

This section discusses the law of conservation of mass within a control volume, expressed in both integral and differential forms. Mathemical descriptions of advective and diffusive fluxes into/out of a control volume are shown, the end result being the all-important mass transport equation. The concept of the total derivative is also introduced, allowing us to relate Eulerian (fixed position) and Lagrangian (moving with the flow) perspectives. Two animations further explain the total derivative, showing the temporal temperature change of a probe moving through a spatial temperature gradient. The example problems require application of both forms of the law of conservation of mass to solve transport problems in both industrial and environmental contexts.

## 1. Conservation of Mass

### 1.1 Conceptual Model for Diffusion

Diffusion is defined as the net transport due to random motion. A model for diffusive flux can be constructed from the following simple example. Consider a one-dimensional system with motion in the X direction only. An interface B-B' separates two regions of different concentration, C 1 and $\mathrm{C} 2=$ particles/volume on the left and right side of the interface, respectively. The motion of each particle is a one-dimensional random walk. In each time interval, $\Delta t$, each particle will move a distance $\pm \Delta X$, moving right $(+\Delta X)$ or left $(-\Delta X)$ with equal probability.


Within each time step, any particle within a distance $\Delta \mathrm{X}$ of the interface B-B' has a $50 \%$ probability of crossing over that interface. The number of particles with the potential to cross $B-B^{\prime}$ from left to right (positive mass flux) is ( $\mathrm{C} 1 \Delta \mathrm{X} A$ ), where A is the area of interface $\mathrm{B}-\mathrm{B}^{\prime}$. On average half of these take a positive step and cross the interface in time $\Delta \mathrm{t}$, such that the flux left to right is $(0.5 \mathrm{C} 1 \Delta \mathrm{X} \mathrm{A})$. Similarly, the number of particles crossing right to left in $\Delta \mathrm{t}$ (negative mass flux) will be ( $0.5 \mathrm{C} 2 \Delta \mathrm{X} \mathrm{A}$ ). The resulting mass flux, $\mathrm{q}_{\mathrm{X}}$, is

$$
\begin{equation*}
\mathrm{q}_{\mathrm{x}}=\frac{0.5 \Delta \mathrm{X} \mathrm{~A}(\mathrm{C} 1-\mathrm{C} 2)}{\Delta \mathrm{t}} . \tag{1}
\end{equation*}
$$

If $\mathrm{C}(\mathrm{x})$ is continuous, then $\mathrm{C} 2 \approx \mathrm{C} 1+\Delta \mathrm{X} \partial \mathrm{C} / \partial \mathrm{x}$, and (1) becomes

$$
\begin{equation*}
\mathrm{q}_{\mathrm{X}} \approx-\left\lfloor\frac{\Delta \mathrm{X}^{2}}{2 \Delta \mathrm{t}}\right\rfloor \mathrm{A} \frac{\partial \mathrm{C}}{\partial \mathrm{x}}=-\mathrm{D} \mathrm{~A} \frac{\partial \mathrm{C}}{\partial \mathrm{x}}=[\text { mass } / \text { time }] . \tag{2}
\end{equation*}
$$

The coefficient of diffusion, $\mathrm{D} \sim(1 / 2) \Delta \mathrm{X}^{2} / \Delta \mathrm{t}$, has units of [length ${ }^{2}$ time $\left.^{-1}\right]$. The diffusivity of a chemical molecule in a given fluid depends on the ease with which the molecule can move, specifically, how far, $\Delta \mathrm{X}$, the molecule can move in a given time
interval. The ease of molecular motion, and thus the diffusivity of a particular chemical, will depend on the molecule size and polarity, the type of fluid and the temperature.

Equation (2) is a mathematical expression of Fick's Law. Fick's Law states that the flux of solute mass crossing a unit area, A, per unit time, $\Delta t$, in a given direction, e.g. $x$, is proportional to the gradient of concentration in that direction, $\partial \mathrm{C} / \partial \mathrm{x}$, and is countergradient, i.e. the net flux is down-gradient. Because the flux in any direction is proportional only to the concentration gradient in that direction, Fick's Law can be directly extended to three-dimensions.

$$
\begin{equation*}
\left(\mathrm{q}_{\mathrm{x}}, \mathrm{q}_{\mathrm{y}}, \mathrm{q}_{\mathrm{z}}\right)=\left(-\mathrm{DA}_{\mathrm{yz}} \frac{\partial \mathrm{C}}{\partial \mathrm{x}},-\mathrm{DA}_{\mathrm{xz}} \frac{\partial \mathrm{C}}{\partial \mathrm{y}},-\mathrm{DA}_{\mathrm{xy}} \frac{\partial \mathrm{C}}{\partial \mathrm{z}}\right) . \tag{3}
\end{equation*}
$$

For molecular diffusion the coefficient for diffusion is isotropic, i.e. the same in all directions. This is not typically true for turbulent diffusion.

