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by

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ABSTRACT

An analytical solution is developed for the problem of one-dimensional diffusion from a porous slab to a closed chamber. Motivation for the work was the study of gas diffusion from soils to a static chamber (a device commonly used to estimate soil-atmosphere gas exchange rates). The solution should also be useful in studies of radon accumulation rates, temperature conduction, and groundwater seepage rates into lakes. Initial concentration is arbitrary, as is length of the slab and the chamber. Gas movement within the chamber headspace is governed by diffusion. Concentrations can be calculated for any time and any location within the slab or chamber.

SOLUTION

The problem can be formally stated as:

$$\frac{\partial c}{\partial t} = D_1 \frac{\partial^2 c}{\partial z^2} \qquad -d_1 < z < 0, \qquad t > 0, \tag{1}$$

$$\Theta_D \frac{\partial c}{\partial t} = D_2 \frac{\partial^2 c}{\partial z^2} \qquad 0 < z < d_2, \qquad t > 0, \tag{2}$$

$$D_1 \frac{\partial c}{\partial z}(-d_1, t) = 0 \qquad t > 0, \tag{3}$$

$$c(d_2, t) = c_d \qquad t > 0, \tag{4}$$

$$D_1 \frac{\partial c}{\partial z}(0-, t) = D_2 \frac{\partial c}{\partial z}(0+, t) \qquad t > 0, \tag{A5}$$

$$c(z, 0) = g(z) \qquad -d_1 < z < d_2, \tag{6}$$

where t is time; $D_1 = D$, $D_2 = \tau\Theta_D D$; $d_1 = h$, and $d_2 = d$. There are no internal sources or sinks, nor any consumption or production. The solution $c(z,t)$ has the form

$$c(z,t) = c_d + \sum_{k=1}^{\infty} \gamma_k \, u_k(z) e^{-\lambda_k^2 t}, \tag{7}$$

where

$$\gamma_k = \frac{\int_{-d_1}^{0} (g(z) - c_d) u_k(z) dz + \Theta_D \int_0^{d_2} (g(z) - c_d) u_k(z) dz}{\int_{-d_1}^{0} u_k(z)^2 dz + \Theta_D \int_0^{d_2} u_k(z)^2 dz}, \tag{8}$$

$$
u_k(z) = \begin{cases} -\sin \dfrac{\lambda_k d_2}{\sqrt{\tilde{D}_2}} \cos \dfrac{\lambda_k (z+d_1)}{\sqrt{D_1}} & \text{if } z \le 0 \text{ and } \sin \dfrac{\lambda_k d_2}{\sqrt{\tilde{D}_2}} \ne 0, \quad (9a) \\ \cos \dfrac{\lambda_k d_1}{\sqrt{D_1}} \sin \dfrac{\lambda_k (z-d_2)}{\sqrt{\tilde{D}_2}} & \text{if } z \ge 0 \text{ and } \sin \dfrac{\lambda_k d_2}{\sqrt{\tilde{D}_2}} \ne 0, \quad (9b) \\ -\sqrt{D_2 \theta_D} \cos \dfrac{\lambda_k d_2}{\sqrt{\tilde{D}_2}} \cos \dfrac{\lambda_k (z+d_1)}{\sqrt{D_1}} & \text{if } z \le 0 \text{ and } \sin \dfrac{\lambda_k d_2}{\sqrt{\tilde{D}_2}} = 0, \quad (9c) \\ \sqrt{D_1} \sin \dfrac{\lambda_k d_1}{\sqrt{D_1}} \sin \dfrac{\lambda_k (z-d_2)}{\sqrt{\tilde{D}_2}} & \text{if } z \ge 0 \text{ and } \sin \dfrac{\lambda_k d_2}{\sqrt{\tilde{D}_2}} = 0, \quad (9d) \end{cases}
$$

$\tilde{D}_2 = D_2/\theta_D$, and the numbers $0 < \lambda_1 < \lambda_2 < \lambda_3 < \ldots$ are the positive solutions λ of the equation

$$
\sqrt{D_1} \sin \frac{\lambda d_1}{\sqrt{D_1}} \sin \frac{\lambda d_2}{\sqrt{\tilde{D}_2}} = \sqrt{D_2 \theta_D} \cos \frac{\lambda d_1}{\sqrt{D_1}} \cos \frac{\lambda d_2}{\sqrt{\tilde{D}_2}} . \tag{10}
$$

