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Authors

Ahn, J

Kim, C.-L.

Chambré, P L

et al.

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Lawrence Berkeley Laboratory

UNIVERSITY OF CALIFORNIA

EARTH SCIENCES DIVISION

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Multiple Areal Sources in Fractured Rock and
Point Sources in Porous Rock**

J. Ahn, C.-L. Kim, P.L. Chambré,
T.H. Pigford, and W.W.-L. Lee

June 1989



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**Intermediate-Field Transport of
Contaminants:
Multiple Areal Sources in Fractured Rock
and Point Sources in Porous Rock**

J. Ahn
University of Tokyo

C.-L. Kim
Korea Advanced Energy Research Institute

P. L. Chambré, T. H. Pigford and W. W.-L. Lee

**Department of Nuclear Engineering
University of California**

and

**Earth Sciences Division
Lawrence Berkeley Laboratory
1 Cyclotron Road
Berkeley, CA 94720**

June 1989

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**The authors invite comments and would appreciate
being notified of any errors in the report.**

**T. H. Pigford
Department of Nuclear Engineering
University of California
Berkeley, CA 94720**

1. Introduction

This report is about "intermediate-field" transport or the migration of contaminants from arrays of discrete waste packages or sources. In constructing nuclear waste repositories in rock, it may be necessary to place a waste package across a rock fracture, or a rock fracture may develop some time after waste packages have been emplaced. To predict the spatial and temporal distribution of contaminant species from a line of waste packages facing a rock fracture may be important, because such fractures may now be considered a preferential pathway for released radionuclides to re-enter the biosphere. In land disposal of hazardous wastes, individual barrels may contain especially toxic material whose dispersion demands special attention. We have published analytic solutions for the multidimensional advective transport of contaminants from arrays of waste packages and multiple areal sources into a planar fracture.^{1,2} The results show a near region in which the concentrations vary greatly in the direction transverse to ground-water flow, an intermediate region in which the array can be treated as an infinite plane source of dissolving species, and a far-field region in which the array can be treated as a plane source of finite extent. The array equations have been developed for both porous and fractured media. These intermediate-field analyses will be useful to projects that require detailed predictions of releases to the environment. In this paper we summarize and compare the work with multiple areal sources facing a planar fracture and an array of point sources in porous media.

2. Multiple Areal Sources Facing a Planar Fracture

Analysis

The situation studied is shown in Figure 1, where a line of waste packages, here assumed to be corroded and releasing radioactive species, is exposed to a planar rock fracture in a water-saturated porous rock.