## Diffusion from a point source

Consider a cloud of $N$ particles (and total mass $M$ ) released at $x=0$ and $t=0$. Under the action of molecular diffusion, the cloud will slowly spread. We use the random walk model to predict the distribution of particle (mass) concentration, $\mathrm{C}(\mathrm{x}, \mathrm{t})$. Note, that if we assume a unit mass per particle, we can conveniently interchange $\mathrm{N}=\mathrm{M}$. For simplicity we again consider a one-dimensional system, with the same rules of random motion described above, i.e. at each time step, $\Delta \mathrm{t}$, each particle will move either $+\Delta \mathrm{X}$ or $-\Delta \mathrm{X}$ with equal probability. Over time each particle will move a bit forward and a bit backward. The probable location of an individual particle after many such steps can be predicted with the Central Limit Theorem (see any basic statistics text). Specifically, in the limit of many steps, the probability that a particle will be located between $\mathrm{m} \Delta \mathrm{X}$ and $(m+1) \Delta X$ approaches a normal distribution with a zero mean and a standard deviation of

$$
\begin{equation*}
\sigma=\sqrt{2 \mathrm{Dt}} \tag{4}
\end{equation*}
$$

where, as above,

$$
\begin{equation*}
\mathrm{D}=(1 / 2) \Delta \mathrm{X}^{2} / \Delta \mathrm{t} . \tag{5}
\end{equation*}
$$

The probability that a particle ends up between $x$ and $x+\Delta X$ is

$$
\begin{equation*}
\mathrm{p}(\mathrm{x}, \mathrm{t}) \Delta \mathrm{X}=\frac{1}{\sigma \sqrt{2 \pi}} \exp \left(-\frac{\mathrm{x}^{2}}{2 \sigma^{2}}\right) \Delta \mathrm{X}=\frac{1}{\sqrt{4 \pi \mathrm{Dt}}} \exp \left(-\frac{\mathrm{x}^{2}}{2 \sigma^{2}}\right) \Delta \mathrm{X} . \tag{6}
\end{equation*}
$$

Now consider the full cloud of $N$ particles. At any time $t$, the number of particles between $x$ and $x+\Delta X$ is expected to be $n(x, t)=N p(x, t) \Delta X$. Thus, the concentration, $C$, at position $X$ is $C(x, t) \approx n(x, t) /(A \Delta X)$, where $A$ is the constant cross-section of the onedimensional system. Exchanging M for N , the concentration distribution, $\mathrm{C}(\mathrm{x}, \mathrm{t})$,

$$
\begin{equation*}
\mathrm{C}(\mathrm{x}, \mathrm{t})=\frac{\mathrm{M}}{\mathrm{~A} \sqrt{4 \pi \mathrm{Dt}}} \exp \left(-\mathrm{x}^{2} / 4 \mathrm{Dt}\right)=\left[\text { mass } / \text { length }{ }^{3}\right] \tag{7}
\end{equation*}
$$

As noted above, this distribution is the normal distribution with zero mean and standard deviation, $\sigma=\sqrt{2 \mathrm{Dt}}$, which should be familiar to you from any basic statistics course. Briefly, the distribution forms a bell-curve, as shown below. At any time, sixty-eight percent of the total mass (total number of particles) falls within $\pm \sigma$ of the mean position $(x=0)$. Ninety-five percent of the mass falls within $\pm 2 \sigma$ of the mean position. And, $99.7 \%$ falls within $\pm 3 \sigma$ of the mean position. Based on these limits, it has become common to define the extent of a concentration patch based on the contour that includes ninety-five percent of the total mass, i.e. the contour at $2 \sigma$ from the center. With this convention the length of a diffusing cloud, $L$, is often taken as $L=4 \sigma$.


It is also useful to note that the concentration level at one standard deviation from the cloud center is $61 \%$ of the maximum concentration, i.e. $C(x= \pm \sigma)=0.61 \mathrm{Cmax}$, where Cmax is the concentration at the center of the cloud. This value provides a useful way to rapidly define the standard deviation of a particle (species) cloud.

## Animation Example of Random Walk:

This animation shows the motion of 500 particles in a one-dimensional random walk with step size $\Delta X=1$ in time $\Delta t=1$. At $t=0$ the particles are at $x=0$. The animation mimics the effect of Fickian Diffusion. As you watch the animation, consider the following.