(In practice, (9c) and (9d) should be used if $\sin(\lambda_k d_2/\sqrt{\tilde{D}_2})$ is moderately small.) The infinite series in (7) is not completely in "closed form" because we do not have analytical expressions for λ_k, $k=1,2,3,\ldots$. However, we can characterize these numbers in a manner that lends itself to accurate evaluation on a computer. Rewrite (10) in the form

$$
\sqrt{D_1} \tan \frac{\lambda d_1}{\sqrt{D_1}} = \sqrt{D_2 \theta_D} \cot \frac{\lambda d_2}{\sqrt{\tilde{D}_2}}, \tag{11}
$$

noting that λ should also be considered a solution of (11) if both sides are infinite (in which case both sides of (10) are 0). List the nonnegative values of λ that make the left-hand side of (11) infinite,

$$\frac{\pi\sqrt{D_1}}{2d_1},\ \frac{3\pi\sqrt{D_1}}{2d_1},\ \frac{5\pi\sqrt{D_1}}{2d_1},\ \ldots,$$

make a similar list for the right-hand side,

$$0,\ \frac{\pi\sqrt{\tilde{D}_2}}{d_2},\ \frac{2\pi\sqrt{\tilde{D}_2}}{d_2},\ \ldots,$$

then intersperse the two lists in ascending order to obtain

$$\mu_0 = 0,\ \mu_1 = \left\{\min\frac{\pi\sqrt{D_1}}{2d_1},\frac{\pi\sqrt{\tilde{D}_2}}{d_2}\right\},\ \mu_2,\ \mu_3,\ \ldots,$$

If the same number appears on both lists (e.g., $\frac{\pi\sqrt{D_1}}{2d_1} = \frac{\pi\sqrt{\tilde{D}_2}}{d_2}$), put it twice on the μ list. (In practice, this should be invoked if the lists agree within a suitable tolerance.) Then $\mu_{k-1} < \lambda_k < \mu_k$ if $\mu_{k-1} < \mu_k$ and $\mu_{k-1} = \lambda_k = \mu_k$ if $\mu_{k-1} = \mu_k$, i.e., there is exactly one solution of (10) between each consecutive pair on the μ list. With these bracketing values for λ_k, one can easily compute it with a combination of bisection and Newton's method. This completes the description of the solution $c(z,t)$.

For completeness, we include the mathematical derivation of the above analytical solution. Letting

$$v(z,t) = c(z,t) - c_d, \tag{12}$$

we see that $v(z,t)$ solves (1)-(6) with c_d and $g(z)$ replaced by 0 and $g(z)-c_d$ in (4) and (6), respectively. Applying separation of variables to the problem for v, we seek solutions $v_k(z,t)$ of the form

$$v_k(z,t) = Z_k(z)\ T_k(t), \tag{13}$$

where

$$\frac{\partial v_k}{\partial t}(z,t) = Z_k(z)\ T_k'(t) = D_1\frac{\partial^2 v_k}{\partial z^2} = D_1\ Z_k''(z)T_k(t), \qquad z < 0,$$

$$\Theta_D\ \frac{\partial v_k}{\partial t}(z,t) = \Theta_D Z_k(z)\ T_k'(t) = D_2\ \frac{\partial^2 v_k}{\partial z^2} = D_2\ Z_k''(z)T_k(t), \qquad z > 0,$$

so that

$$D_1\ \frac{Z_k''(z)}{Z_k(z)} = \frac{T_k'(t)}{T_k(t)} = \lambda_k^2, \qquad z < 0, \tag{14a}$$

$$D_2\ \frac{Z_k''(z)}{Z_k(z)} = \Theta_D\ \frac{T_k'(t)}{T_k(t)} = -\Theta_D\ \lambda_k^2, \qquad z > 0. \tag{14b}$$

For the solution $v_k(z,t)$ to be a continuous function, the same constant $-\lambda_k^2$ must appear in both parts of (14); otherwise the two sides would decay at different exponential rates and $v_k(z,t)$ would be discontinuous at $z=0$. The spatial function $Z_k(z)$ is then a solution of the Sturm-Liouville eigenvalue problem (Courant and Hilbert, 1989, Vol. I, pp. 291-295)

$$D_1 Z'' + \lambda^2 Z = 0, \qquad -d_1 < z < 0, \tag{15}$$

$$D_2 Z'' + \theta_D \lambda^2 Z = 0, \qquad 0 < z < d_2, \tag{16}$$

$$D_1 Z'(-d_1) = 0, \tag{17}$$

$$Z(d_2) = 0, \tag{18}$$

$$Z(0-) = Z(0+), \tag{19}$$

$$D_1 Z'(0-) = D_2 Z'(0+). \tag{20}$$

For $-d_1 < z < 0$, (15) and (17) require an expression of the form

$$Z(z) = \alpha \cos \frac{\lambda(z+d_1)}{\sqrt{D_1}}, \qquad z < 0. \tag{21}$$

Similarly, for $0 < z < d_2$, (16) and (18) yield

$$Z(z) = \beta \sin \frac{\lambda(z-d_2)}{\sqrt{\tilde{D}_2}}, \qquad z > 0. \tag{22}$$