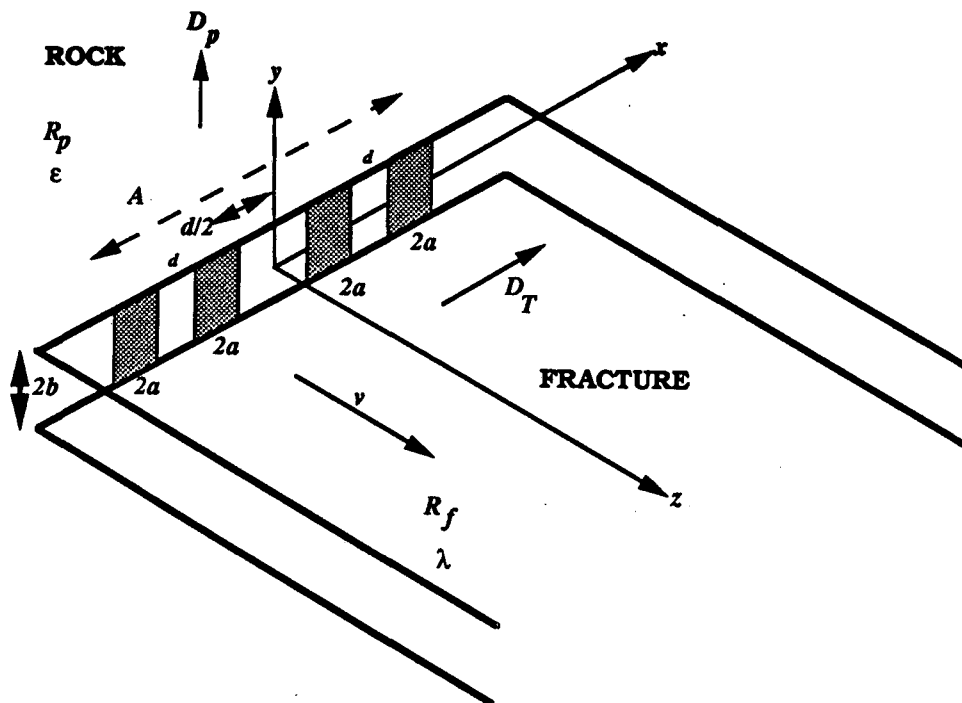


Fig. 1 Multiple Areal Sources Facing a Planar Fracture

Consider a single areal source along the fracture in Figure 1. After a contaminant species is released, several transport processes are important in tracing its eventual fate. First, there is advection in the rock fracture. Second, there is transverse dispersion in the planar fracture. Longitudinal dispersion is conservatively neglected.³ Radioactive species can sorb on the rock surface in the fracture, and they can diffuse into and out of pores in the rock matrix and sorb on the matrix. These transport processes can be described by the following coupled differential equations. In the rock fracture the mass balance is

$$R_f \frac{\partial N}{\partial t} + u \frac{\partial N}{\partial z} - D_T \frac{\partial^2 N}{\partial x^2} + R_f \lambda N + q/b = 0 \quad t > 0, z > 0, -\infty < x < \infty \quad (1)$$

where $N(x, z, t)$ is the species concentration in the fracture water, [M species/L³ fracture water]

$2b$ is the aperture of the fracture, [L]

u is the pore velocity in the fracture, [L/t]

D_T is the transverse dispersion coefficient, [L²/t]

R_f is the dimensionless retardation coefficient in the fracture, defined as $R_f = 1 + K_f/b$

K_f is the species distribution coefficient, [(M species/L² fracture wall)/(M species/L³ fracture water)], and

q is the diffusive flux into the rock matrix, [M/L²-t].

We also write a mass balance for the species inside the porous rock matrix

$$R_p \frac{\partial M}{\partial t} - D_p \frac{\partial^2 M}{\partial y^2} + R_p \lambda M = 0 \quad t > 0, y > b, z > 0, -\infty < x < \infty \quad (2)$$

where $M(x, y, z, t)$ is the concentration of the species in the matrix-pore water, [M species/L³ pore water]

D_p is the species diffusion coefficient in the matrix pore water, [L²/t]

R_p is a dimensionless retardation coefficient defined as $R_p = 1 + a_p K_p/\epsilon$

K_p is a distribution coefficient, [(M species/L² pore surface)/(M species/L³ pore water)]

a_p is the pore surface area per unit volume of rock, [L² pore surface/L³ rock matrix]

ϵ is the matrix porosity.

The two governing equations are coupled by two relationships. The first is flux continuity at the surface of the rock fracture

$$q(x, z, t) = -\epsilon D_p \left. \frac{\partial M}{\partial y} \right|_{y=b}, \quad t > 0, z > 0, -\infty < x < \infty \quad (3)$$

The second preserves the continuity of concentration at the fracture/rock interface

$$M(x, b, z, t) = N(x, z, t), \quad t > 0, z > 0, -\infty < x < \infty, \quad (4)$$

We solve eq. (1) and (2), subject to (3), (4) and the following initial conditions

$$N(x, z, 0) = 0, \quad z > 0, -\infty < x < \infty, \quad (5)$$

$$M(x, y, z, 0) = 0, \quad y > b, z > 0, -\infty < x < \infty, \quad (6)$$

and boundary conditions

$$N(x, 0, t) = \varphi(t)[h(x+a) - h(x-a)], \quad t > 0, -\infty < x < \infty, \quad (7)$$

$$N(x, \infty, t) = 0, \quad t > 0, -\infty < x < \infty, \quad (8)$$

$$N(\pm\infty, z, t) = 0, \quad z > 0, t > 0, \quad (9)$$

$$M(x, +\infty, z, t) = 0, \quad t > 0, z > 0, -\infty < x < \infty \quad (10)$$

where $\varphi(t)$ represents the time-dependent concentration at the surface of an areal source and can be in the form $N^0 e^{-\lambda t} \{h(t) - h(t-T)\}$, with $h(\cdot)$ the Heaviside step function, T the leach time and N^0 is the initial concentration. Equation (7) states that the center of an areal source of dimensions $2a \times 2b$ is located at the

origin of the system. The solution to the above system of equations is given in Ahn *et al.*,¹ and summarized below.

