Environmental transport phenomena: Lecture IV

Benoît Crouzy
(benoit.crouzy@meteoswiss.ch)

EPFL

Schweizerische Eidgenossenschaft
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Diffusion equation: superposition principle

The diffusion equation is linear $$\frac{\partial C(x,t)}{\partial t} = D\frac{\partial^2 C(x,t)}{\partial x^2}$$

- If $C_1(x,t)$ and $C_2(x,t)$ are solution of the diffusion equation then their sum is also a solution of the diffusion equation.

- Solution in the presence of several point sources in an infinite 1D domain

$$C(x,t) = \sum_{i=1}^{N} \frac{M_i}{A\sqrt{4\pi Dt}} e^{-\frac{(x-\mu_i)^2}{4Dt}}$$

With μ_i the position of the i^{th} source (N in total).

Diffusion equation: continuous initial condition

We assume an **infinite** 1D domain and a **continuous** initial condition $C_0(x)$

- Evolution equation

$$\frac{\partial C(x,t)}{\partial t} = D\frac{\partial^2 C(x,t)}{\partial x^2}$$

- Domain boundary concentrations

$$C(x = \pm\infty, t) = 0 \qquad \forall t$$

- Initial concentration distribution

$$C(x,0) = C_0(x)$$

Using the linearity of the diffusion equation, we will obtain the solution satisfying the initial continuous boundary condition from the solution for a **point release**.

Diffusion equation: continuous initial condition

- General solution obtained from the **point source** solution

$$C(x,t) = \int_{-\infty}^{\infty} \frac{C_0(\xi)}{\sqrt{4\pi D t}} e^{-\frac{(x-\xi)^2}{4Dt}} d\xi$$

- By linearity it is easy to verify that this is a solution of the diffusion equation.

- Intuitively, the integral can be seen as the sum of an **infinite number of local contributions** (~ point sources). Each of those contributions is **weighed** by the value of the initial concentration $C_0(x)$.

Diffusion equation: continuous initial condition

$$C(x,t) = \int_{-\infty}^{\infty} \frac{C_0(\xi)}{\sqrt{4\pi D t}} e^{-\frac{(x-\xi)^2}{4Dt}} d\xi$$

- In order to prove that the continuous initial condition is satisfied we use the property of the Dirac distribution (blackboard derivation).

$$\int \delta(x - x_0) f(x) dx = f(x_0)$$

- In addition, we use the Leibniz integral rule

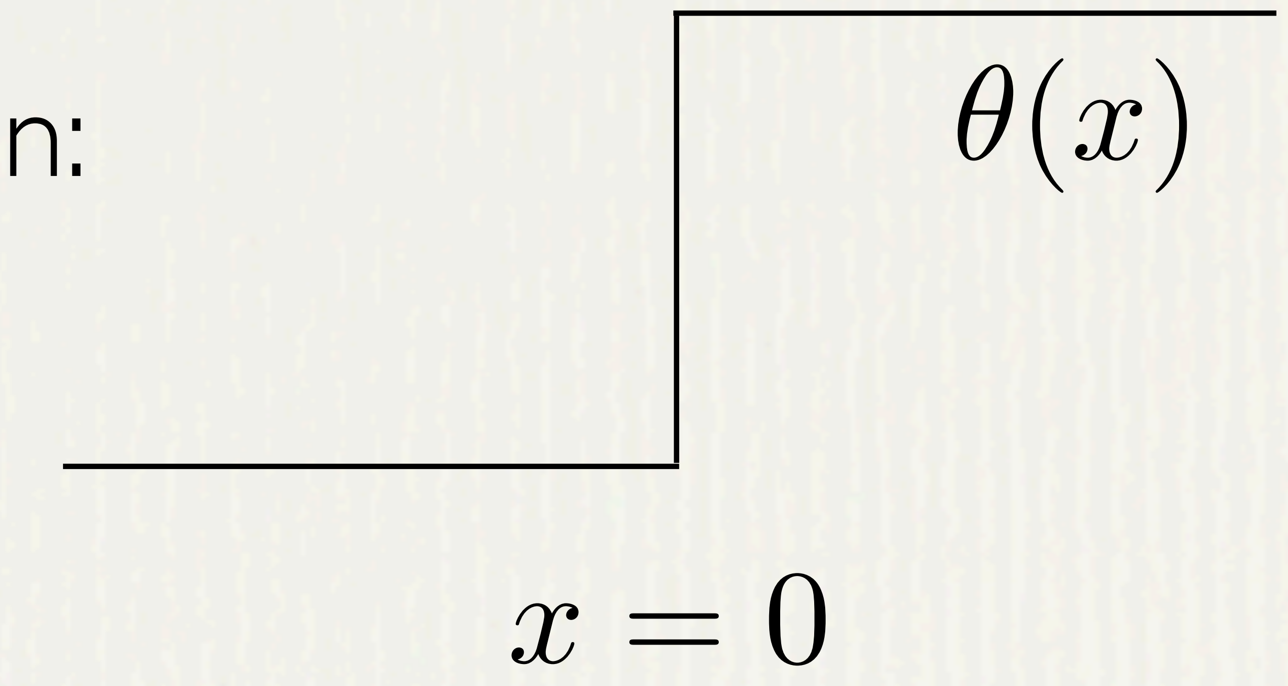
$$\frac{d}{dx}\int_{f(x)}^{g(x)} C(x,t)dt = C(g(x),t)g'(x) - C(f(x),t)f'(x) + \int_{f(x)}^{g(x)} \frac{\partial C(x,t)}{\partial x} dt$$

