Environmental transport phenomena: Lecture V

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2D ADE, point source solution

The advection **diffusion equation** (ADE) can be written

$$\frac{\partial C}{\partial t} + u\frac{\partial C}{\partial x} + v\frac{\partial C}{\partial y} = D_x\frac{\partial^2 C}{\partial x^2} + D_y\frac{\partial^2 C}{\partial y^2}$$

The **boundary** condition is

$$C(x,y,t) \to 0 \qquad \text{for} \qquad \sqrt{x^2+y^2} \to \infty$$

As **initial** condition we have (we assume a release uniform over a depth H)

$$C(x,y,0) = \frac{M}{H}\delta(x)\delta(y)$$

2D ADE, point source solution

The form of the initial condition suggests to look for a solution in the form of

$$C(x,y,t) = \frac{M}{H} C_1(x,t) C_2(y,t)$$

With **boundary** conditions

$$C_{1,2}(\infty,t) = 0$$

And **initial** conditions

$$C_1(x,0) = \delta(x) \qquad\qquad C_2(y,0) = \delta(y)$$

This technique, called "**separation of variables**" only works for certain types of PDE and boundary conditions (no universal method).

2D ADE, point source solution

Inserting
$$C(x,y,t) = \frac{M}{H} C_1(x,t) C_2(y,t)$$

into the advection diffusion equation, we obtain.

$$C_2 \left[\frac{\partial C_1}{\partial t} + u \frac{\partial C_1}{\partial x} - D_x \frac{\partial^2 C_1}{\partial x^2} \right] + C_1 \left[\frac{\partial C_2}{\partial t} + v \frac{\partial C_2}{\partial y} - D_y \frac{\partial^2 C_2}{\partial y^2} \right] = 0$$

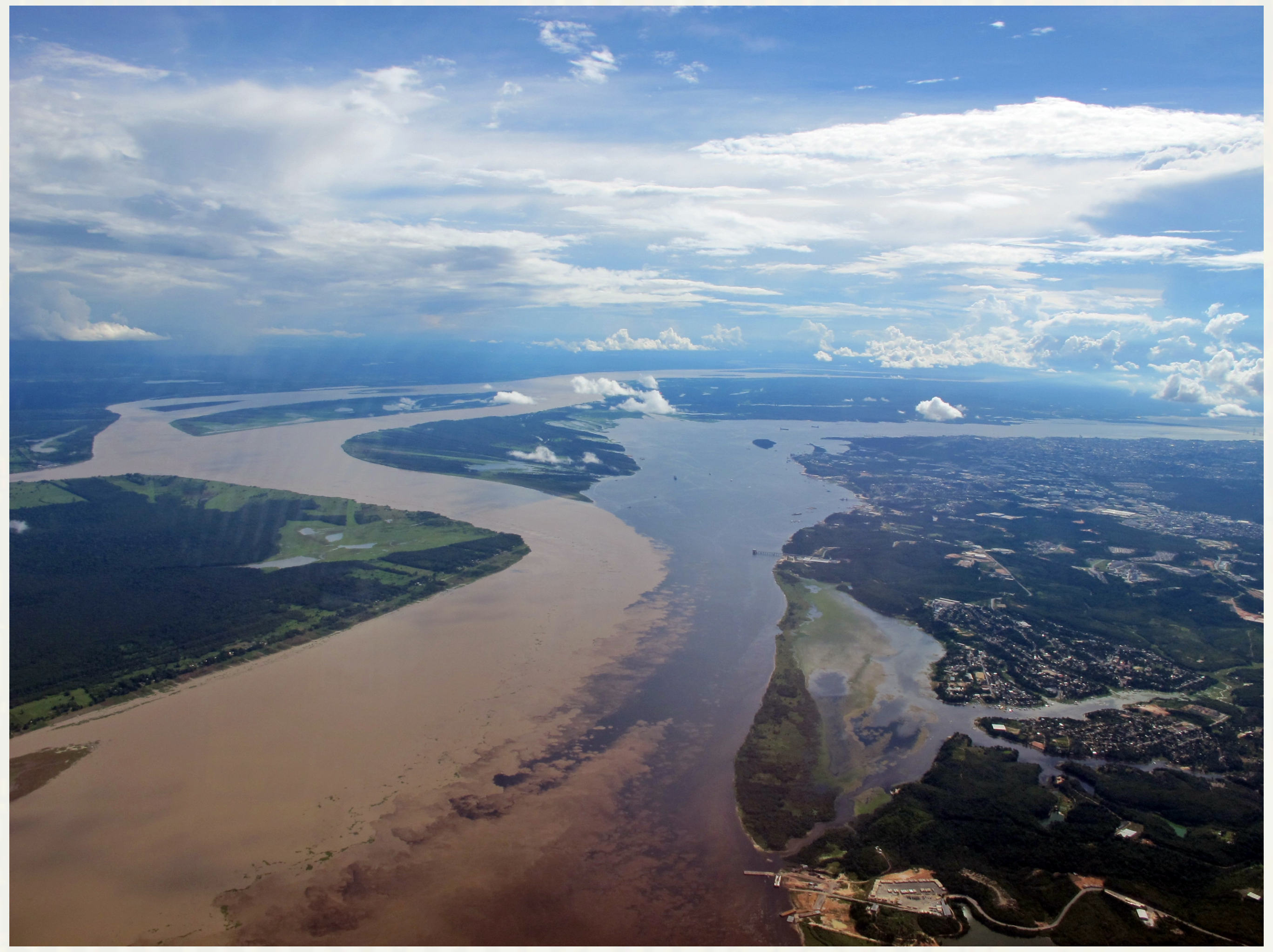
To simplify notation, we take u, v = 0 (no advection). Setting

