Answer 4.4

a) Estimate the time at which the concentration at A and A’ begin to diverge?
The concentrations at A and A’ diverge when the boundary impacts the solution in System 1. This occurs when the diffusing cloud reaches the boundary. Estimate this time by equating the edge of the cloud with the length scale $\sigma$. That is, the cloud will touch the boundary when $3\sigma = \sqrt{2D} = 50\text{cm}$, such that $t = (50\text{cm})^2 / 18 \cdot 2\text{cm}^2\text{s}^{-1} = 70\text{ seconds}$.

b) What is the final concentration at A (A’), and when is this concentration achieved?
The final concentration in System 1 will be $C = (100\text{g}) / (1\text{m} \times 1\text{m} \times 0.1\text{m}) = 1000\text{ ppm}$. It is achieved when the mass is fully mixed across the domain. Using the largest dimension to estimate this time-scale, $t = (L)^2 / (4D) = 1250\text{ s}$. As noted in the text, this is a conservative estimate, and $t = (L)^2 / (8D) = 625\text{ s}$, is also a reasonable estimate. Because System 2 is unbounded, infinite dilution is possible and the final concentration is $C = 0\text{ ppm}$, but theoretically this will take infinite time. Because the probe has a detection limit of 10 ppm, zero concentration will be recorded for any concentration $C < 10\text{ ppm}$, which occurs in a finite time.

c) Describe the evolution of the concentration field in each system, i.e. $C(x,y,z,t)$.
In both systems the concentration is uniform in z by $t = (10\text{cm})^2 / (4 \times 2\text{cm}^2\text{s}^{-1}) = 12.5\text{ s}$ after release. Because this is short relative to other time scales of interest (1250 sec), we neglect the 3-D phase and use a two-dimensional solution. For System 1, an infinite number of image sources is needed to satisfy the no-flux boundaries.

$$C_1(x,y,t) = \frac{M}{L_z} \frac{1}{4\pi D t} \left[ \exp \left( -\frac{x^2 + y^2}{4D} \right) + \sum_{n=1}^{\infty} \exp \left( -\frac{x^2 + (y \pm 2nL)^2}{4D} \right) + \sum_{n=1}^{\infty} \exp \left( -\frac{(x \pm 2nL)^2 + y^2}{4D} \right) \right]$$

The images in the second line are located at the corners (see sketch), to offset the losses of y-axis images across the boundaries at $x = \pm L/2$; and the loss of x-axis images across the boundaries at $y = \pm L/2$. In practice an infinite number of images is not needed. For time less than required to reach a well-mixed condition between the boundaries ($t < L^2 / 4D$), three images per boundary is sufficient to approximate the full solution with infinite images. Beyond this time, the concentration is steady and uniform, and the detailed solution above is no longer needed. System 2 is described by a simple two-dimensional slug-release,

$$C_2(x,y,t) = \frac{M}{L_z} \frac{1}{4\pi D t} \exp \left( -\frac{x^2 + y^2}{4D} \right).$$

See the animation link which compares the solutions given above for System 1 (bounded) and System 2 (unbounded).