In this case the limits of integration do not depend on the position, those two terms are thus zero.

Example 1: gate opening

- We consider the following initial concentration distribution:

$$C_0(x) = C_0\theta(x)$$



With θ(x) = 1 for positive values of x and zero otherwise (**Heaviside** function). This corresponds to a gate closed at x=0 and t<0.

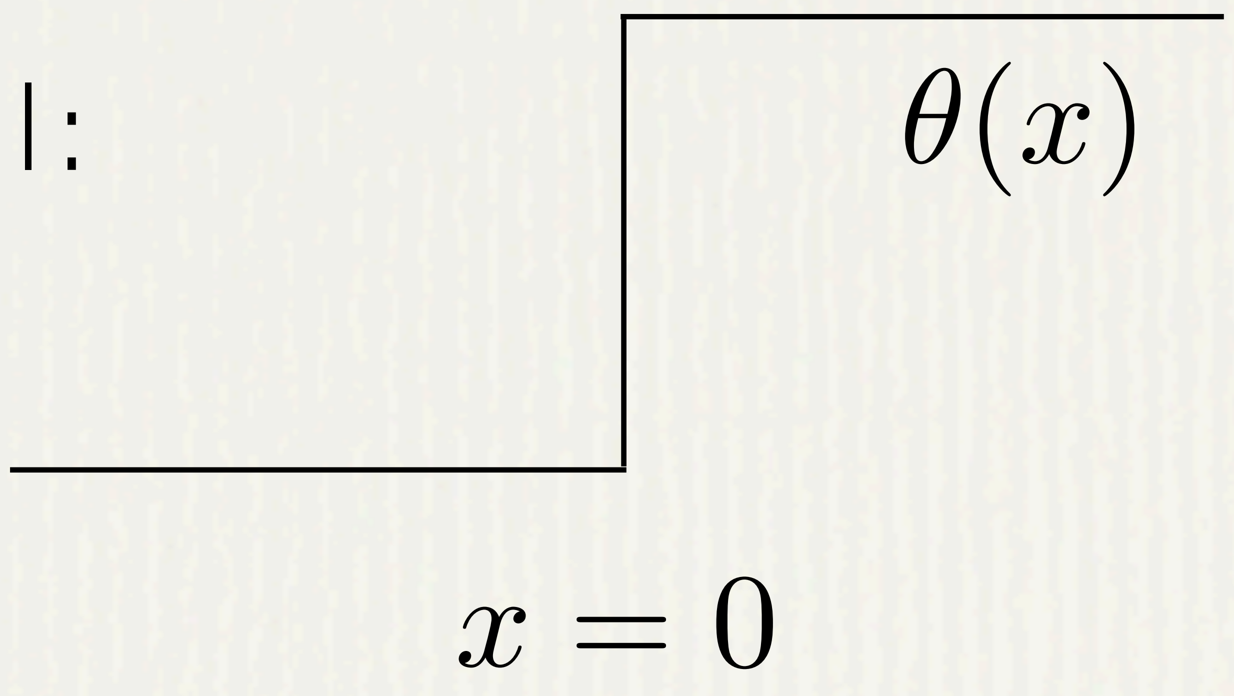
- At t=0 the gate is **opened** and the substance diffuses toward negative values of x.