$$C_1 = \frac{1}{\sqrt{4\pi D_x t}} e^{-\frac{x^2}{4D_x t}} \qquad C_2 = \frac{1}{\sqrt{4\pi D_y t}} e^{-\frac{y^2}{4D_y t}}$$

Satisfies the diffusion equation, the I.C and the B.C. The final solution is then (generalization to 3D and u, v ≠ 0 is immediate):

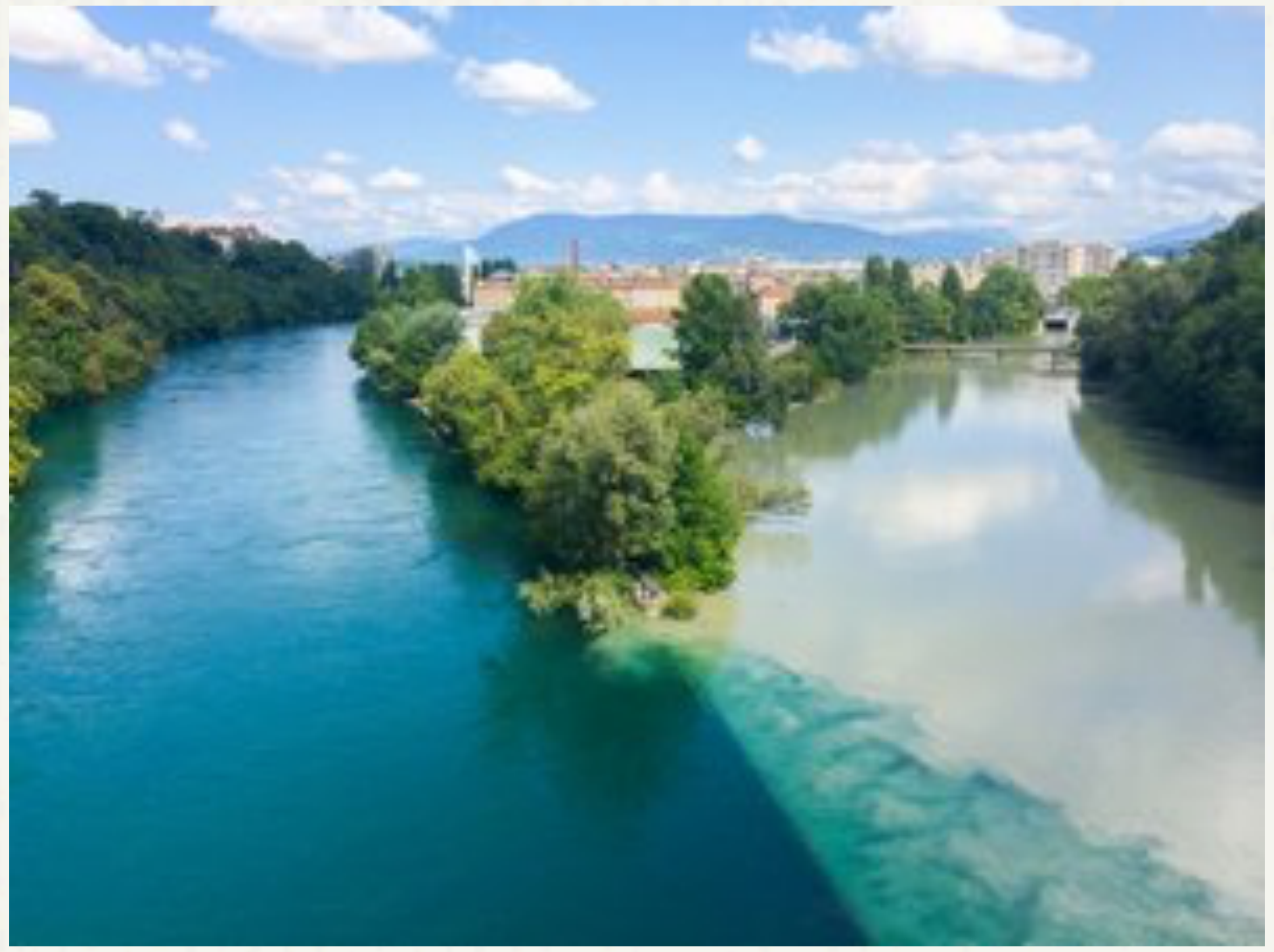
$$C(x,y,t) = \frac{M}{H} \frac{1}{4\pi \sqrt{D_x D_y} t} e^{-\left[\frac{x^2}{4D_x t} + \frac{y^2}{4D_y t} \right]}$$

2D diffusion equation, joining rivers



- Two rivers **joining**, one contains a **uniform concentration** C_0 of a given substance.

- **Advection** is assumed to prevail along the flow direction. In the transverse direction transport occurs due to (turbulent) **diffusion**. We assume that a **steady** state is reached. Flow in rivers is typically **turbulent** and thus **unsteady** by definition but can be **statistically stationary** (all statistics time invariant).



- **Regional** example: Rhone-Arve junction in Geneva

Joining rivers: modeling

- We start with the 2D ADE, with x coordinate along the flow (y transverse coordinate). We assume a straight river geometry and a **small junction angle**.

$$\cancel{\frac{\partial C}{\partial t}} + u\frac{\partial C}{\partial x} + v\cancel{\frac{\partial C}{\partial y}} = D_x\cancel{\frac{\partial^2 C}{\partial x^2}} + D_y\frac{\partial^2 C}{\partial y^2}$$

steady state

no advection transverse to the flow due to small angle

$Pe_x << 1$

Advection dominates along the flow

- **Only B.C.** matter because we are interested in steady-state solution. We set x=0 and y=0 at the junction. We also assume a situation with **wide and shallow river**, or equivalently we remain in a domain where the concentration front has not reached the opposite side of the river.