It remains to determine those λ for which α and β can be found that will satisfy (19) and (20). These constraints respectively imply that

$$\alpha \cos \frac{\lambda d_1}{\sqrt{D_1}} = -\beta \sin \frac{\lambda d_2}{\sqrt{\tilde{D}_2}}, \tag{23}$$

$$-\alpha\lambda \sqrt{D_1} \sin \frac{\lambda d_1}{\sqrt{D_1}} = \beta\lambda \sqrt{D_2 \theta_D} \cos \frac{\lambda d_2}{\sqrt{\tilde{D}_2}}. \tag{24}$$

Dividing (24) by (23) yields (11); if both sides of (23) are 0, then α and β can be chosen to satisfy (24), and (10) covers this case. For a specific λ_k that solves (10), by (23) we can choose

$$\alpha = -\sin \frac{\lambda_k d_2}{\sqrt{\tilde{D}_2}}, \qquad \beta = \cos \frac{\lambda_k d_1}{\sqrt{D_1}}, \tag{25}$$

unless both sides of (23) vanish, in which case we use (24) instead and take

$$\alpha = -\sqrt{D_2 \theta_D} \cos \frac{\lambda_k d_2}{\sqrt{\tilde{D}_2}}, \qquad \beta = \sqrt{D_1} \sin \frac{\lambda_k d_1}{\sqrt{D_1}}. \tag{26}$$

Substituting (25) into (21) and (22) and denoting $Z(z)$ by $u_k(z)$ leads to (9a) and (9b), respectively; (9c) and (9d) are obtained analogously from (26) in (21) and (22).

To see that there is exactly one solution of (10) between each consecutive pair of μ's, consider the difference (left side minus right side) of the two sides of (11). If $\mu_{k-1}<\mu_k$, this is a strictly increasing function of λ that tends to $-\infty$ at μ_{k-1} and to $+\infty$ at μ_k, hence it is zero exactly once. The degenerate case of $\mu_{k-1} = \mu_k$ was covered above.

By Sturm-Liouville theory (Courant and Hilbert, 1989), the eigenfunctions $u_k(z)$ behave like Fourier modes in the sense that they are orthogonal,

$$\int_{-d_1}^{d_2} u_j(z)\ u_k(z)\ w(z)\ dz = 0, \qquad j \neq k, \tag{27}$$

where $w(z) = 1$ for $-d_1 < z < 0$ and $w(z) = \theta_D$ for $0 < z < d_2$, and that the initial data $g(z) - c_d$ can be represented as an infinite linear combination

$$g(z) - c_d = \sum_{k=1}^{\infty} \gamma_k\ u_k(z). \tag{28}$$

Multiplying (28) by $u_k(z)\ w(z)$, integrating, and using (27), we obtain (8). Finally, from (14) we have

$$T_k(t) = e^{-\lambda_k^2 t}, \tag{29}$$

and thus (12), (13), and (29) give

$$c(z,0) - c_d = v(z,0) = \sum_{k=1}^{\infty} \gamma_k\ u_k(z)\ T_k(0), \tag{30}$$

whence (7) follows.

EXAMPLES

To demonstrate use of the solution we assume a generic gas with $D = 1.52\ m^2/d$, $d = 0.3$ m, $h = 0.2$m, and $\tau = \theta_D^{1/3}$. Initial soil-gas concentration changes linearly with depth from $c_d = 1$ at $z{=}d$ to $c_a = 0$ (atmospheric concentration) at land surface. In the absence of the chamber, the atmosphere at $z = 0$ is treated as a fixed concentration which gives $f_T = \theta_D^{4/3}\, D/.3 = 5.067\ \theta_D^{4/3}$. Initial concentration of the chamber is uniform at 0. These conditions are similar to those assumed by Matthias et al. (1978) as well as others. Figure 1 shows concentration vs depth profiles near soil surface at times of 0 and 30 min as calculated by the analytical solution ($\theta_D = 0.3$). Also shown are the concentrations calculated with a numerical finite-difference solution (Ishii et al., 1989) to the diffusion equation. Figure 2 shows analytically and numerically calculated gas accumulation rates in the chamber, f, relative to f_T for $\theta_D = 0.1$, 0.3, and 0.5.