- From the general solution for a continuous initial condition, we can derive (blackboard).

$$C(x,t) = \frac{C_0}{2}\left[1 + \mathrm{erf}\left(\frac{x}{\sqrt{4Dt}}\right)\right] \quad \text{with} \quad \mathrm{erf}(x) = \frac{2}{\sqrt{\pi}}\int_0^x e^{-t^2}dt.$$

Example 2: semi-infinite domain and fixed concentration (e.g. oxygen diffusion in lake)

- We consider the same initial concentration as in example 1:



$$C_0(x) = C_0\theta(x)$$

With $\theta(x) = 1$ for positive values of x and zero otherwise (Heaviside function).

- Instead of opening the gate we **fix** the boundary concentration.

$$C(x = 0, t) = C_0 \qquad \forall t$$

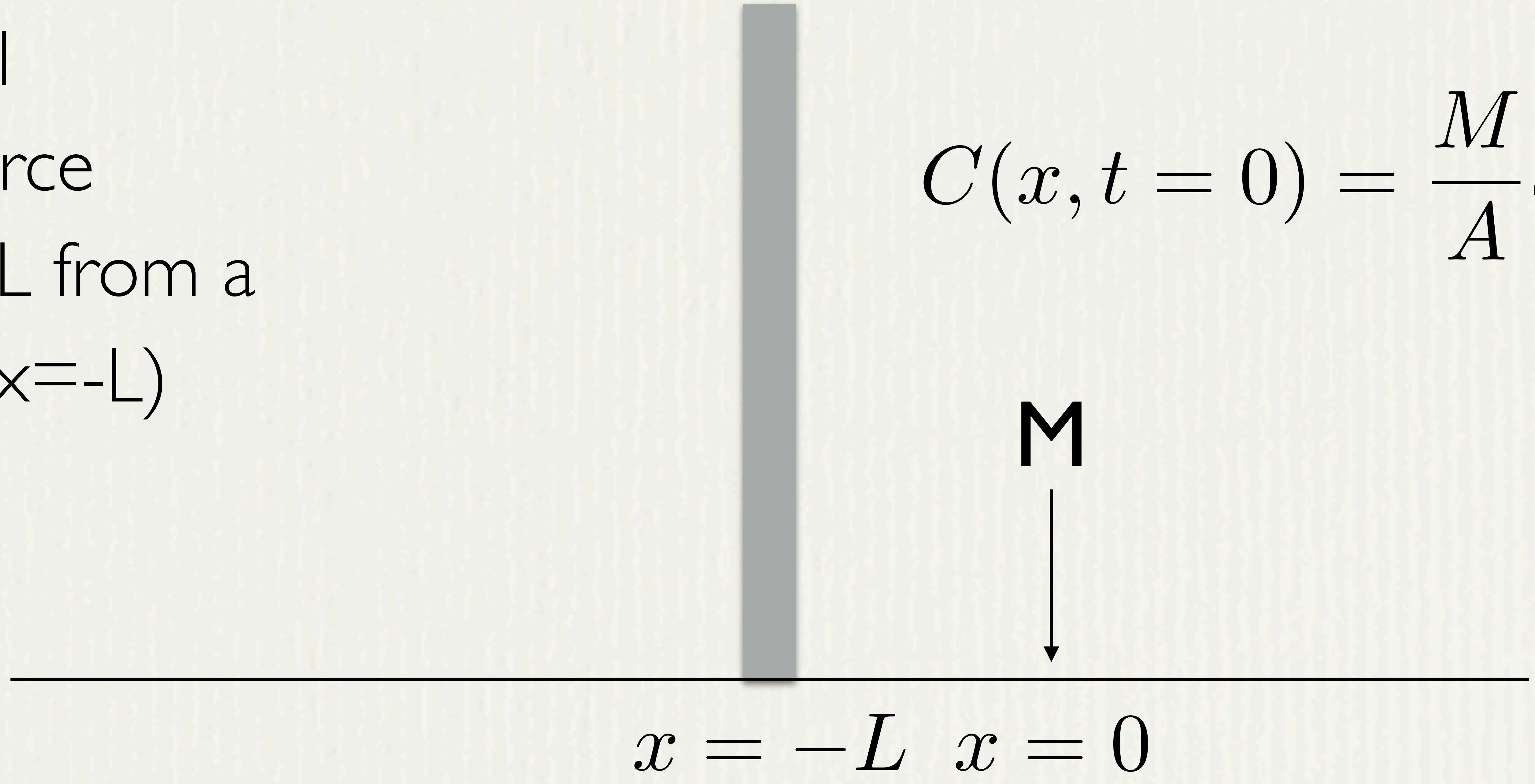
- Noting that the solution from example 1 is constant at x=0 (**symmetry**), we obtain directly (note the factor 2 difference)

