Modeling Microbial Fate & Transport

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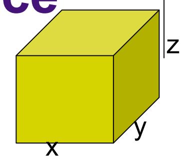
Outline

- Concept of Mass Balance
- Fluxes and Rates
- General Mass Balances
- Illustrative example to a simple room
- More complex situations

Concept of a Mass Balance



- A region in space (cartesian)
- Concentration within is uniform
- Principle of conservation of mass dictates:
  - Change of mass within =(things entering)–(things leaving) +/– (stuff that happens inside)
- (things entering), (things leaving)-> “Fluxes”
- (stuff that happens inside)->”Rates”
- Units-each term is amount/time. We are looking at viable organisms so units are #/time.

Aside

- At a finer level of detail, we would want to look at force balances on each particle and get their equations of motion (Lagrangian approach)
- For this presentation, treat particles as a continuum (Eulerian) which is a bit of a simplification

Concept of Fluxes

- Movement of stuff in and out of system
  - J: #/area/time (area is the area perpendicular to the movement)
- Most common - due to bulk flow
  - $v \cdot C_{in}$: flux into system due to flow
  - $v \cdot C_{out}$: flux out of system due to flow
- Many other examples -->

Other Fluxes (1)

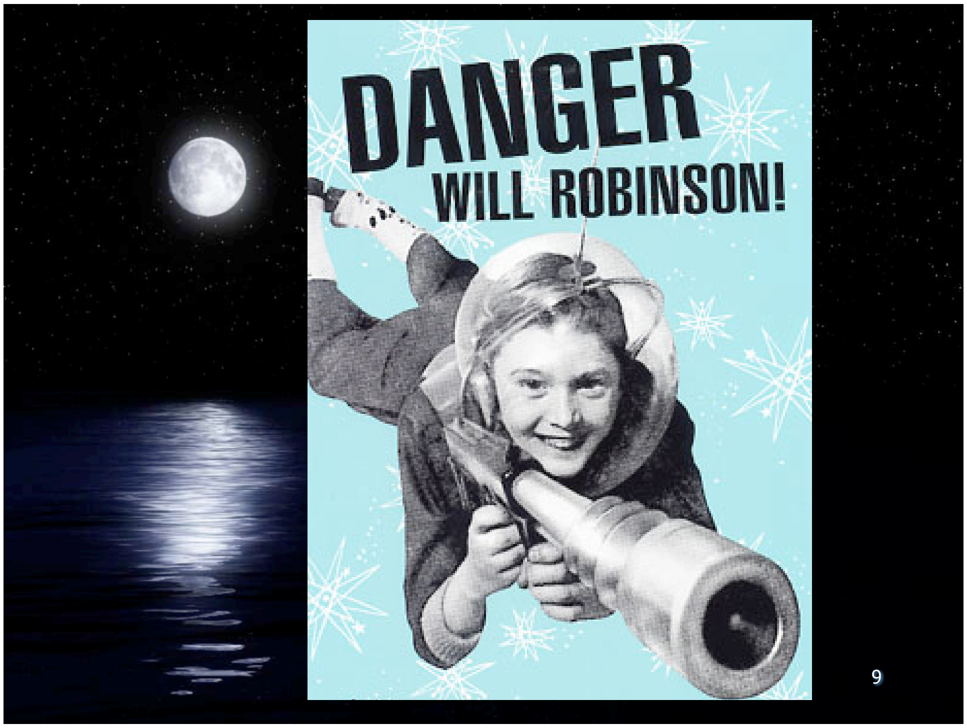
- Dispersion
  - Proportional to concentration gradient, induced by turbulence and mixing
- Gravitational
  - Time scale hours for micron size particles in air (longer for water). Results in effective downward velocity. Balanced by particle drag forces and buoyancy.
- Wall collisions (all surfaces)
  - Driven by convection. Can write in terms of an effective velocity (mass transfer coefficient, “deposition velocity”) to the surfaces

Other Fluxes (2)

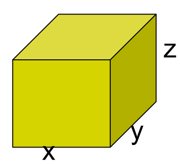
- Electrostatic
  - Charged particles in an electric field will experience a Coulomb force which results in an effective velocity
- Resuspension
  - "lifting" of particles at a surface by fluid motion near a surface.
  - This is one particular area that needs **a lot** of additional study

Concept of Rates

- Units generally #/volume-time (symbol r)
  - Death
    - Typically first order in viable conc, $r_{death}=-k_{death}\bullet C$
    - k_{death} may be function of environment (including disinfectants)
    - (note could also have death on surfaces)
  - Collisions
    - Causes particle growth which may affect settling
    - Typically second order
    - At the low concentrations we expect this may be minor
      - Unless a lot of intert particles are also present
  - (Growth)
    - We typically would not expect this of pathogens (but in favorable environments, e.g. food with temperature abuse) this can occur



Some mathematics



- Change of mass within =(things entering)–(things leaving) +/– (stuff that happens inside)
- Look at what happens during a time Δt

=xyz

$$(\Delta C)(V) = QC_{in}\Delta t - QC\Delta t + \sum_i J_i A_i \Delta t + \sum_j r_j V \Delta t$$