## Graph of Absolute Particle Location (lower left window).

This graph shows the number of particles located at each position of the x-axis. The number of particles per location is analogous to a concentration.
a) Over time how does the peak particle number, N , (concentration, C ) change under the influence of random particle motion (diffusion)?
b) Over time how does the gradient in particle number (concentration), i.e. $\mathrm{dN} / \mathrm{dx}$ ( $\mathrm{dC} / \mathrm{dx}$ ) change under the influence of random particle motion (diffusion)?
c) What is the sign of the particle number (concentration) gradient $(\mathrm{dN} / \mathrm{dx})$ for $\mathrm{x}>0$ ? Consider the animation of individual particle motion (uppermost window). For $\mathrm{x}>0$,
is the net particle flux positive (to the right) or negative (to the left)? Is the direction of flux up-gradient of down-gradient? Is the relationship between the direction of flux and the concentration gradient consistent with Fick's Law (equation 3)?
d) Estimate the diffusion coefficient, D, using equation (4) above, and the values of $\sigma$ given in the upper left corner of this graph. You can pause the animation. How does the realized value of D compare with the theoretical value given in equation (5). Note that no specific units are given here, such that D will simply have unit $\mathrm{L}^{2} \mathrm{~T}^{-1}$, where L is an arbitrary length unit and T is the arbitrary time unit.

## Graph of Particle Location in Terms of $\sigma$.

This graph plots the distribution of particle location with the position normalized by the standard deviation, $\sigma$. The solid curve is the Gaussian distribution.
e) Note that at early time (first few time steps) the real distribution of particles does not approximate a Gaussian distribution very well. This is because the Gaussian distribution is only valid after a sufficient number of steps (Central Limit Theorem). Use the animation to estimate how many steps are required for the distribution to consistently fit the Gaussian distribution.

## Key Aspects of Diffusion

- Diffusion is the net flux due to random motion.
- Diffusive flux is proportional but opposite in sign to the gradient of concentration.
- Diffusion acts to dilute concentration and reduce gradients of concentration.


### 1.2 Conservation of Mass

The equation of mass conservation expresses a budget for the addition and removal of mass from a defined region of fluid. Consider a fixed, non-deforming volume of fluid, $\forall$, called the control volume (cv), which has a defined surface boundary, called the control surface (cs). Conservation of mass requires that the time rate of change of mass within the control volume equals the rate at which mass enters the control volume plus the rate at which mass is gained or lost within the control volume due to sources and sinks. A mathematical expression of this law is described below.

Within the control volume there is a distribution of some species defined by the concentration field, $\mathrm{C}(\mathrm{x}, \mathrm{y}, \mathrm{z})$. The total mass within the control volume is
(8) $\quad \mathrm{M}=\int_{c v} \mathrm{C} d \forall$.
$M$ can change over time due to sources and sinks located within the volume, or due to fluxes of mass across the control volume boundaries. In a fluid system there are two forms of mass flux, advection and diffusion. The net flux of mass out of the control volume due to advection is described by the integral,

$$
\begin{equation*}
\int_{\mathrm{cs}} \mathrm{C} \overrightarrow{\mathrm{~V}} \cdot \overrightarrow{\mathrm{n}} \mathrm{dA} \tag{9}
\end{equation*}
$$



Here, $\overrightarrow{\mathrm{V}}=(\mathrm{u}, \mathrm{v}, \mathrm{w})$ is the velocity vector and $\overrightarrow{\mathrm{n}}$ is the outward pointing normal for surface segment $\mathrm{dA} . \overrightarrow{\mathrm{V}} \cdot \overrightarrow{\mathrm{n}}$ represents the velocity component perpendicular to the area segment dA . The definition of $\overrightarrow{\mathrm{n}}$ as the outward facing normal makes equation 9 the net flux out of $\forall$. That is, flow out of $\forall$ (same direction as $\overrightarrow{\mathrm{n}}$ ) contributes positively to the integral, and flows into $\forall$ (opposite to $\overrightarrow{\mathrm{n}}$ ) contribute negatively. The net flux out of the control volume due to diffusion is defined using Fick's Law.

$$
\begin{equation*}
-\int_{\mathrm{cs}} \mathrm{D}_{\mathrm{n}} \frac{\partial \mathrm{C}}{\partial \mathrm{n}} \mathrm{dA}, \tag{10}
\end{equation*}
$$

Note that the concentration gradients are defined along the axis $\overrightarrow{\mathrm{n}}$, i.e. everywhere perpendicular to the surface, and position outward. Denoting $\mathrm{D}_{\mathrm{n}}$ as the diffusion coefficients along the axis $\overrightarrow{\mathrm{n}}$ allows for anisotropy in D. For molecular diffusion and/or isotropic turbulence D is not a function of direction and the subscript may be dropped. The final mathematical expression for conservation of mass combines (8), (9), and (10).