$$C(x,t) = C_0 \left[1 + \mathrm{erf}\left(\frac{x}{\sqrt{4Dt}}\right)\right]$$

Example 3: presence of boundaries method of images

- We consider as initial condition a point source located at a distance L from a reflecting boundary (x=-L)

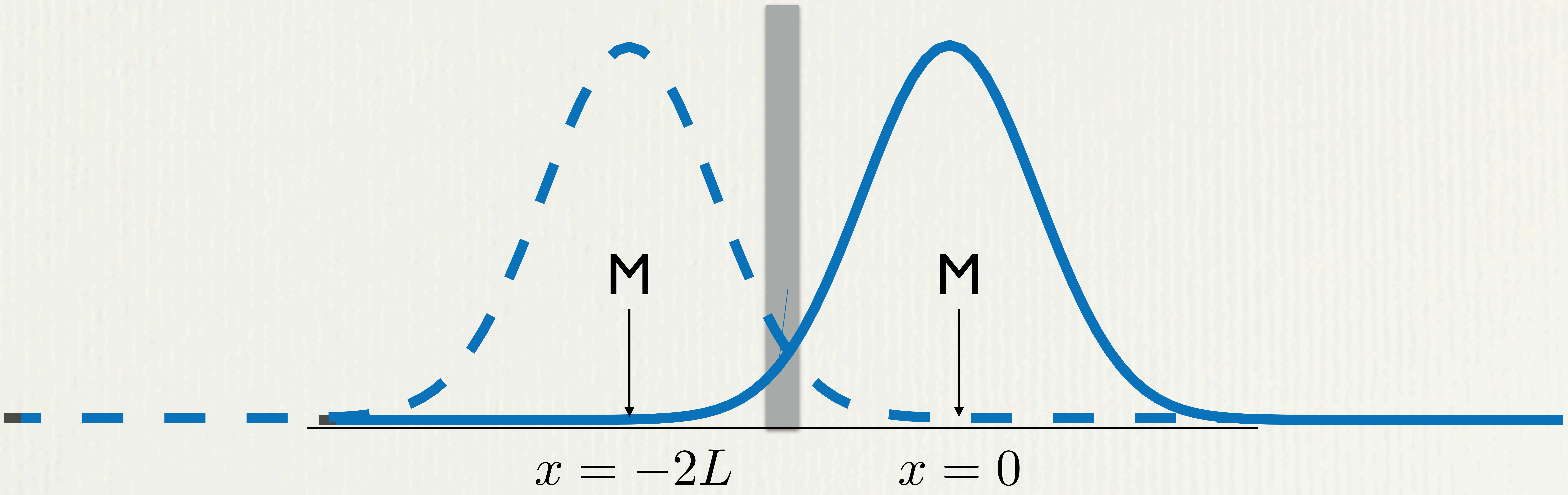
$$C(x, t=0) = \frac{M}{A}\delta(x)$$



- As boundary condition we impose a zero flux at the reflecting boundary

$$\left.\frac{\partial C(x,t)}{\partial x}\right|_{x=-L} = 0 \qquad \forall t$$

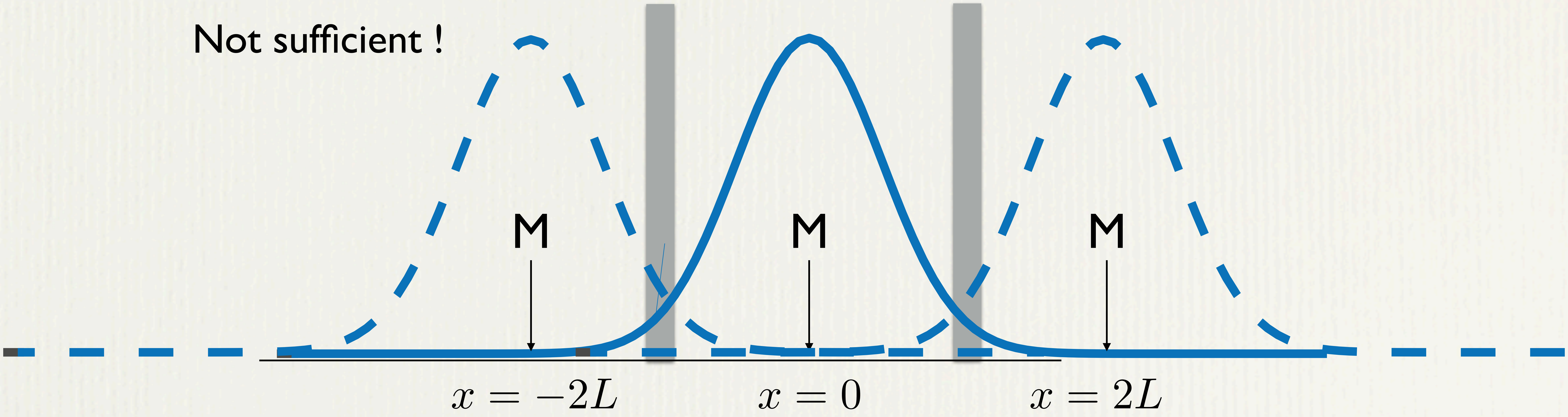
Example 4: presence of boundaries method of images



- Both boundary conditions can be satisfied by introducing an imaginary source at x=-2L.

$$C(x,t) = \frac{M}{A\sqrt{4\pi Dt}}\left[e^{-\frac{x^2}{4Dt}} + e^{-\frac{(x+2L)^2}{4Dt}}\right]$$

Example 4: multiple boundaries



- In the presence of two boundaries, **multiple** reflections have to be accounted for

$$C(x,t) = \frac{M}{A\sqrt{4\pi D t}} \sum_{n=-\infty}^{\infty} \left[e^{-\frac{(x+2nL)^2}{4Dt}} \right]$$

Advection diffusion equation

- We start from the continuity equation

$$\frac{\partial C}{\partial t} + \nabla \cdot \mathbf{J} = 0$$

- We assume that at each time the concentration profile results in a flux coming from diffusion **and** from advection. In addition both processes need to be independent.

$$\mathbf{J}(x,y,z,t) = \mathbf{J}_{adv}(x,y,z,t) + \mathbf{J}_{diff}(x,y,z,t)$$

With $$\mathbf{J}_{diff} = -D\nabla C \qquad \mathbf{J}_{adv} = \mathbf{U}C$$

- For solenoidal flow (incompressible flow, with zero divergence of velocity field) we obtain

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

Advection diffusion equation (e.g. polluant in river)

- We consider now the **1D** advection diffusion equation with **constant** advection velocity v_{adv}

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

- We assume in addition a **point source** located at x=0 as initial condition.
- If we choose a moving (inertial) reference frame **following** the fluid (e.g. observer on boat dragged by the current), we have the usual solution of the diffusion equation **without advection**.
- **Transforming back** to the reference frame for which the fluid is moving (e.g. observer standing on the side of the river) with v_{adv} we get

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

centerline moves with the fluid