Diffusion Across Channels and Along Pores

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Purpose of Computational Diffusion Experiment:

Learn about the rate at which diffusion transports reactant chemicals across channels and through porous regions

Model Assumptions for Computational Fluid Dynamic Experiment:

1. Fluid has a single phase - liquid
2. The reactant has a diffusion coefficient in water of 1e-9 m^2 / sec
3. A concentration of 1 mol/liter is maintained at the inlet border of the diffusion region

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Boundary Conditions

• The diffusion equation is a 2nd-order PDE and requires two boundary or initial conditions to obtain a unique solution.

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

1) Initial state:
$C = 0$, for $x > 0$, $t = 0$.

2) Left-hand boundary:
At $x = 0$, C_0 is maintained for all $t > 0$.

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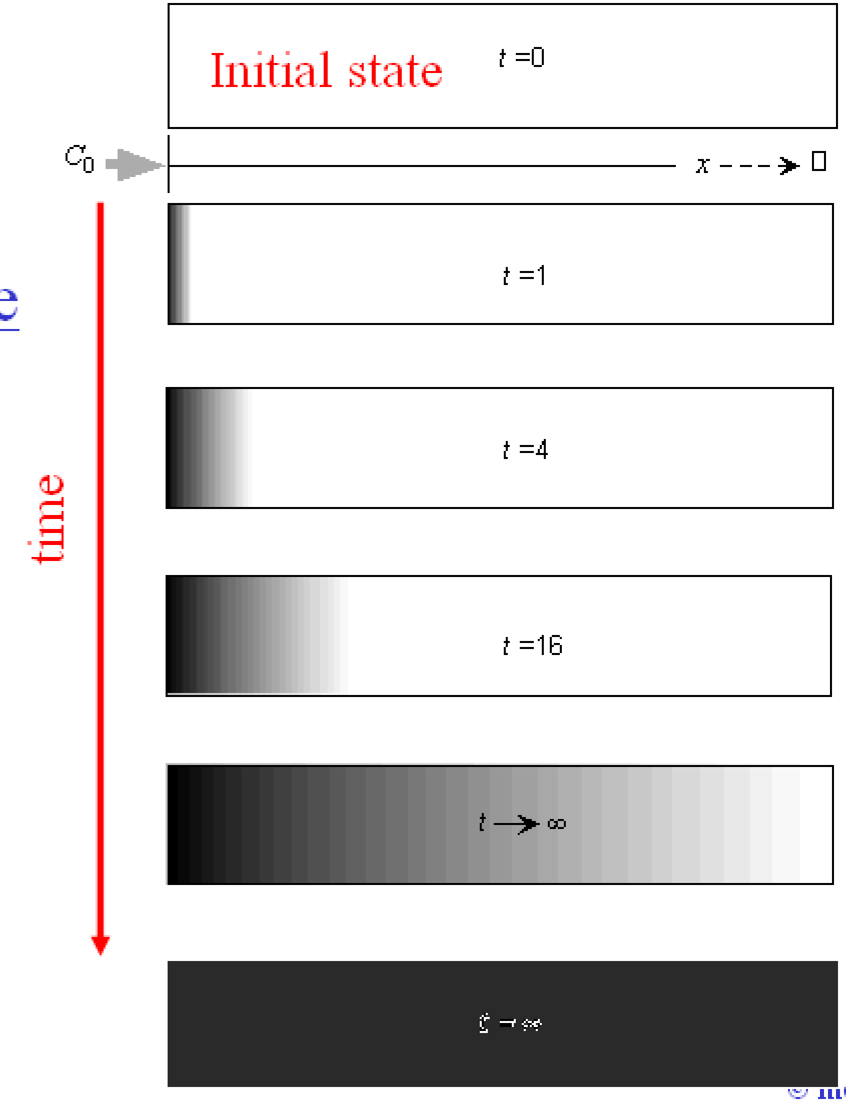
Linear diffusion into a semi-infinite medium



