Mass Conservation and Compartmental Analysis

"There is no reason anyone would want a computer in their home," Ken Olson, president, chairman, and founder of Digital Equipment Corp., 1977

Compartmental Analysis

Compartmental Analysis: Examine transport of mass (or other items) across physical or nonphysical compartments

- Onion, coffee, …
- Acoustics
- Fluid flow (mix cups of milk and water)
- Chemical Transport
- Traffic flow
- Related processes: population dynamics, biological models

Assumptions:

- Constant volumes: $V_1 \neq V_2$ but $\frac{dV_1}{dt} = \frac{dV_2}{dt} = 0$
- Well-mixed
- Transport constant across membranes

Conservation of Stuff

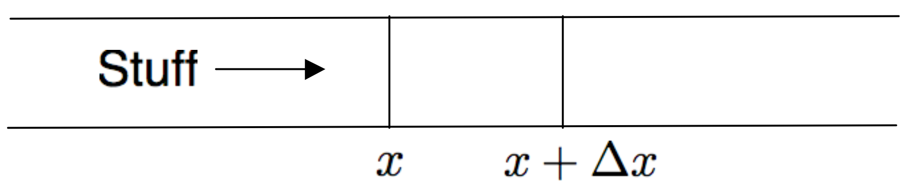
Basic Idea: "Stuff" flowing along a conduit is conserved

Conduit	Stuff
air	mass
rod	heat
pipe	water
highway	cars
river	pollution
sidewalk	people

Fundamental Concept:

$$\frac{d\text{Stuff}}{dt} = \text{Stuff in} - \text{Stuff out} + \text{Stuff created} - \text{Stuff destroyed}$$

Strategy: Consider flow of Stuff through a control volume (x to $x + \Delta x$ in 1-D)



Note: Thanks to Kurt Bryan for motivating the consideration of Stuff

Conservation of Stuff

Density: $\rho(t,x)$ – Amount of Stuff per unit length (linear density) or unit volume (regular density)

e.g., Mass density: kg/m^3

Cars per unit length of road

People per unit length of sidewalk

Rate of Flow: $q(t,x)$ – Rate at which Stuff flows past x at time t (Units: Stuff per second)

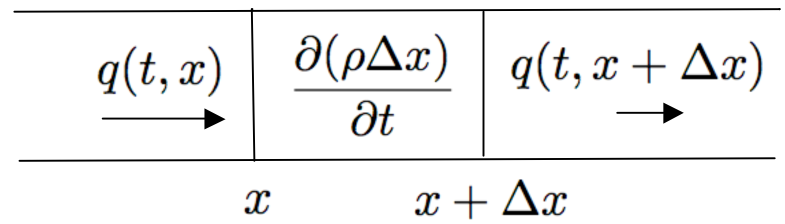
e.g., Cars or people per second

Flux: $\mu(t,x)$ – Rate at which Stuff crosses unit area A at x and time t (Units: Stuff per area per second)

e.g., Mass flux: $kg/m^2/s$ or $\frac{kg}{m^2 s}$

Continuity Equations:1-D

Case 1: Rate of flow



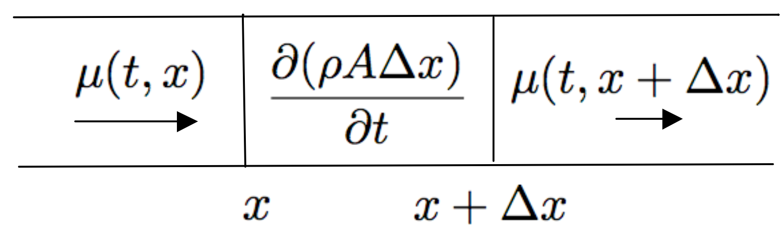
$$\frac{\partial(\rho\Delta x)}{\partial t} = q(t,x) - q(t,x+\Delta x)$$

$$\Rightarrow \lim_{\Delta x\to 0}\frac{\partial\rho}{\partial t} = \lim_{\Delta x\to 0}\frac{q(t,x)-q(t,x+\Delta x)}{\Delta x}$$

$$\boxed{\Rightarrow \frac{\partial\rho}{\partial t} + \frac{\partial q}{\partial x} = 0}$$

Continuity Equation

Case 2: Flux



$$\frac{\partial(\rho A\Delta x)}{\partial t} = A\mu(t,x) - A\mu(t,x+\Delta x)$$

$$\boxed{\Rightarrow \frac{\partial(\rho A)}{\partial t} + \frac{\partial(\mu A)}{\partial x} = 0}$$