Conservation of Mass in Integral (Control Volume) Form

$$
\begin{array}{cccc}
\frac{\partial}{\partial \mathrm{t}} \int_{\mathrm{cv}} \mathrm{C} \mathrm{~d} \forall & = & -\int_{\mathrm{cs}} \mathrm{C} \overrightarrow{\mathrm{~V}} \cdot \overrightarrow{\mathrm{n}} \mathrm{dA} & +\int_{\mathrm{cs}} \mathrm{D}_{\mathrm{n}} \frac{\partial \mathrm{C}}{\partial \mathrm{n}} \mathrm{dA}
\end{array} \quad \pm \mathrm{S}
$$

Example: South Meadow Power Station, Connecticut, burns 2000 tons of municipal solid waste per day to generate electricity. Cooling water is drawn from and returned to the Connecticut River at $\mathrm{Q}_{\mathrm{c}}=250 \mathrm{ft}^{3} \mathrm{~s}^{-1}$. The cooling cycle raises the temperature of the water by $\Delta \mathrm{T}=20^{\circ} \mathrm{F}$ before it is returned to the river. Because thermal pollution can be damaging to aquatic life, we want to know how the inflow affects temperature downstream of the station. The median flow of the river is $Q_{R}=20,000 \mathrm{ft}^{3} \mathrm{~s}^{-1}$.


This problem can be solved using the integral form of conservation of energy. The control volume is above as a dashed-box. Conservation of Energy is derived as (11), but with energy replacing mass. The 'concentration' of heat energy is $\mathrm{C}_{\text {heat }}\left[\mathrm{J} \mathrm{m}^{-3}\right]=\rho \mathrm{C}_{\mathrm{p}} \mathrm{T}$, where, $\rho$ is the fluid density $\left[\mathrm{kgm}^{-3}\right], C_{P}$ is the specific heat $[\mathrm{J} /($ degree kg$)]$, and $T$ [degrees] is temperature. Replacing C with $\rho \mathrm{C}_{\mathrm{p}} \mathrm{T}$ in (4), gives

## Conservation of Thermal Energy

$$
\begin{equation*}
\frac{\partial}{\partial \mathrm{t}} \int_{\mathrm{cv}} \rho \mathrm{C}_{\mathrm{p}} \mathrm{Td} \forall=-\int_{\mathrm{cs}} \rho \mathrm{C}_{\mathrm{p}} T \overrightarrow{\mathrm{~V}} \cdot \overrightarrow{\mathrm{n}} \mathrm{dA} \quad+\int_{\mathrm{cs}} \mathrm{D}_{\mathrm{n}} \frac{\partial}{\partial \mathrm{n}}\left(\rho \mathrm{C}_{\mathrm{p}} \mathrm{~T}\right) \mathrm{dA} \quad \pm \mathrm{S} \tag{12}
\end{equation*}
$$

We assume there are no sources or sinks of heat inside the control volume, i.e. $\mathrm{S}=0$. At each of the inflow/outflow points around the volume, the advective flux is $\mathrm{U}_{\mathrm{i}} \mathrm{A}_{\mathrm{i}} \rho \mathrm{C}_{\mathrm{p}} \mathrm{T}$, where $A_{i}$ and $U_{i}$ are the respective area and velocity. We assume that the diffusive flux across each inlet/outlet area is negligible. With these assumptions (4.1) can be written,

$$
\begin{equation*}
\rho \mathrm{C}_{\mathrm{p}} \forall \frac{\partial \mathrm{~T}}{\partial \mathrm{t}}=\sum_{\text {inlets }} \mathrm{UA} \rho \mathrm{C}_{\mathrm{p}} \mathrm{~T}-\sum_{\text {outlets }} \mathrm{UA} \rho \mathrm{C}_{\mathrm{p}} \mathrm{~T} . \tag{13}
\end{equation*}
$$

We assume the power plant discharge has been turned on long enough that the system is at steady state, then $\partial \mathrm{T} / \partial \mathrm{t}=0$. Finally, it is reasonable to assume that $\mathrm{C}_{\mathrm{P}}$ and $\rho$ are approximately constant (only weak functions of T), so they cancel across (4.2). Then, using the definitions in our sketch, (4.2) becomes

$$
\begin{gathered}
0=\mathrm{Q}_{\mathrm{R}} \mathrm{~T}_{\mathrm{R}}+\mathrm{Q}_{\mathrm{C}}\left(\mathrm{~T}_{\mathrm{R}}+\Delta \mathrm{T}_{\mathrm{C}}\right)-\mathrm{Q}_{\mathrm{C}} \mathrm{~T}_{\mathrm{R}}-\mathrm{Q}_{\mathrm{R}}\left(\mathrm{~T}_{\mathrm{R}}+\Delta \mathrm{T}_{\mathrm{R}}\right) \text {, and } \\
\Delta \mathrm{T}_{\mathrm{R}}=\mathrm{T}_{\mathrm{R}}+\left(-\mathrm{Q}_{\mathrm{R}} \mathrm{~T}_{\mathrm{R}}-\mathrm{Q}_{\mathrm{C}}\left(\mathrm{~T}_{\mathrm{R}}+\Delta \mathrm{T}_{\mathrm{C}}\right)+\mathrm{Q}_{\mathrm{C}} \mathrm{~T}_{\mathrm{R}}\right) / \mathrm{Q}_{\mathrm{R}}=\mathrm{Q}_{\mathrm{C}} \Delta \mathrm{~T}_{\mathrm{C}} / \mathrm{Q}_{\mathrm{R}}=1^{0} \mathrm{~F} .
\end{gathered}
$$