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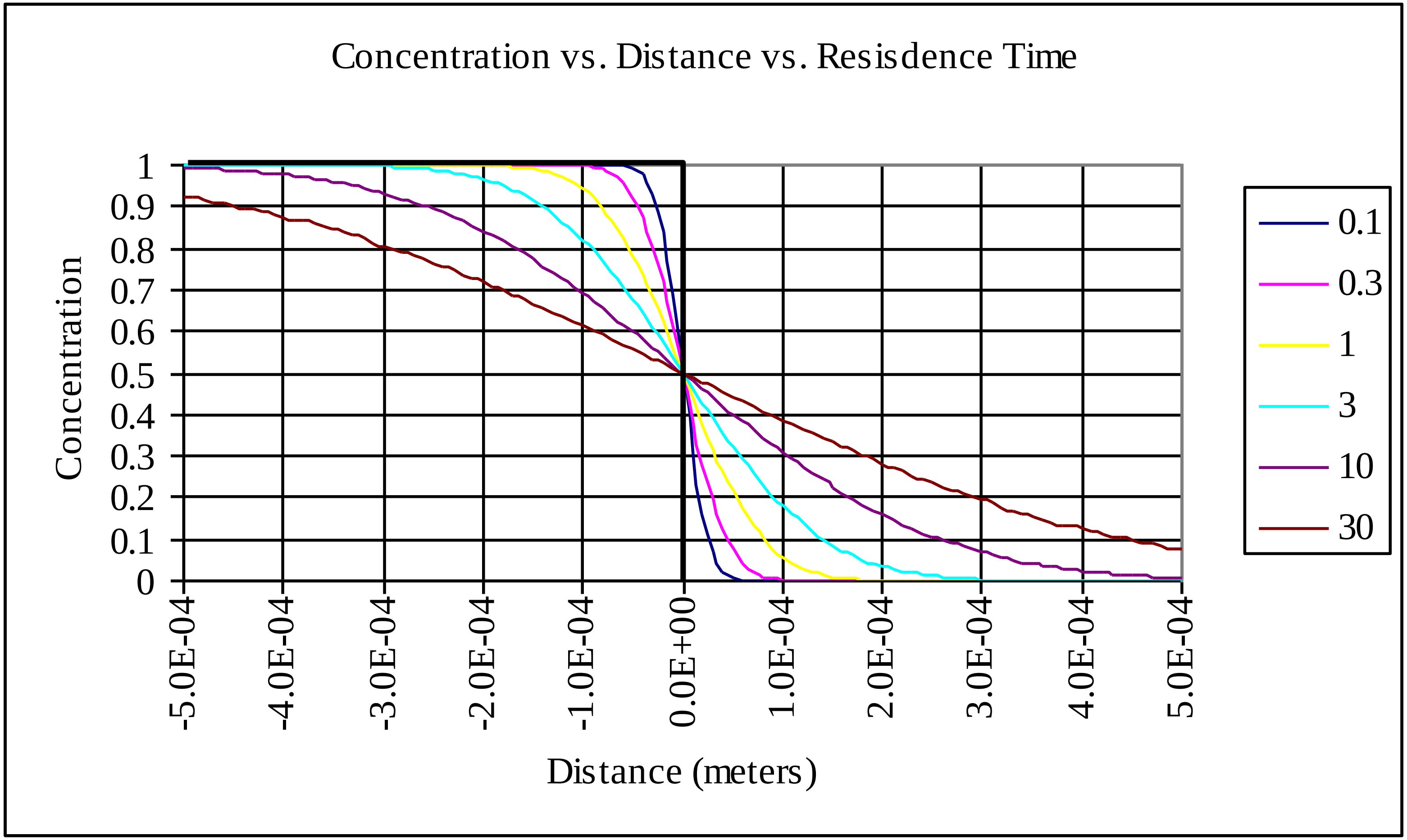
Laplace Transforms

The concentration field associated with the image field is found by inverting the transform either by formal means, a look-up table, or using a computer-based mathematics package.