Continuity Equation

$\Rightarrow \frac{\partial\rho}{\partial t} + \frac{\partial\mu}{\partial x} = 0$ if A is constant

Continuity Equations: 1-D

Continuity Equations with Production and Destruction of Stuff:

$$\frac{\partial \rho}{\partial t} + \frac{\partial q}{\partial x} = b - d$$

$$\frac{\partial (\rho A)}{\partial t} + \frac{\partial (\mu A)}{\partial x} = (b - d)A$$

b: rate of production per unit length or volume

d: rate of destruction per unit length or volume

Problem:

- One equation with two unknowns ρ and q or μ

Constitutive Relations:

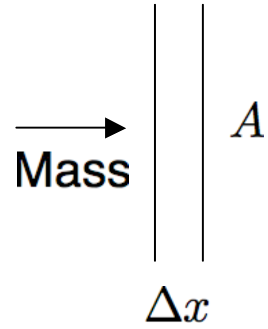
- Need constitutive relations or equations of state to relate unknowns
- This depends upon Stuff being considered
- Consider first relation between mass density and mass flux

Compartmental Analysis: Mass Flow

Transport across Membrane:

$$K \propto \frac{A}{\Delta x} = D\frac{A}{\Delta x}$$

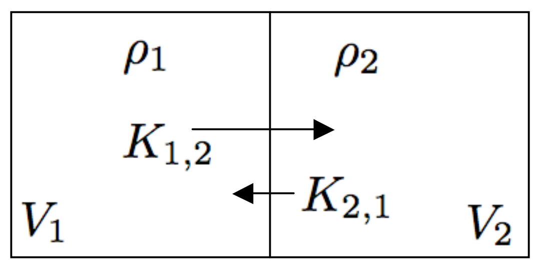
K: Volumetric Rate (m^3/s)



Mass Transport:

$$\frac{dm}{dt} = K\rho$$

Two Compartment Model:



- Mass Balance

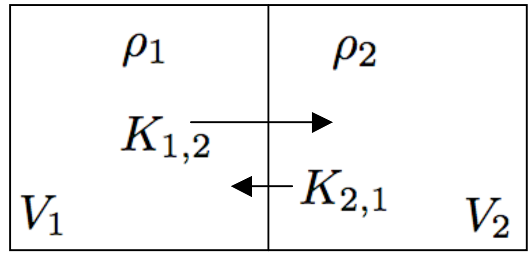
$$\frac{dm_1}{dt} = K_{2,1}\rho_2 - K_{1,2}\rho_1$$
$$\frac{dm_2}{dt} = K_{1,2}\rho_1 - K_{2,1}\rho_2$$

- Mass Balance $(K = K_{1,2} = K_{2,1})$

$$\frac{dm_1}{dt} = K(\rho_2 - \rho_1)$$
$$\frac{dm_2}{dt} = K(\rho_1 - \rho_2)$$

Compartmental Analysis: Mass Flow

Two Compartment Model:



- Density Balance

$$\frac{d\rho_1}{dt} = \frac{1}{V_1}\left[K_{2,1}\rho_2 - K_{1,2}\rho_1\right]$$

$$\frac{d\rho_2}{dt} = \frac{1}{V_2}\left[K_{1,2}\rho_1 - K_{2,1}\rho_2\right]$$

- Density Balance ($K = K_{1,2} = K_{2,1}$)

$$\frac{d\rho_1}{dt} = \frac{K}{V_1}(\rho_2 - \rho_1)$$

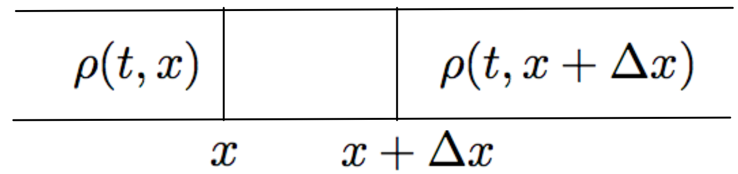
$$\frac{d\rho_2}{dt} = \frac{K}{V_2}(\rho_1 - \rho_2)$$

Note:

- $\dfrac{dm_1}{dt} + \dfrac{dm_2}{dt} = 0$ so Conservation of Mass
- $\dfrac{d\rho_1}{dt} + \dfrac{d\rho_2}{dt} \neq 0$ unless $V_1 = V_2$