The thermal plume shown below has not yet mixed fully with the river. Considering the cross-section marked in red, the mean plume temperature rise is $\approx 6^{\circ} \mathrm{F}$ and the plume occupies approximately $1 / 3$ of the river width. Since the plume is warmer (less dense) then the river, it floats at the surface, occupying only about half the channel depth. Thus, the plume reasonable occupies $1 / 6$ of the channel cross-sectional area. Using these
approximations, we estimate that the downstream temperature rise once the plume has fully mixed into the river will be $(7 / 6)=1.2^{\circ} \mathrm{F}$, consistent with our calculation.


Figure 1. Contours of thermal plume observed downstream of South Meadow Station, Conn. Adapted from Thermal Survey at South Meadow Station, Hartford Electric Light Company, October 1974, prepared by Lawler, Matusky \& Skelly Engineers, Tappan, New York. December 1975.

## Differential Form of Conservation of Mass

The differential form of conservation of mass is derived by evaluating (11) for an infinitely small, cubic volume. The volume is sufficient small that we assume the concentration within the volume is essential uniform. The volume is rigid, so that the dimensions $\partial \mathrm{x}, \partial \mathrm{y}$, and $\partial \mathrm{z}$ are constant. The two surface integrals (terms 2 and 3 in equation (11)) reduce to a sum of fluxes across each of the six cube faces.

$$
\begin{equation*}
\frac{\partial \mathrm{C}}{\partial \mathrm{t}} \partial \mathrm{~V}=\sum_{\mathrm{i}=1}^{6}\left[-\mathrm{C} \overrightarrow{\mathrm{~V}} \cdot \overrightarrow{\mathrm{n}} \mathrm{dA}+\mathrm{D}_{\mathrm{n}} \frac{\partial \mathrm{C}}{\partial \mathrm{n}} \mathrm{dA}\right]_{\mathrm{i}} \pm \mathrm{S} \tag{14}
\end{equation*}
$$

As an example, consider fluxes in the $x$-direction across the faces numbered 1 and 2 , and located at $x=x_{1}$ and $x_{2}$, respectively.


On face $1 \overrightarrow{\mathrm{n}}$ points in the negative x direction, such that $\overrightarrow{\mathrm{V}} \cdot \overrightarrow{\mathrm{n}}=-\mathrm{u}$, and $\partial \mathrm{C} / \partial \mathrm{n}=-\partial \mathrm{C} / \partial \mathrm{x}$. The evaluation of the surface integral for face 1 is then,
(15) Flux across $1=(u C)_{1} \partial y \partial z-\left(D_{x} \partial C / \partial x\right)_{1} \partial y \partial z$.

Similarly for face 2 , but noting that $\overrightarrow{\mathrm{n}}$ points in the positive x direction,
(16) Flux across $2=-(u C)_{2} \partial y \partial z+\left(\mathrm{D}_{\mathrm{x}} \partial \mathrm{C} / \partial \mathrm{x}\right)_{2} \partial \mathrm{y} \partial \mathrm{z}$

The net $x$-direction flux into the control volume is the sum of (15) and (16).
(17) Net flux in $\mathrm{x}=\left((\mathrm{uC})_{1}-(\mathrm{uC})_{2}-\left(\mathrm{D}_{\mathrm{x}} \partial \mathrm{C} / \partial \mathrm{x}\right)_{1}+\left(\mathrm{D}_{\mathrm{x}} \partial \mathrm{C} / \partial \mathrm{x}\right)_{2}\right) \partial \mathrm{y} \partial \mathrm{z}$.

If we assume that $C, u, \partial C / \partial x$, and $D_{x}$ are continuous functions of $x$, a Taylor expansion may be used to express each parameter at $\mathrm{x}_{2}$ as a function of the same parameter at $\mathrm{x}_{1}$.

$$
\begin{align*}
& (\mathrm{uC})_{2}=(\mathrm{uC})_{1}+\frac{\partial}{\partial \mathrm{x}}(\mathrm{uC}) \partial \mathrm{x}+\text { higher order terms }  \tag{18}\\
& \left(\mathrm{D}_{\mathrm{x}} \frac{\partial \mathrm{C}}{\partial \mathrm{x}}\right)_{2}=\left(\mathrm{D}_{\mathrm{x}} \frac{\partial \mathrm{C}}{\partial \mathrm{x}}\right)_{1}+\frac{\partial}{\partial \mathrm{x}}\left(\mathrm{D}_{\mathrm{x}} \frac{\partial \mathrm{C}}{\partial \mathrm{x}}\right) \partial \mathrm{x}+\text { higher order terms } \tag{19}
\end{align*}
$$