$$N(x, z, t) = N^0 F(b, z, t) G(x; \theta, a, 0), \quad t \geq 0, -\infty < x < \infty, \quad (11)$$

$$M(x, y, z, t) = N^0 F(y, z, t) G(x; \theta, a, 0), \quad t \geq 0, y \geq b, z \geq 0, -\infty < x < \infty, \quad (12)$$

where

$$F(y, z, t) = f(y, z, t) - e^{-\lambda T} f(y, z, t - T), \quad (13)$$

$$f(y, z, t) = e^{-\lambda t} h(t - ZA) \operatorname{erfc}[\{Z + B(y - b)\}/2\sqrt{t - ZA}], \quad (14)$$

$$G(x; \theta, a, x_1) = \frac{1}{2} \left[\operatorname{erf}\left(\frac{x - x_1 + a}{2\theta}\right) - \operatorname{erf}\left(\frac{x - x_1 - a}{2\theta}\right) \right] \quad (15)$$

$$Z = \frac{R_f z}{uA}, \quad A = \frac{bR_f}{\epsilon\sqrt{D_p R_p}}, \quad B = \sqrt{R_p/D_p}, \quad \theta = \sqrt{\frac{zD_T}{u}}. \quad (16)$$

These equations give the concentration field of the radioactive species in both the fracture and the rock matrix, as a function of space and time.

If there are multiple areal sources along the fracture, as shown in Figure 1, the solution is obtained by superposing the solutions for single areal sources. For areal sources each of width $2a$ separated by a *pitch* d , and the same release characteristics, the solution is

$$M(x, y, z, t, c) = N^0 F(y, z, t) \sum_{k=1}^c G(x; \theta, a, x_k), \quad t > 0, y \geq b, z \geq 0, -\infty < x < \infty \quad (17)$$

where c is the number of areal sources, and x_k [L] is the location of the center of the k^{th} areal source on the transverse axis x and is

$$x_k = d[k - (c + 1)/2], \quad k = 1, \dots, c \quad (18)$$

Numerical Illustrations

Figure 2 shows the normalized contaminant concentration in rock in the transverse direction. The ordinate shows the concentration predicted by eq. (17) normalized by the concentration predicted by an infinitely long source with equivalent strength, defined as

$$M^\infty(y, z, t) = (2a/d)N^0 F(y, z, t), \quad t > 0, y \geq b, z \geq 0, -\infty < x < \infty \quad (19)$$

Combining eq. (17) and (19), the ordinate in Figure 2 shows

$$\frac{M(x, y, z, t, c)}{M^\infty(y, z, t)} = (d/2a) \sum_{k=1}^c G(x; \theta, a, x_k), \quad t > 0, y \geq b, z \geq 0, -\infty < x < \infty \quad (20)$$

The normalized concentrations in Figure 2 are for four values of the distance parameter $\theta = \sqrt{(zD_T)/u}$ and for ten areal sources separated on ten-meter centers, or a total "repository" of 100 meters. The following parameter values are used in the calculations,

a , half-width of the areal sources, 0.14 m
 d , pitch or separation between areal sources, 10 m
 D_p , diffusion coefficient, 10^{-2} m²/a
 R_f , fracture retardation coefficient, 1
 c , number or count of areal sources, 10

b , half-aperture of the fracture, 0.005 m
 u , ground-water pore velocity, 10 m/a
 D_T , transverse dispersion coefficient, 0.05 m²/a
 R_p , matrix retardation coefficient, 100
 ϵ , porosity, 0.01.