Constitutive Relation and Mass Flow Model

Case 1: Stationary fluid -- 1-D



$$\dot{m} = AD\,\frac{\rho(x) - \rho(x+\Delta x)}{\Delta x}$$

$$\Rightarrow \dot{m} = -DA\frac{\partial \rho}{\partial x}$$

- **Mass flux:** $\mu = \dfrac{\dot{m}}{A}$

Constitutive Relation:

$$\boxed{\mu = -D\frac{\partial \rho}{\partial x}}$$

Fick's First Law of Diffusion

Model: Constant A and no production or destruction of mass

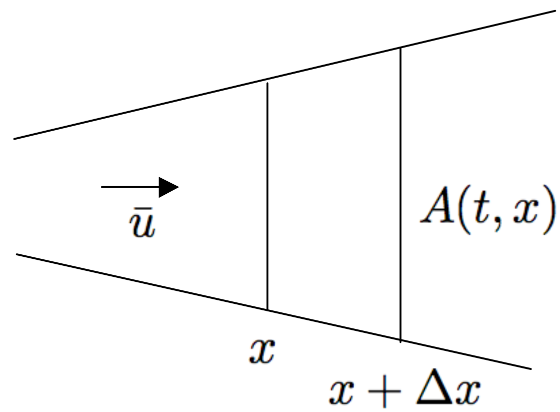
$$\boxed{\frac{\partial \rho}{\partial t} = \frac{\partial}{\partial x}\left(D\frac{\partial \rho}{\partial x}\right)}$$

Diffusion Equation

Mass Flow Model: 1-D Moving Fluid

Constitutive Relation: Average fluid velocity $\bar{u}$

$$\mu = -D\frac{\partial \rho}{\partial x} + \rho\bar{u}$$



Mass Sources and Sinks:

b: rate of production per unit volume

d: rate of destruction per unit volume

Model:

$$\frac{\partial(\rho A)}{\partial t} + \frac{\partial(\rho\bar{u}A)}{\partial x} = \frac{\partial}{\partial x}\left(DA\frac{\partial \rho}{\partial x}\right) + (b-d)A$$

or

$$\frac{\partial \rho}{\partial t} + \frac{\partial(\rho\bar{u})}{\partial x} = \frac{\partial}{\partial x}\left(D\frac{\partial \rho}{\partial x}\right) + b - d$$

if A is constant

Mass Flow Model: 1-D Moving Fluid

Special Cases: A is constant, $b = d = 0$

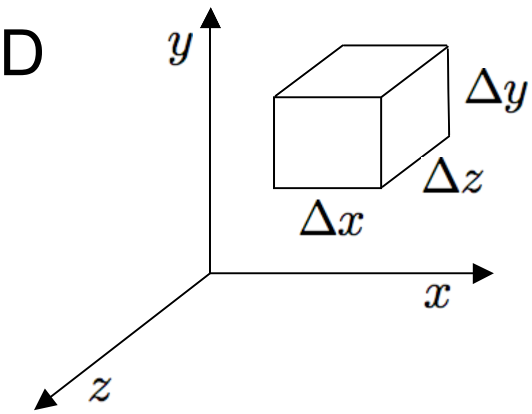
- Ignore diffusion

$$\frac{\partial \rho}{\partial t} + \frac{\partial (\rho \bar{u})}{\partial x} = 0 \qquad \text{Continuity of Mass}$$

- ρ constant

$$\frac{\partial \bar{u}}{\partial x} = 0 \qquad \text{Incompressible Fluid}$$

Mass Conservation in 3-D



Constitutive Relation: Take $\vec{u} = [u \ , \ v \ , \ w]$

$$\mu = \rho \vec{u}$$

Mass Balance:

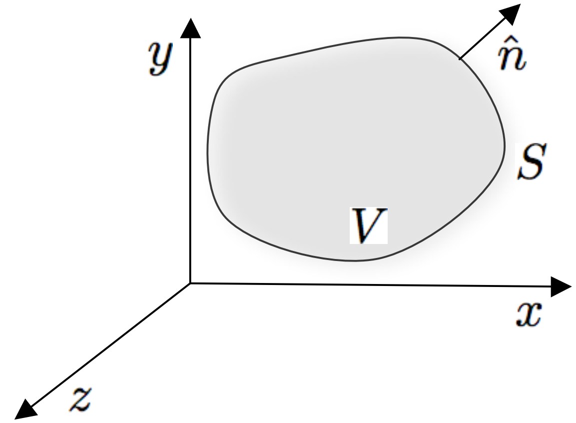
$$\left\{ \begin{array}{c} \text{Rate of change} \\ \text{of mass in } \Delta V \end{array} \right\} = \left\{ \begin{array}{c} \text{Rate of mass} \\ \text{convected into } \Delta V \end{array} \right\} - \left\{ \begin{array}{c} \text{Rate of mass} \\ \text{convected out of } \Delta V \end{array} \right\}$$