If we drop the higher order terms and replace $(\mathrm{uC})_{2}$ and $\left(\mathrm{D}_{\mathrm{x}} \partial \mathrm{C} / \partial \mathrm{x}\right)_{2}$ in (17) with the expressions in (18) and (19), then (17) becomes,

$$
\begin{equation*}
\text { Net flux in } x=\left\lceil-\frac{\partial u C}{\partial x}+\frac{\partial}{\partial x} D_{x} \frac{\partial C}{\partial x}\right\rfloor \partial x \partial y \partial z \tag{20}
\end{equation*}
$$

Similar expressions can be found for flux across the remaining four faces. Combining these in (14) and noting $\partial \forall=\partial x \partial y \partial z$,

## Conservation of Mass in Differential Form

$$
\begin{equation*}
\frac{\partial \mathrm{C}}{\partial \mathrm{t}}=-\frac{\partial \mathrm{uC}}{\partial \mathrm{x}}-\frac{\partial \mathrm{vC}}{\partial \mathrm{y}}-\frac{\partial \mathrm{wC}}{\partial \mathrm{z}}+\frac{\partial}{\partial \mathrm{x}} \mathrm{D}_{\mathrm{x}} \frac{\partial \mathrm{C}}{\partial \mathrm{x}}+\frac{\partial}{\partial \mathrm{y}} \mathrm{D}_{\mathrm{y}} \frac{\partial \mathrm{C}}{\partial \mathrm{y}}+\frac{\partial}{\partial \mathrm{z}} \mathrm{D}_{\mathrm{z}} \frac{\partial \mathrm{C}}{\partial \mathrm{z}} \pm \mathrm{S} \tag{21}
\end{equation*}
$$

This expression can be simplified under the following conditions.
First, consider the expansion of the advective fluxes in (21),

$$
\begin{equation*}
\frac{\partial u \mathrm{uC}}{\partial \mathrm{x}}+\frac{\partial \mathrm{vC}}{\partial \mathrm{y}}+\frac{\partial \mathrm{wC}}{\partial \mathrm{z}}=\left[\frac{\partial \mathrm{u}}{\partial \mathrm{x}}+\frac{\partial \mathrm{v}}{\partial \mathrm{y}}+\frac{\partial \mathrm{w}}{\partial \mathrm{z}}\right\rceil \mathrm{C}+\mathrm{u} \frac{\partial \mathrm{C}}{\partial \mathrm{x}}+\mathrm{v} \frac{\partial \mathrm{C}}{\partial \mathrm{y}}+\mathrm{w} \frac{\partial \mathrm{C}}{\partial \mathrm{z}} \tag{22}
\end{equation*}
$$

If the flow field is incompressible, then from continuity

$$
\frac{\partial \mathrm{u}}{\partial \mathrm{x}}+\frac{\partial \mathrm{v}}{\partial \mathrm{y}}+\frac{\partial \mathrm{w}}{\partial \mathrm{z}}=0
$$

This eliminates the bracketed term in (22). Thus, conservation of mass for incompressible flow may be expressed as follows. By convention, advective terms are brought to the left.

## Conservation of Mass for Incompressible Flow

$$
\begin{equation*}
\frac{\partial C}{\partial t}+u \frac{\partial C}{\partial x}+v \frac{\partial C}{\partial y}+w \frac{\partial C}{\partial z}=\frac{\partial}{\partial x} D_{x} \frac{\partial C}{\partial x}+\frac{\partial}{\partial y} D_{y} \frac{\partial C}{\partial y}+\frac{\partial}{\partial z} D_{z} \frac{\partial C}{\partial z} \pm S \tag{23}
\end{equation*}
$$

Furthermore, when the coefficients of diffusion are homogeneous, $D_{i} \neq f(x, y$, or $z)$,

$$
\begin{equation*}
\frac{\partial \mathrm{C}}{\partial \mathrm{t}}+\mathrm{u} \frac{\partial \mathrm{C}}{\partial \mathrm{x}}+\mathrm{v} \frac{\partial \mathrm{C}}{\partial \mathrm{y}}+\mathrm{w} \frac{\partial \mathrm{C}}{\partial \mathrm{z}}=+\mathrm{D}_{\mathrm{x}} \frac{\partial^{2} \mathrm{C}}{\partial \mathrm{x}^{2}}+\mathrm{D}_{\mathrm{y}} \frac{\partial^{2} \mathrm{C}}{\partial \mathrm{y}^{2}}+\mathrm{D}_{\mathrm{z}} \frac{\partial^{2} \mathrm{C}}{\partial \mathrm{z}^{2}} \pm \mathrm{S} \tag{24}
\end{equation*}
$$