$$C(x,t) = C_0 \operatorname{erfc}\left(\frac{x}{2\sqrt{Dt}}\right)$$

The error function, erf (z), and its complement, erfc (z), are defined

$$\operatorname{erfc}(z) = 1 - \operatorname{erf}(z) = 1 - \frac{2}{\sqrt{\pi}}\int_0^z e^{-\eta^2}\,d\eta$$



Diffusion from a Center Line with Diffusion Coefficient = 1e-9 m^2 / sec

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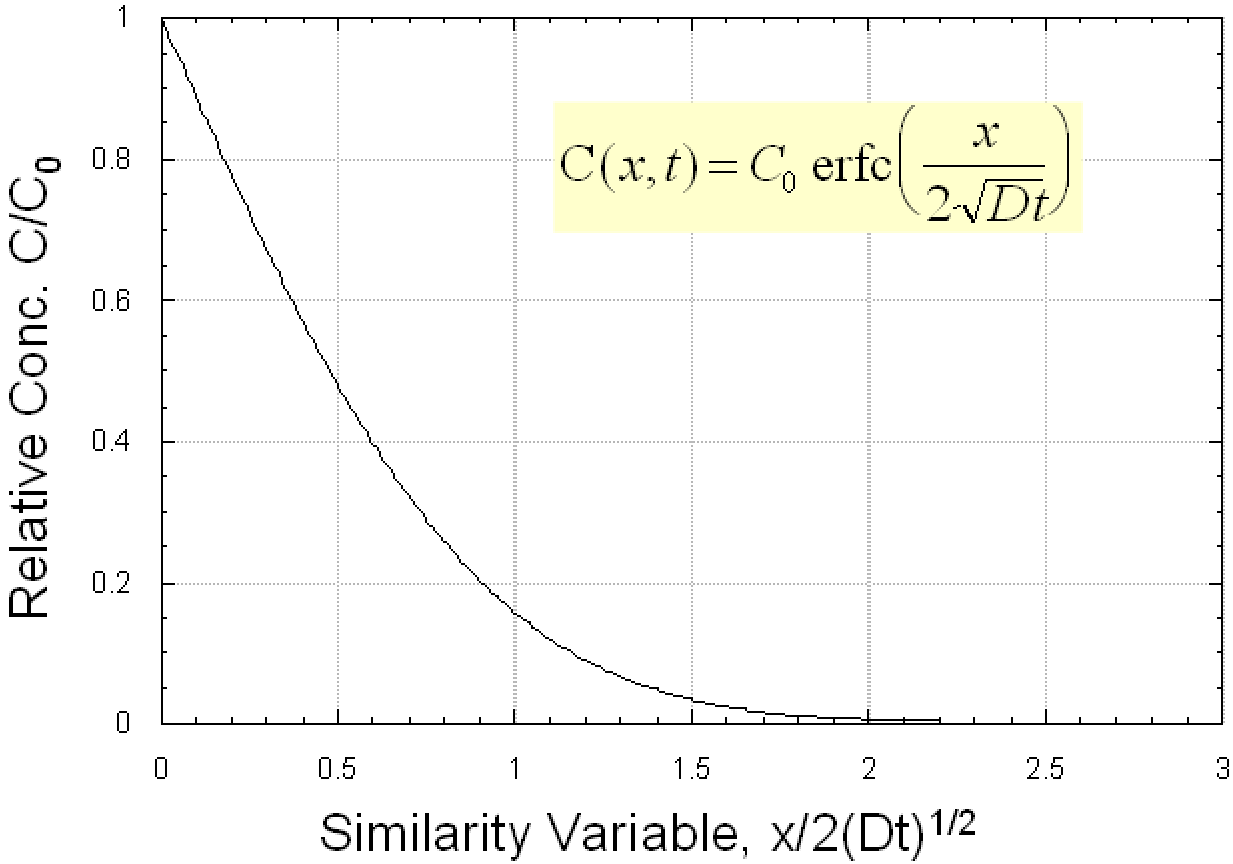
Concentration versus the similarity variable