$$\begin{aligned} \Rightarrow \Delta x \Delta y \Delta z \frac{\partial \rho}{\partial t} &= \Delta y \Delta z \left[(\rho u)|_x - (\rho u)|_{x+\Delta x} \right] \\ &+ \Delta x \Delta z \left[(\rho v)|_y - (\rho v)|_{y+\Delta y} \right] \\ &+ \Delta x \Delta y \left[(\rho w)|_z - (\rho w)|_{z+\Delta z} \right] \end{aligned}$$

$$\Rightarrow \frac{\partial \rho}{\partial t} + \frac{\partial}{\partial x}(\rho u) + \frac{\partial}{\partial y}(\rho v) + \frac{\partial}{\partial z}(\rho w) = 0$$

$$\boxed{\Rightarrow \frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \vec{u}) = 0}$$

Mass Conservation in 3-D



Arbitrary Control Volume: Continuity equation

$$\frac{d}{dt}\int_V \rho dV = -\int_S \hat{n}\cdot(\rho\vec{u})dS$$

Divergence Theorem: Continuous vector field $\vec{B}$

$$\int_V \nabla\cdot\vec{B}dV = \int_S \hat{n}\cdot\vec{B}dS = \int_S \vec{B}\cdot d\vec{A}$$

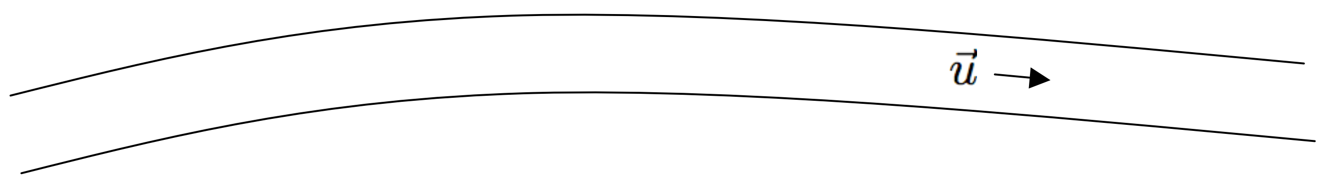
Continuity Equation:

$$\int_V \left[\frac{\partial\rho}{\partial t} + \nabla\cdot(\rho\vec{v})\right] dV = 0$$

$$\boxed{\Rightarrow \frac{\partial\rho}{\partial t} + \nabla\cdot(\rho\vec{u}) = 0}$$ Since control volume is arbitrary

Eulerian Versus Lagrangian Reference Frames

Eulerian Specification: Describe phenomenon at a specific spatial location by specifying flow velocity; e.g., sit on bank of river and watch river flow.



Lagrangian Specification: Follow individual fluid particles as they move through space and time; e.g., sit in boat and drift down river.

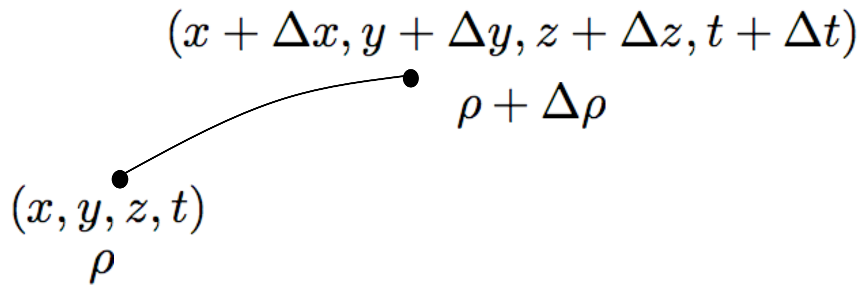
Substantive, Material or Total Derivative: Relates the two specifications

Framework: Let $f(x(t), y(t), z(t), t)$ denote any function of position and time (can be scalar or vector)

Material or Substantive Derivative

Example: Let $\rho = f(x, y, z, t)$

Velocity: $\vec{u} = [u\,,\, v\,,\, w] = \left[\frac{dx}{dt}, \frac{dy}{dt}, \frac{dz}{dt}\right]$