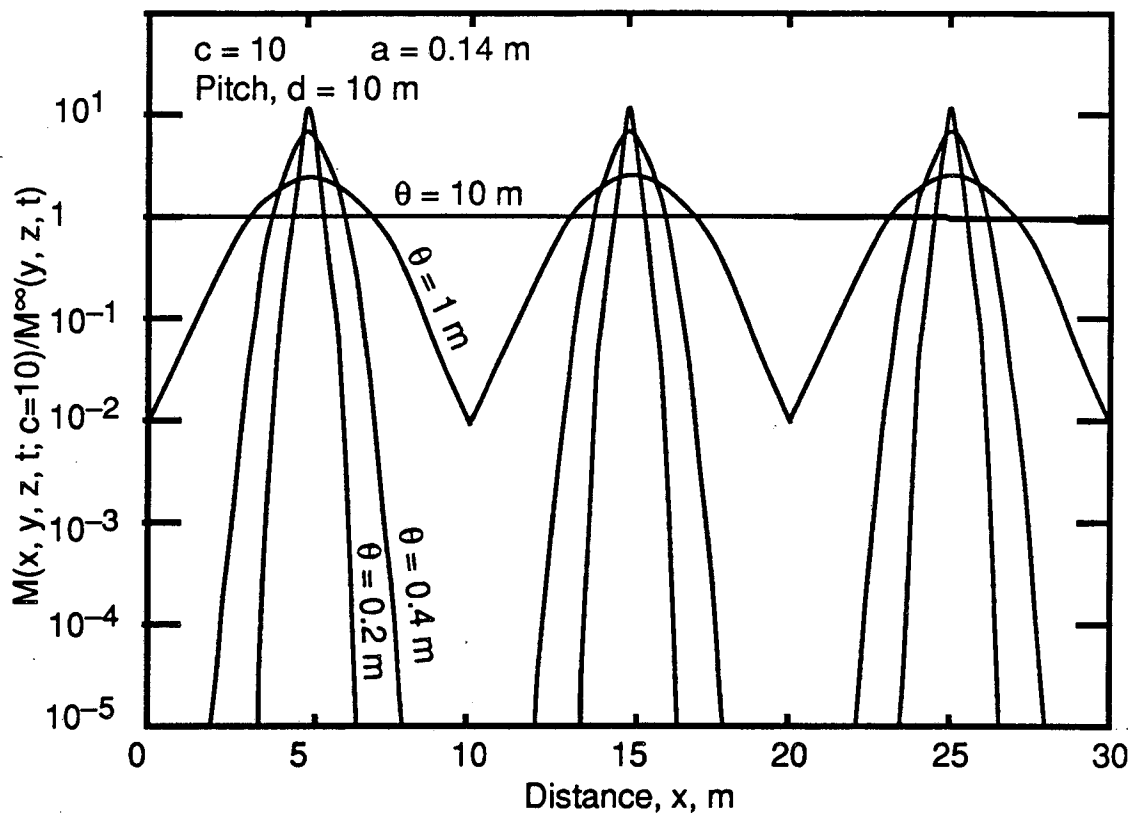


Fig. 2 Normalized Concentrations Along the Transverse Axis, Multiple Areal Sources/Infinite Source

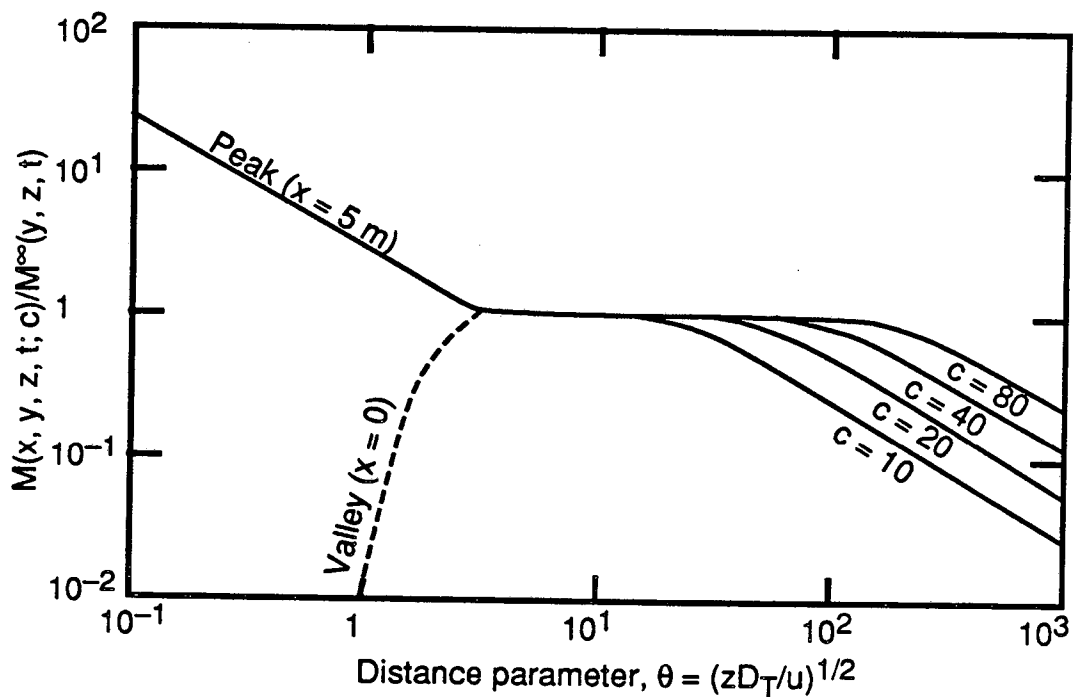


Fig. 3. Normalized Concentrations in the Rock Matrix as a Function of the Distance Parameter and the Number of Areal Sources

The differences between the concentrations fields predicted by the two models are illustrated more clearly in Figure 3. Here the concentration ratio of eq. (20) is plotted against the distance parameter θ , with a constant spacing of areal sources 10 meters apart, the number of areal sources are $c = 10, 20, 40$ and 80 .

