y^{n+2/3} + D_z^{n+1/3},\\ \frac{C_i^n - C_i^{n+2/3}}{\frac{1}{3}\Delta t} &= D_x^{n+2/3} + D_y^{n+2/3} + D_z^{n+1}.\end{aligned}\right\} \tag{81}$$

Adding these equations gives a consistent representation of Eq. (80) which is second order accurate in space and time. This is an alternating-direction implicit (ADI) method.