Note: At time $t + \Delta t$:

$$
\begin{aligned}
\rho + \Delta\rho &= f(x + \Delta x, y + \Delta y, z + \Delta z, t + \Delta t) \\
&= f(x + u\Delta t, y + v\Delta t, z + w\Delta t, t + \Delta t) \\
&= f(x, y, z, t) + \left(u\frac{\partial f}{\partial x} + v\frac{\partial f}{\partial y} + w\frac{\partial f}{\partial z} + \frac{df}{\partial t}\right)\Delta t + \mathcal{O}((\Delta t)^2)
\end{aligned}
$$

Material Derivative:

$$
\begin{aligned}
\frac{D\rho}{Dt} &= \lim_{\Delta t \to 0} \frac{\Delta\rho}{\Delta t} \\
&= u\frac{\partial\rho}{\partial x} + v\frac{\partial\rho}{\partial y} + w\frac{\partial\rho}{\partial z} + \frac{df}{\partial t} \\
&= \vec{u} \cdot \nabla\rho + \frac{\partial\rho}{\partial t}
\end{aligned}
$$

Note:

- $\vec{u} \cdot \nabla\rho$: Convective rate of change due to spatial changes
- $\frac{\partial\rho}{\partial t}$: Local rate of change
- $\vec{u}$: Flow velocity

Material or Substantive Derivative

Note: The material derivative is the *total derivative*

$$\begin{aligned}\frac{d}{dt}f(x(t),y(t),z(t),t) &= \frac{\partial f}{\partial x}\frac{dx}{dt}+\frac{\partial f}{\partial y}\frac{dy}{dt}+\frac{\partial f}{\partial z}\frac{dz}{dt}+\frac{\partial f}{\partial t}\\ &= \frac{Df}{Dt}(x(t),y(t),z(t),t)\end{aligned}$$

Continuity Equation: Differentiation yields

$$\boxed{\frac{D\rho}{Dt} = -\rho(\nabla\cdot\vec{u})}$$

Material or Substantive Derivative

Example: Consider temperature in Yellowstone Lake; $T = f(x, y, z, t)$

Case i: Swimmer stands in one place and feels water get warmer as sun rises;

Note: $\frac{d\vec{x}}{dt} = 0$

Case ii: Swimmer swims through regions with warmer *steady state* temperatures due to underwater hot springs. Note that temperatures at a given spatial point remain constant.

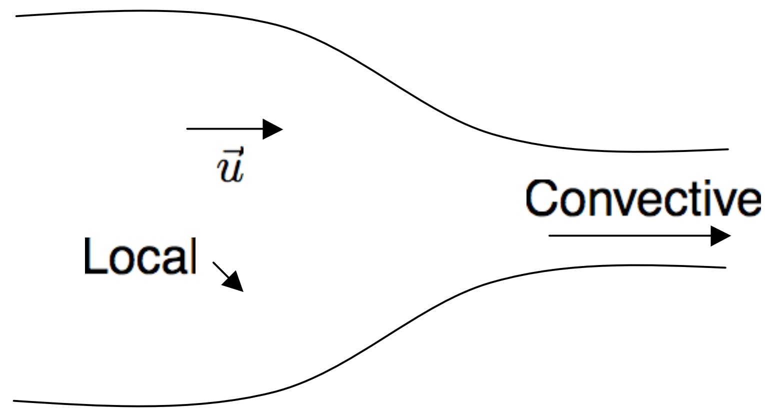
Case iii: Swimmer goes through water that is warming due to the sun and has gradients due to hot pools… Material Derivative

$$\frac{DT}{Dt} = \frac{\partial T}{\partial t} + \vec{u} \cdot \nabla T$$

Material or Substantive Derivative

Example: Let $u = f(x, y, z, t)$. Then

$$a_x = \frac{Du}{Dt} = \vec{u} \cdot \nabla u + \frac{\partial u}{\partial t}$$



More Generally:

$$\vec{a} = \frac{D\vec{u}}{Dt} = \vec{u} \cdot \nabla \vec{u} + \frac{\partial \vec{u}}{\partial t}$$

Note: Be careful with notation for covariant derivative; e.g., non-Cartesian system

Interpretation: Material derivative is rate of change measured by observer traveling with specific particles under investigation; e.g., floating on river

Material or Substantive Derivative

Example: Here we examine the difficulties faced by a tourist who jumps into the Yellowstone river a few meters above the lower falls. If we assume that the river is flowing at 10 m/s, what does his local velocity have to be in order for him to swim upriver?