Near the areal sources, that is for small values of θ , the plumes are evident and the concentration field for discrete areal sources differs considerably from that for the infinitely long source. The "peaks" are the local plumes, opposite the location of the areal sources and the "valleys" are where the local plumes are absent, opposite the region in between areal sources. However, farther away from the areal sources, $\theta \approx 3$ meters, the plumes from the areal sources have merged completely due to transverse dispersion. At greater distances and until the concentrations ratio becomes less than unity in Figure 3, the simpler, infinite-source model³ predicts the concentration field just as well as the detailed areal-source model. For larger values of θ , when the concentration ratio becomes less than unity, the infinite-source model predicts a concentration that is higher than is accurate but on the conservative side. In this region the concentration field can be predicted accurately by replacing the discrete areal sources with a single finite-area source of equivalent strength and with the same overall dimensions as the array of discrete sources. These observations are independent of contaminant, rock type and time.

Discussion

The numerical implementation of the analytic solutions shows that three regions exist, in terms of the distance parameter $\theta = \sqrt{(zD_T)/u}$. For the parameter values used in this study, at $\theta \leq 3$ meters the detailed multiple-area-source solution should be used to give accurate predictions of the concentration field. For θ between 3 meters to 100 meters, the concentration field predicted by a simpler infinite-line source model is applicable. For θ greater than 100 meters, the simpler infinite-line source model overestimates conservatively and an equivalent single finite-area source will yield the correct concentration field. This is an illustration of the ability of analytic solutions to provide results in a most economical manner, by the use of dimensionless groups.

3. Contaminant Migration from an Array of Sources in Porous Media

Analysis

For contaminant dispersion in porous media, we develop solutions for an array source by superpositioning solutions for individual point sources. For a single point source in an infinite porous medium, the governing equation for the dispersion of a contaminant species is

$$R \frac{\partial N}{\partial t} + \hat{u}_x \frac{\partial N}{\partial x} + \hat{u}_y \frac{\partial N}{\partial y} + \hat{u}_z \frac{\partial N}{\partial z} = \frac{\partial}{\partial x} \hat{D}_x \left(\frac{\partial N}{\partial x} \right) + \frac{\partial}{\partial y} \hat{D}_y \left(\frac{\partial N}{\partial y} \right) + \frac{\partial}{\partial z} \hat{D}_z \left(\frac{\partial N}{\partial z} \right) - \lambda RN, \quad (21)$$

$$x, y, z \in \mathcal{D}_\infty, \quad t > 0;$$

where the Cartesian coordinates are labeled x, y, z , N is the radioactive species concentration, \hat{D}_i the dispersion coefficient in the i^{th} direction, $i = x, y, z$, R is the retardation coefficient of the radioactive species and \mathcal{D}_∞ the unbounded space. Some solutions to this problem, without limit on the velocity field u_x, u_y, u_z , and for radioactive chains of arbitrary lengths, have been obtained by P. L. Chambré.⁴

The solution, for an uniform flow along the z axis of pore velocity of u , is

$$N(x, y, z, t) = \int_0^t \frac{\dot{M}(\tau) e^{-\lambda(t-\tau)}}{\epsilon R (4\pi D(t-\tau))^{3/2}} \exp \left\{ \frac{-1}{4(t-\tau)} \left[\frac{\{z - u(t-\tau)\}^2}{D_z} + \frac{y^2}{D_y} + \frac{x^2}{D_x} \right] \right\} d\tau \quad (22)$$

where $\dot{M}(\tau)$ is the contaminant input rate at time τ

D_i is the normalized dispersion coefficient in the i^{th} direction, $D_i = \hat{D}_i/K, i = x, y, z$

u is the normalized ground-water pore velocity in the z direction, $u = \hat{u}_z/K$

[M/t]

[L²/t]

[L/t]

λ is the species decay constant

[t⁻¹]

ϵ is the porosity

$$D = (D_x D_y D_z)^{1/3}$$

The dispersion coefficients and the ground-water velocity have been normalized by dividing them by the retardation coefficient of the radioactive species.

If the rate of nuclide input is temporally constant, the solution in (22) can be simplified by the substitution of a constant input rate \dot{M} , and integrated to give

$$\begin{aligned}
 N(x, y, z, t) = & \frac{\dot{M} e^{zu/2D_z}}{8\pi\epsilon RD^{3/2} [x^2/D_x + y^2/D_y + z^2/D_z]^{1/2}} \\
 & \times \left[\exp \left(-\sqrt{(x^2/D_x + y^2/D_y + z^2/D_z) \left(\lambda + \frac{u^2}{4D_z} \right)} \right) \right. \\
 & \times \left\{ 2 - \operatorname{erfc} \left(\sqrt{\left(\lambda + \frac{u^2}{4D_z} \right) t} - \sqrt{(x^2/D_x + y^2/D_y + z^2/D_z) \left(\frac{1}{4t} \right)} \right) \right\} \\
 & + \exp \sqrt{(x^2/D_x + y^2/D_y + z^2/D_z) \left(\lambda + \frac{u^2}{4D_z} \right)} \\
 & \times \operatorname{erfc} \left(\sqrt{\left(\lambda + \frac{u^2}{4D_z} \right) t} + \sqrt{(x^2/D_x + y^2/D_y + z^2/D_z) \left(\frac{1}{4t} \right)} \right) \Big]
 \end{aligned} \tag{23}$$