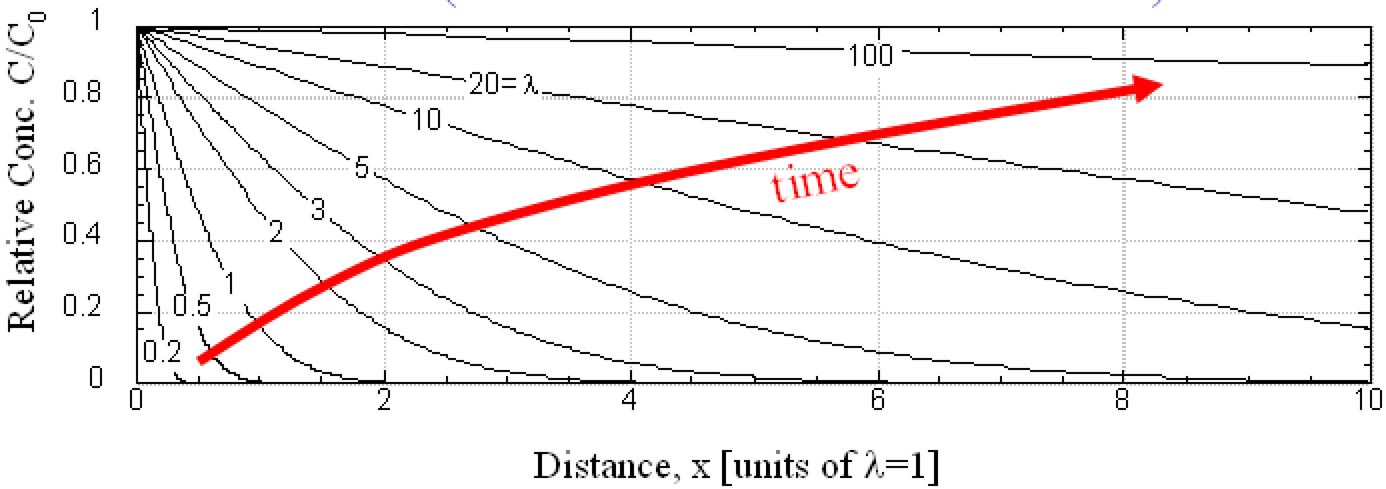


$$C(x,t) = C_0 \operatorname{erfc}\left(\frac{x}{2\sqrt{Dt}}\right)$$

Concentration field versus distance

$\lambda = 2(Dt)^{1/2}$ is the "time tag"

(Note: λ has the units of distance!)



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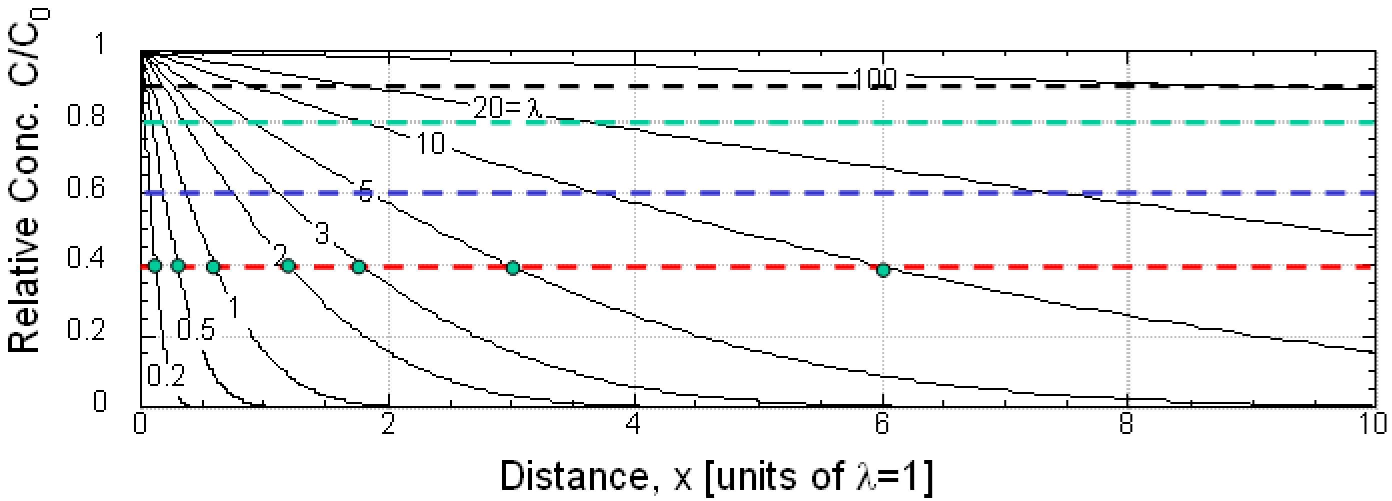
Diffusion Penetration X^*