$$C(x=0, y>0) = 0 \qquad C(x, y\to\infty) = 0$$

$$C(x=0, y<0) = C_0 \qquad C(x, y\to-\infty) = C_0$$

Joining rivers: model solution

- Performing the change of variables

$$\eta = \frac{x}{u} \qquad\qquad \xi = y$$

reduces the advection diffusion equation to the simpler diffusion equation

$$u\frac{\partial C}{\partial x} = D_y \frac{\partial^2 C}{\partial y^2} \quad \longrightarrow \quad \frac{\partial C}{\partial \eta} = D_y \frac{\partial^2 C}{\partial \xi^2}$$

- The variable η has the dimension of a time that corresponds to the flow time from the junction to the position x.

- From the solution for the gate opening we directly obtain the solution

$$C(x,y) = \frac{C_0}{2}\left[1 - \mathrm{erf}\left(\frac{y}{\sqrt{4D\frac{x}{u}}}\right)\right]$$

Advection Diffusion Reaction equation

- Production/Loss of mass through **physical** (e.g. sediment deposition, radioactive decay), **chemical** (e.g. stoichiometric reactions) and **biological** processes (e.g. respiration).

- We distinguish between homogeneous (occur everywhere in the domain) and heterogeneous (occur at boundaries) processes.

homogeneous reactions -> source/sink terms in the continuity equation

$$\frac{\partial C}{\partial t} + \nabla \cdot \mathbf{J} = \sum_i S_i$$

heterogeneous reactions -> time-dependent boundary condition

$$C(x = x_i, t) = f(t)$$

- **Reaction rate** R relevant for deciding whether reaction have to be considered or not (for times t << 1/R reaction can be neglected).

Reaction kinetics

- Consider the reaction

$$aA + bB \to cC + dD$$

A, B **reactants**
C, D **products**

a, b, c, d **stoichiometric coefficients**

example $$CH_4 + 2O_2 = CO_2 + 2H_20$$

- We introduce the **rate of change** R_A of a substance A (depletion corresponds to negative rate)

$$\frac{d[A]}{dt} = \frac{dC_A}{dt} = R_A$$

at **equilibrium** we have

$$bR_A = aR_B \Rightarrow R_A = \frac{a}{b}R_B$$

$$cR_A = -aR_C \Rightarrow R_A = -\frac{a}{c}R_C$$

Reaction kinetics

- In general product i formed by j reactants

from **experiment**, dimensional quantity

$$\frac{d[i]}{dt} = \frac{d[C_i]}{dt} = R_i = k_i C_1^{n_1} C_2^{n_2} \ldots C_j^{n_j}$$

$$O_i = \sum_{l=1}^{j} n_l$$

overall reaction order

- The n_l are not necessarily equal to the stoichiometric coefficients (can even be **fractional**) -> to be determined experimentally.

First order (linear) reactions

- Important simple case (e.g. radioactive decay)

$$\frac{dC}{dt} = \pm kC \qquad [k] = \frac{1}{T}$$

- Initial condition $C(t=0) = C_0$

- Solution $C(t) = C_0 e^{\pm kt}$

- Decay **half-life** (or doubling period) independent of initial condition

$$t_{1/2} = \frac{\ln 2}{k}$$

Advection Diffusion Reaction equation

- From the continuity equation we obtain the **ADR equation**

$$\frac{\partial C}{\partial t} + \mathbf{U}\nabla C = D\nabla^2 C + R$$

- Example 1: 1D linear ADR equation, point source in an infinite domain

$$\frac{\partial C}{\partial t} + v_{adv}\frac{\partial C}{\partial x} = D\frac{\partial^2 C}{\partial x^2} \pm kC$$

- Solution (blackboard derivation) $C(x,t) = \frac{M}{A\sqrt{4\pi D t}} e^{-\frac{(x - v_{adv}t)^2}{4Dt}} e^{\pm kt}$

- Example 2: 1D linear ADR equation, steady release (blackboard)