For the special case of no consumption, the solution of Samuelsson (1987) for a completely mixed chamber headspace can be obtained from Equation 7 by setting $D_1 = \infty$ (in practice, some unrealistically high number will suffice). This effectively induces instantaneous mixing within the chamber making all concentrations uniform. The analytical solution to a 1-dimensional diffusion equation developed here should be of use not only in studies of soil-gas movement, but also in studies of temperature conduction. groundwater flow, and other phenomena which involve diffusional processes. Copies of a computer program for evaluating the analytical expression can be obtained from the authors.

List of Figures

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Figure 1

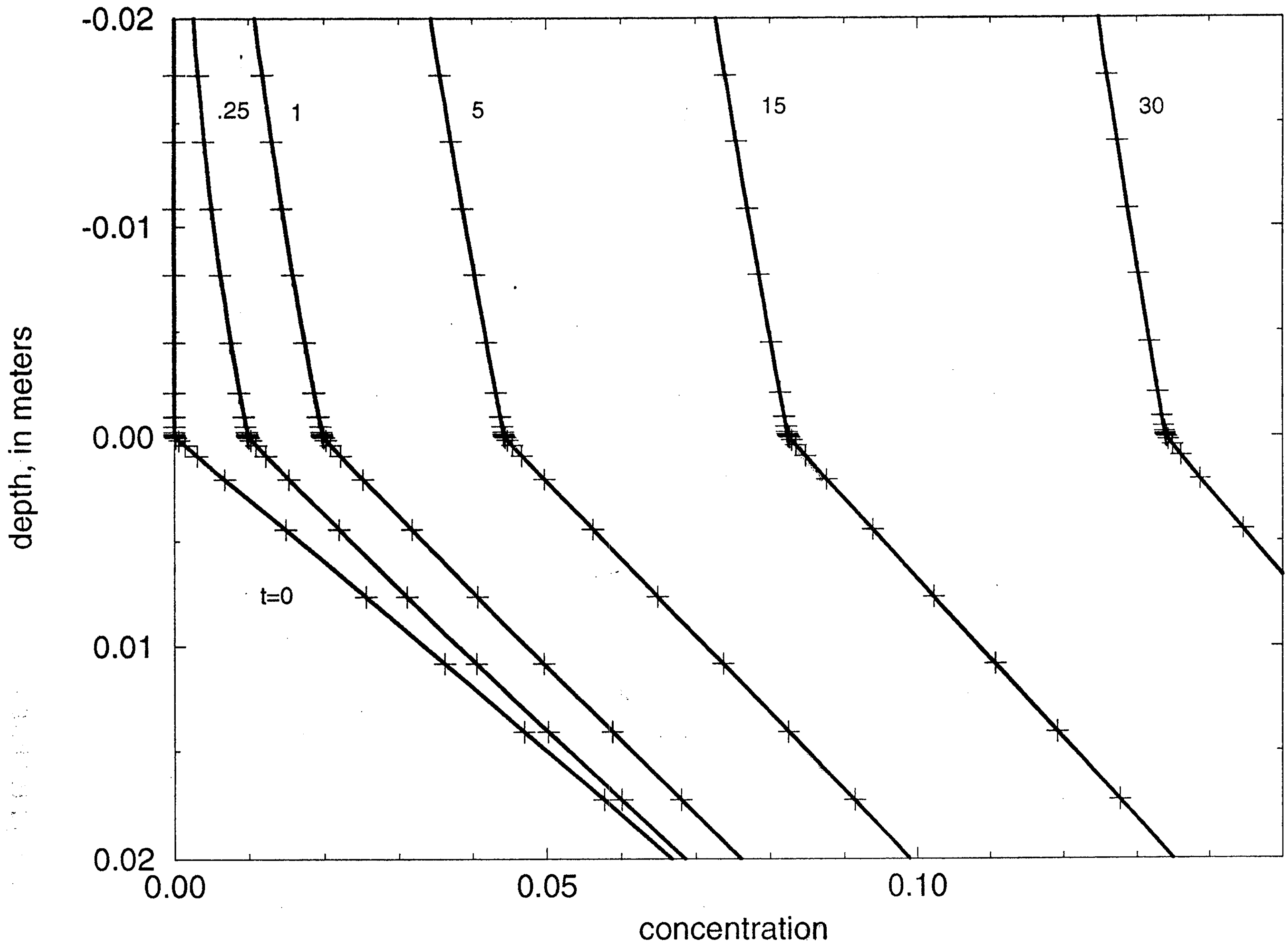
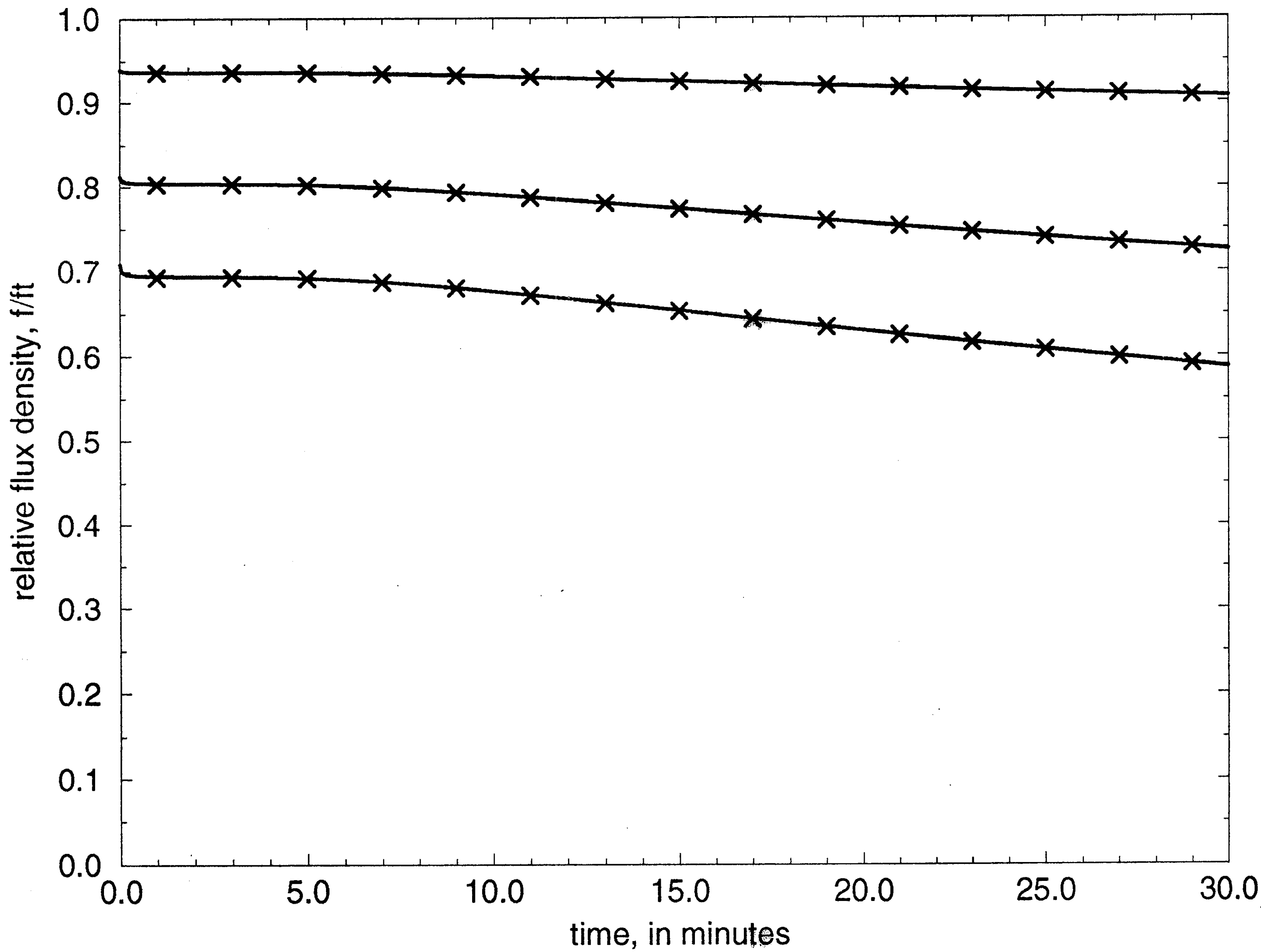

-0.02
-0.01
0.00
0.01
0.02
depth, in meters
0.00
0.05
0.10
concentration
.25
1
5
15
30
t=0

Figure 2



relative flux density, f/ft
1.0
0.9
0.8
0.7
0.6
0.5
0.4
0.3
0.2
0.1
0.0
0.0
5.0
10.0
15.0
20.0
25.0
30.0
time, in minutes

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