$$X^* = K\, t^{1/2}$$



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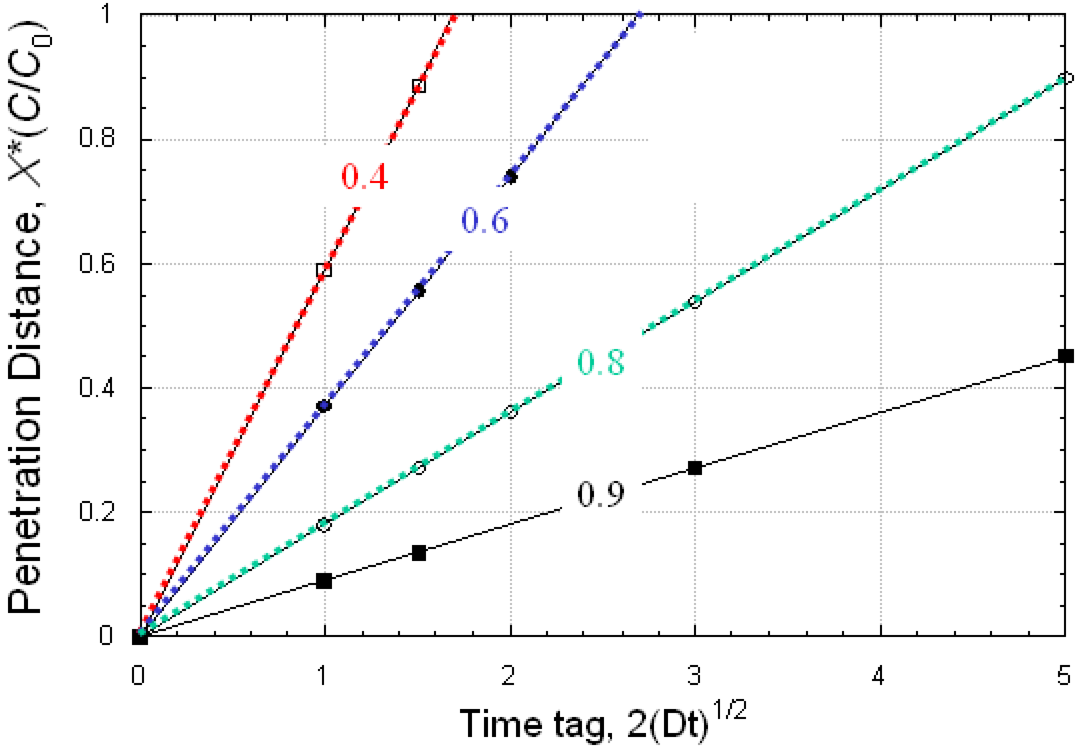
Penetration versus square-root of time