If the diffusion coefficients are additionally isotropic, $D_{x}=D_{y}=D_{z}$, then

$$
\begin{equation*}
\frac{\partial \mathrm{C}}{\partial \mathrm{t}}+\mathrm{u} \frac{\partial \mathrm{C}}{\partial \mathrm{x}}+\mathrm{v} \frac{\partial \mathrm{C}}{\partial \mathrm{y}}+\mathrm{w} \frac{\partial \mathrm{C}}{\partial \mathrm{z}}=\mathrm{D}\left[\frac{\partial^{2} \mathrm{C}}{\partial \mathrm{x}^{2}}+\frac{\partial^{2} \mathrm{C}}{\partial \mathrm{y}^{2}}+\frac{\partial^{2} \mathrm{C}}{\partial \mathrm{z}^{2}}\right] \pm \mathrm{S} \tag{25}
\end{equation*}
$$

For laminar flow molecular diffusion controls the diffusive flux. In general, molecular diffusion is both homogeneous and isotropic, so that (25) is appropriate. For turbulent flow turbulent transport dominates the diffusive flux. Commonly the turbulence field is both heterogeneous and anisotropic and the diffusion coefficients will be as well.

## Material Derivative

Fluid motion and any constituent (temperature, concentration) transported by fluid motion can be described from two frames of reference, one which is stationary or one which is moving along with the flow. In the Eulerian perspective, the flow and its scalar constituents are described with respect to fixed spatial positions, $\overrightarrow{\mathrm{X}}=(\mathrm{x}, \mathrm{y}, \mathrm{z})$ and with respect to time $(\mathrm{t})$, and are written, e.g. $\overrightarrow{\mathrm{V}}(\overrightarrow{\mathrm{X}}, \mathrm{t})$ and $\mathrm{C}(\overrightarrow{\mathrm{X}}, \mathrm{t})$. In the Lagrangian perspective moves with the flow, and traces the history of individual fluid particles. Unlike the Eulerian description, in which spatial position is a fixed reference, in the Lagrangian perspective, the spatial position is another variable of the particle. The flow variables are written with respect to time and a single, initial reference position, e.g. $\overrightarrow{\mathrm{X}}_{0}$ the particle position at $t=0$, such that the variables are recorded $\vec{X}\left(\vec{X}_{0}, t\right)$ and $C\left(\vec{X}_{0}, t\right)$.

The Eulerian perspective is generally easier to represent, and therefore is more common in analysis and flow description. However, the physics and transport of flow are
more fundamentally related to the Lagrangian perspective. For example, the NavierStokes equations essentially represent Newton's Second Law ( $\overrightarrow{\mathrm{F}}=\mathrm{m} \overrightarrow{\mathrm{a}}$ ) applied to fluid particles. For transport problems, e.g., tracking the evolution of a phytoplankton patch as is grows (source), is preyed upon (sink) and diffuses, one again sees the conceptual advantage of a Lagrangian perspective - predicting concentration following the patch. It is important to understand how these perspectives are related.

Consider $\mathrm{F}(\mathrm{x}, \mathrm{y}, \mathrm{z}, \mathrm{t})$ to be any variable of the flow described in terms of fixed Eulerian coordinates, $(\mathrm{x}, \mathrm{y}, \mathrm{z})$. We wish to relate this description to a Lagrangian perspective, specifically to describe the rate of change in F observed while following an individual particle through the flow. First, we can describe a change in F, namely dF, due to a small change in spatial position ( $\mathrm{d} \overline{\mathrm{X}}$ ) and/or time (dt), as

$$
\begin{equation*}
d F=\frac{\partial \mathrm{F}}{\partial \mathrm{t}} \mathrm{dt}+\frac{\partial \mathrm{F}}{\partial \mathrm{x}} \mathrm{dx}+\frac{\partial \mathrm{F}}{\partial \mathrm{y}} \mathrm{dy}+\frac{\partial \mathrm{F}}{\partial \mathrm{z}} \mathrm{dz} \tag{26}
\end{equation*}
$$

Next, we constrain the increments dt andd $\overline{\mathrm{X}}$ such that they follow the trajectory of an individual particle, specifically, $\mathrm{dx}=\mathrm{udt}$, $\mathrm{dy}=\mathrm{vdt}$, and $\mathrm{dz}=\mathrm{wdt}$. Then (26) becomes,

$$
\begin{equation*}
\mathrm{dF}=\frac{\partial \mathrm{F}}{\partial \mathrm{t}} \mathrm{dt}+\mathrm{u} \frac{\partial \mathrm{~F}}{\partial \mathrm{x}} \mathrm{dt}+\mathrm{v} \frac{\partial \mathrm{~F}}{\partial \mathrm{y}} \mathrm{dt}+\mathrm{w} \frac{\partial \mathrm{~F}}{\partial \mathrm{z}} \mathrm{dt} . \tag{27}
\end{equation*}
$$