The solution for the contaminant concentration field from an array of point sources can be obtained by superpositioning single point sources. Figure 4 shows a typical planar array of point sources. For an array of $\Gamma \times \Xi \times \Omega$ point sources, the contaminant concentration field resulting from the array is given by

$$\begin{aligned}
 N^a(x, y, z, t) = & \frac{\dot{M}}{8\pi\epsilon RD^{3/2}} \sum_{\gamma=1}^{\Gamma} \sum_{\xi=1}^{\Xi} \sum_{\omega=1}^{\Omega} \exp\{(z - \omega z)u/2D_z\} \left[\frac{(x - \gamma x)^2}{D_x} + \frac{(y - \xi y)^2}{D_y} + \frac{(z - \omega z)^2}{D_z} \right]^{-1/2} \\
 & \times \left[\exp -\sqrt{\left(\frac{(x - \gamma x)^2}{D_x} + \frac{(y - \xi y)^2}{D_y} + \frac{(z - \omega z)^2}{D_z} \right) \left(\lambda + \frac{u^2}{4D_z} \right)} \right. \\
 & \times \left\{ 2 - \operatorname{erfc} \left(\sqrt{\left(\lambda + \frac{u^2}{4D_z} \right) t} - \sqrt{\left(\frac{(x - \gamma x)^2}{D_x} + \frac{(y - \xi y)^2}{D_y} + \frac{(z - \omega z)^2}{D_z} \right) \left(\frac{1}{4t} \right)} \right) \right\} \\
 & + \exp \sqrt{\left(\frac{(x - \gamma x)^2}{D_x} + \frac{(y - \xi y)^2}{D_y} + \frac{(z - \omega z)^2}{D_z} \right) \left(\lambda + \frac{u^2}{4D_z} \right)} \\
 & \times \operatorname{erfc} \left(\sqrt{\left(\lambda + \frac{u^2}{4D_z} \right) t} + \sqrt{\left(\frac{(x - \gamma x)^2}{D_x} + \frac{(y - \xi y)^2}{D_y} + \frac{(z - \omega z)^2}{D_z} \right) \left(\frac{1}{4t} \right)} \right) \Big]
 \end{aligned} \tag{24}$$

where N^a is the concentration from the array source.