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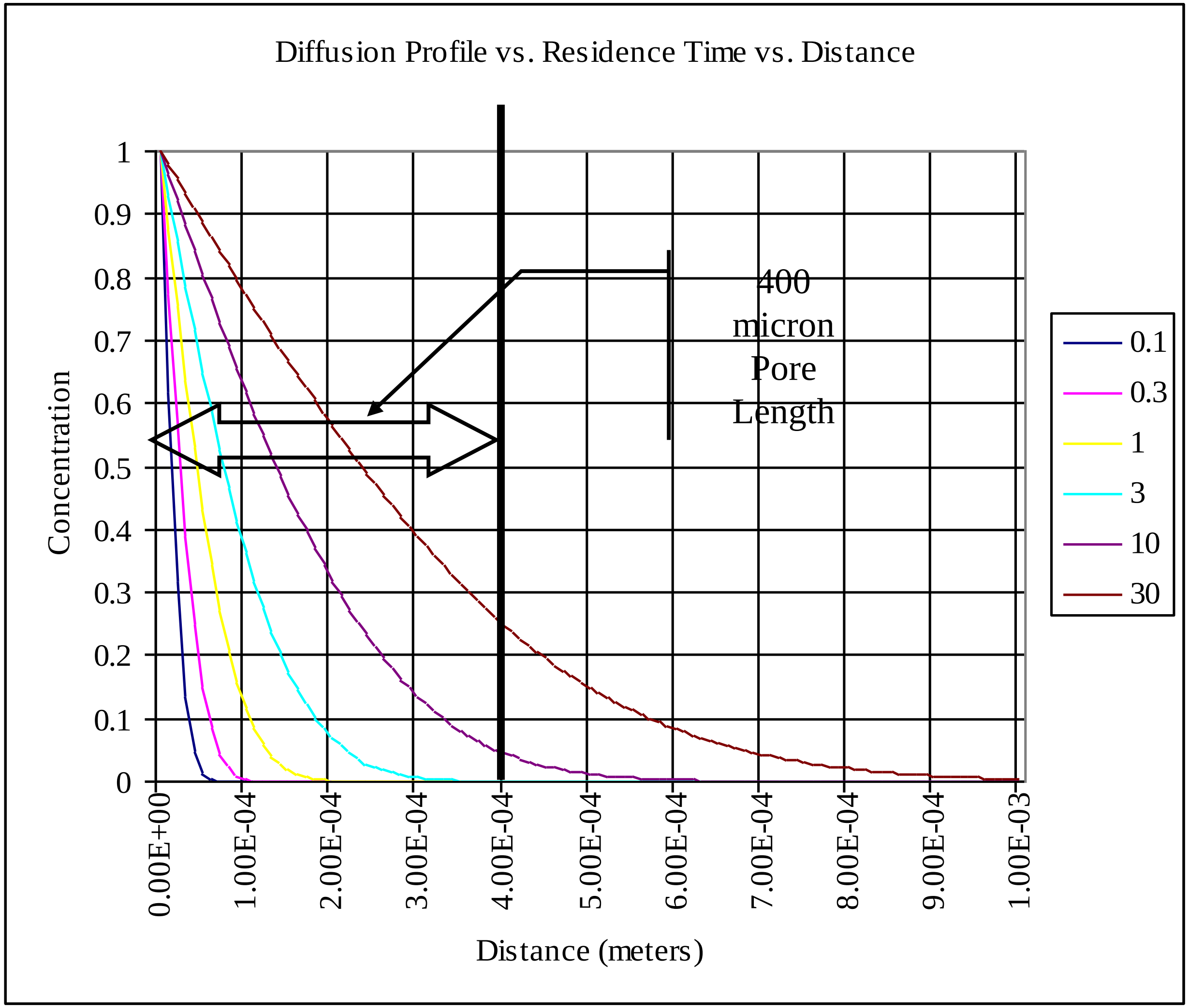

Diffusion from a Center Line with Diffusion Coefficient = 1e-9 m^2 / sec

Summary of Results for Diffusion Analysis

Apparently it takes about 100 seconds for diffusion from one side of a center channel to the other to give a concentration of about 5 % on the far side if no membrane is interposed.

Apparently it takes about 10 seconds for diffusion from one end of a 400 micron pore to the other to give a concentration at the far end of about 5 %

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