Dividing by dt produces a derivative that represents the rate of change in F observed when following the trajectory of a fluid particle. To emphasize this special definition the derivative is given the notation $\mathrm{DF} / \mathrm{Dt}$, i.e.

$$
\begin{equation*}
\frac{\mathrm{DF}}{\mathrm{Dt}}=\frac{\partial \mathrm{F}}{\partial \mathrm{t}}+\mathrm{u} \frac{\partial \mathrm{~F}}{\partial \mathrm{x}}+\mathrm{v} \frac{\partial \mathrm{~F}}{\partial \mathrm{y}}+\mathrm{w} \frac{\partial \mathrm{~F}}{\partial \mathrm{z}} \tag{28}
\end{equation*}
$$

The notation $\mathrm{DF} / \mathrm{Dt}$ is called the material derivative (also the particle derivative, the substantial derivative, and the total derivative) to emphasize that it is taken following a fluid particle. The material derivative has two parts. First, $\partial \mathrm{F} / \partial \mathrm{t}$, called the local derivative, represents the rate of change at any fixed point. For steady flow, $\partial / \partial \mathrm{t}=0$. The remaining terms, $\mathrm{u} \partial \mathrm{F} / \partial \mathrm{x}+\mathrm{v} \partial \mathrm{F} / \partial \mathrm{y}+\mathrm{w} \partial \mathrm{F} / \partial \mathrm{z}$, are called the advective derivative, because they record changes in F which arise as the fluid element advects through a spatial gradients in F . The following animations demonstrate the material derivative.

Animation -Steady Temperature Field: This animation shows a one-dimensional system with a spatial gradient of temperature, $\mathrm{T}(\mathrm{x})$. A temperature probe (white dot) moves with the flow, making a Lagrangian observation. The probe records the material (total) derivative, which in one dimension is,

$$
\begin{equation*}
\frac{\mathrm{DT}}{\mathrm{Dt}}=\frac{\partial \mathrm{T}}{\partial \mathrm{t}}+\mathrm{u} \frac{\partial \mathrm{~T}}{\partial \mathrm{x}} \tag{29}
\end{equation*}
$$

Probes located at the fixed positions A, B, and C make Eulerian observations. They show a steady temperature field, i.e. $\partial \mathrm{T} / \partial \mathrm{t}=0$, such that the material derivative is equal to the
advective derivative, $\mathrm{DT} / \mathrm{Dt}=\mathrm{u} \partial \mathrm{T} / \partial \mathrm{x}$. This is quantified in the lower right corner of the animation. The temperature field shown here could result from a steady, uniform flow through a heating element. The temperature of the fluid rises steadily as heat is added along the flow path.

Animation -Unsteady Temperature Field: This animation shows a one-dimensional system with an unsteady temperature field, $\mathrm{T}(\mathrm{x}, \mathrm{t})$. One temperature probe is moving with the flow (white dot) at velocity $u$, and it records the material derivative given in (29). Three additional probes are located at the fixed positions A, B, and C. These probes record the local derivative, $\partial \mathrm{T} / \partial \mathrm{t}$, which is non-zero (unsteady), but is the same at each position. The value of each derivative is given in the lower right hand corner.

Animation - Spatially Accelerating Flow in a Pipe: In this animation, flow through a pipe accelerates downstream as the pipe cross-section decreases, i.e. $\partial \mathrm{u} / \partial \mathrm{x}>0$. Three probes measuring the flow at fixed positions, $\mathrm{A}, \mathrm{B}$, and C , show that the flow is steady, $\partial \mathrm{u} / \partial \mathrm{t}=0$ at every position. Another velocity probes is moving with the flow (blue dot) and records the material (total) derivative, $\mathrm{Du} / \mathrm{Dt}$. Within each section of the pipe, $\mathrm{Du} / \mathrm{Dt}=0$, as shown by the blue trace in the Velocity vs. Time graph. At the step changes in area, the fluid locally accelerates, $\partial u / \partial x>0$, and at these positions $D u / D t=u \partial u / \partial x$.

What is the mean velocity in this system? From the perspective of transport, the best definition of mean velocity is a Lagrangian definition, i.e. the mean velocity experienced by a probe moving with the flow. The probe takes 109 s to traverse the $90-\mathrm{m}$ pipe. This gives a velocity of $90 / 109=0.83 \mathrm{~ms}^{-1}$. One may be tempted to define a mean Eulerian velocity based on a spatial average of velocity within the three sections. As the segment lengths are equal, the average is straightforward, $(0.50+0.89+2.0) / 3=1.13 \mathrm{~m} / \mathrm{s}$. This value is meaningless, however, from the perspective of transport, because it does not predict the travel time through the system, i.e. $90-\mathrm{m} / 1.13-\mathrm{ms}^{-1}=80 \mathrm{~s} \neq 109 \mathrm{~s}$.