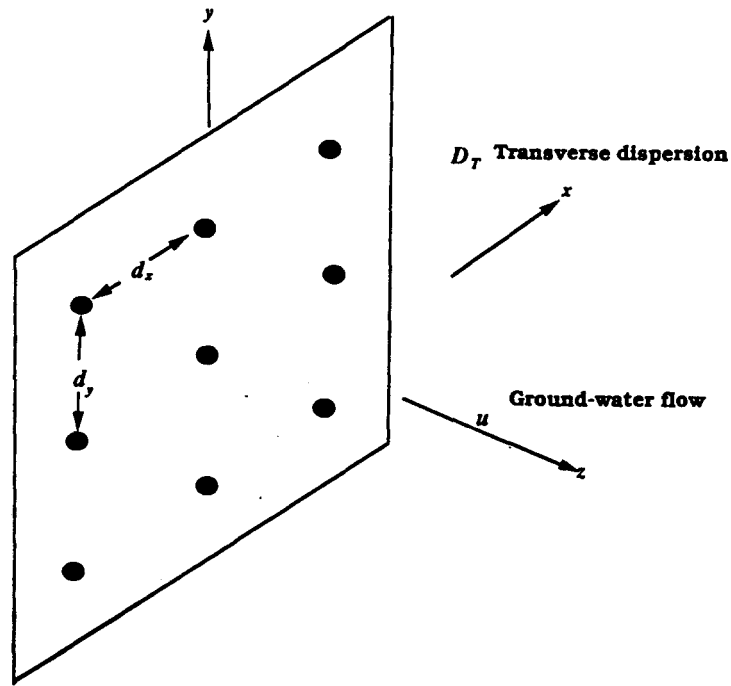


Fig. 4 An Array of Point Sources in Porous Media

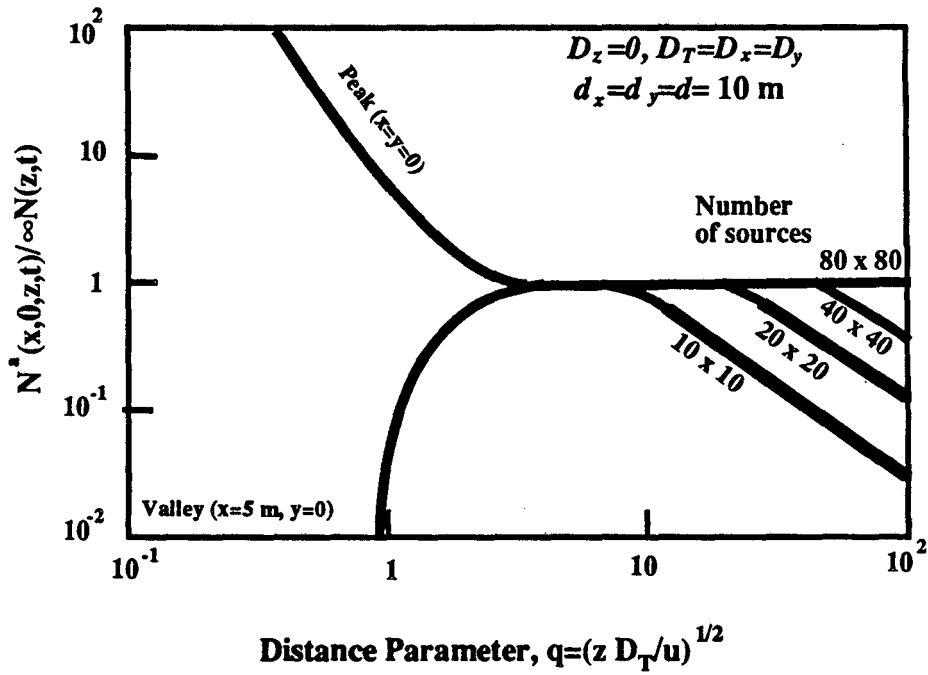


Fig. 5 Steady-State Concentrations, Normalized to that Predicted by an Infinite-Plane Source, as a Function of the Distance Parameter and the Number of Point Sources

The location of the individual point sources in the array is given by

$$\gamma x = d_x \left(\gamma - \frac{\Gamma + 1}{2} \right), \quad \gamma = 1, \dots, \Gamma \quad (25)$$

$$\xi y = d_y \left(\xi - \frac{\Xi + 1}{2} \right), \quad \xi = 1, \dots, \Xi \quad (26)$$

$$\omega z = d_z \left(\omega - \frac{\Omega + 1}{2} \right), \quad \omega = 1, \dots, \Omega \quad (27)$$

where d_x, d_y, d_z are the separations or pitches along the coordinates.

Numerical Illustrations

In Figure 4 we present numerical illustrations for a 3 x 3 planar array of point sources in porous media, perpendicular to the flow of ground water.

In these calculations we assumed

- Each point source is of equal and time-invariant strength.
- The center of the array is at the origin of the axes.
- The constant source strength was derived from a separate model based on solubility-limited dissolution of the contaminant from the source. The details are given in Chambré, *et al.*⁵
- Ground-water velocity is along z only and is constant.
- The dispersion coefficients are constant in space and time. This is not a requirement of the solutions. Actually, in the solutions as stated above, the dispersion coefficients can be functions of velocity, although not of position.

The separations between sources have been chosen arbitrarily as

$$d_y = 3.7 \text{ meters}$$

$$d_x = 36.7 \text{ meters}$$

The other parameter values used in the calculation are

$$D_x = 50 \text{ m}^2/\text{a} \quad D_T = D_x = D_y = 5 \text{ m}^2/\text{a}$$

$$u = 1 \text{ m/a}$$

$$\dot{M} = 0.48 \text{ g/a}$$

$$\lambda = 0$$

$$R = 1$$

$$\epsilon = 0.05$$

In Figure 5 the ordinate is the steady-state contaminant concentration along the z axis predicted for the discrete array sources, normalized to the concentration predicted for an infinite-plane source of the same dissolution rate, plotted as a function of a distance parameter $\theta = \sqrt{zD_T/u}$. When the ratio is unity, the two models give identical predictions. For a value of the distance parameter of approximately ten meters, the ratio is above unity and the detailed array-source model should be used. Beyond this region, the infinite-plane source model either gives identical predictions, or it overestimates, conservatively. Where the concentration ratio becomes less than unity with increasing θ , the concentration field can be accurately predicted by replacing the discrete-source array by an equivalent finite plane source.