- Which becomes

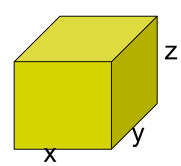
$$\Delta C = \left(\frac{C_{in} - C}{\Theta} + \frac{\sum_i J_i A_i}{V} + \sum_j r_j \right) \Delta t$$

How do I evaluate this?

$$\Delta C = \left(\frac{C_{in} - C}{\Theta} + \frac{\sum_i J_i A_i}{V} + \sum_j r_j \right) \Delta t$$

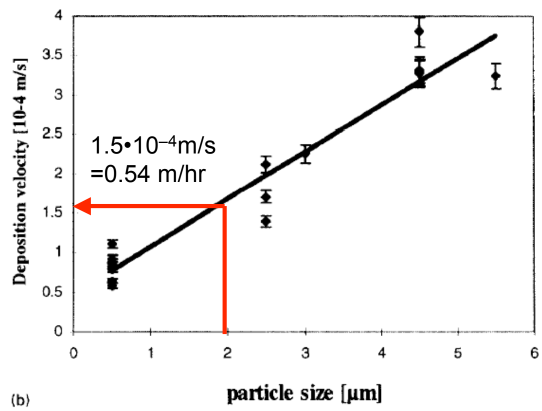
- First I need the terms (r's, J's)
- I could start with what I know at t=0, and calculate the ΔC for a small Δt, and repeat the process (finite difference)
- Or by calculus, as Δt->0, this becomes a differential equation which I can solve

An Example



- Consider a small room
  - x=5 m, y=4 m, z=2.5 m (volume=50 m^3)
  - Total surface area (for deposition)=85 m^2
- Airflow 0.5 airchanges/hr
  - Θ=2 hrs
- Micron sized aerosol
- Assume dieoff with $T_{1/2}$=1 hr
  - -> k=-ln(.5)/1hr = 0.69 hr^{-1}
- We will consider surface deposition as well-->

Indoor Deposition Velocity



Furnished room
Fogh et al.,
Atmospheric
Environment
31:15(2193) 1997

Plugging in the Numbers

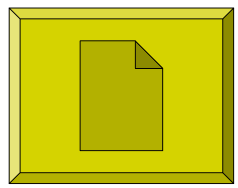
$$\Delta C = \left(\frac{C_{in} - C}{\Theta} + \frac{\sum_i J_i A_i}{V} + \sum_j r_j \right) \Delta t$$

$$\Delta C = \left(\frac{C_{in} - C}{2} - \frac{0.54(85)C}{50} - 0.69 \bullet C \right) \Delta t$$

$$\Delta C = \left(\frac{C_{in}}{2} - 2.608 \bullet C \right) \Delta t$$

Scenario

- Pulse release into room
  - @t=0, C=0
  - @t=<0, 2hr>, C_{in}=0
  - @t=<2hr, 2.5hr>, C_{in}=100,000/m^3
  - @t>2.5hr, C_{in}=0



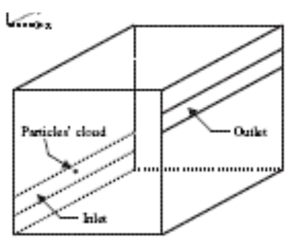
So what?

- We could integrate with respect to breathing rate and activity patterns to get dose.
- Impact of mitigation and change in room characteristics.

More Complex Geometries

- What we have done is an example of a “zone” or “box” model.
  - More complex systems could be modeled with multizone models
  - Even more complex systems by direct calculation of fluid motion using computational fluid dynamics
    - Or Project I analog with Markov Chain models
- More spatially complex systems need full model of fluid flow and for particles going back to Lagrangian form to consider all forces

CFD (courtesy S Hoque)



Room dimensions: 2.5m x 2.5m x 2.5m

Mesh: 57*x* x 82y x 57z

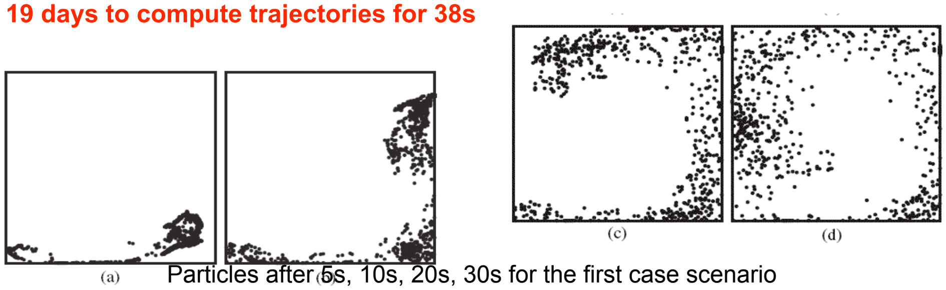
Inlet and outlet:0.07m

Air velocity: 0.886m/s

Particle density: 1000 kg/m^3

Particle diameter: 5μm and 20μm

19 days to compute trajectories for 38s



Particles after 5s, 10s, 20s, 30s for the first case scenario

Beghein, C., Y. Jiang, and Q.Y. Chen, *Using large eddy simulation to study particle motions in a room.* Indoor air, 2005. **15**: p. 281-290