4. Comparison

It is instructive to compare the results for contaminant dispersion from an array in porous media with that from multiple areal sources into a planar fracture. Figure 3 and Figure 5 are remarkably similar. It can be seen that for both areal sources releasing contaminants into a planar fracture and for point sources releasing contaminants into porous media the behaviors are similar. Three distinct regions can be identified. In close proximity to the sources, the detailed solutions available can trace the contaminant concentration fields accurately. Very far away from the sources finite equivalent sources provide valid estimations more simply. There is a mid-region where an infinite-source solution provides valid estimation, also with simpler calculations. The common delimiter of these regions is the distance parameter, $\theta = \sqrt{zD_T/u}$ where z is the downstream distance, D_T the transverse dispersion coefficient and u the pore velocity.

The similarity can also be approached analytically. For the point sources, consider a square array of dimension d^2 , i. e. $d_x = 0, d_y = d_x = d$, we can assemble an infinite planar source of equivalent strength. The ratio of contaminant concentration resulting from the array source to the concentration from the infinite plane source is⁵

$$\frac{N^a(x, y, z, t)}{N^\infty(z, t)} = \frac{\epsilon d^2}{4\pi\theta^2} \sum_{\xi=1}^{\Xi} \sum_{\gamma=1}^{\Gamma} \exp \left[-\frac{(x-\gamma x)^2 + (y-\xi y)^2}{4\theta^2} \right] \quad (28)$$

where $N^\infty(z, t)$ is the concentration resulting from the infinite-plane source, and the other terms as defined in (24)-(27). When (28) is compared with (20), there is an obvious similarity. We can re-write (20) as

$$\frac{M(x, y, z, t, c)}{M^\infty(y, z, t)} = \frac{d}{2a\sqrt{\pi}} \sum_{k=1}^c \int_{\beta-\alpha}^{\beta+\alpha} e^{-t^2} dt, \quad \text{where } \beta = \frac{y-\xi y}{2\theta} \text{ and } \alpha = \frac{a}{2\theta} \quad (29)$$

Because the width $2a$ of an areal source is very small compared to the separation d between sources, as θ becomes large we can approximate the integral as

$$\int_{\beta-\alpha}^{\beta+\alpha} e^{-t^2} dt = \frac{a}{\theta} e^{-\beta^2} \quad (30)$$

and now the similarity between (28) and (20) becomes more obvious.

5. Conclusions

We have provided both the mechanics for analyzing multiple sources of contaminants, as well as criterion for valid simplification.

Acknowledgement

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NOTATION

$2a$ is the width of an areal source, [L]

a_p is the pore surface area per unit volume of rock, [L^2 pore surface/ L^3 rock matrix]

$2b$ is the aperture of the fracture, [L]

c is the number of areal sources

d_x, d_y, d_z are the separations or pitches along the coordinates, [L]

$$D = (D_x D_y D_z)^{1/3}$$

\mathcal{D}_∞ is the unbounded space

\hat{D}_i is the dispersion coefficient in the i^{th} direction, $i = x, y, z$

D_i is the normalized dispersion coefficient in the X_i direction, $D_i = \hat{D}_i/K, i = x, y, z, [L^2/t]$

D_p is the species diffusion coefficient in the matrix pore water, [L^2/t]

D_T is the transverse dispersion coefficient, [L^2/t]

K_f is the species distribution coefficient, [(M species/ L^2 fracture wall)/(M species/ L^3 fracture water)]

K_p is a distribution coefficient, [(M species/ L^2 pore surface)/(M species/ L^3 pore water)]

$\dot{M}(\tau)$ is the contaminant input rate at time τ , [M/t]

$M(x, y, z, t)$ is the concentration of the species in the matrix-pore water, [M species/ L^3 pore water]

$N(x, z, t)$ is the species concentration in the fracture water, [M species/ L^3 fracture water]

q is the diffusive flux into the rock matrix, [M/ L^2 -t]

R is the retardation coefficient of the species

R_f is the dimensionless retardation coefficient in the fracture, defined as $R_f = 1 + K_f/b$

R_p is a dimensionless retardation coefficient defined as $R_p = 1 + a_p K_p/\epsilon$

x_k is the location of the center of the k^{th} areal source on the transverse axis x , [L]

x, y, z the Cartesian coordinates

u is the pore velocity in the fracture and the normalized ground-water pore velocity in the z direction,

$$u = \hat{u}_z/K, [L/t]$$

ϵ is the matrix porosity

$\varphi(t)$ is the time-dependent concentration at the surface of an areal source

λ is the species decay constant [t^{-1}]

$\Gamma \times \Xi \times \Omega$ is the point sources array size

$$\theta = \sqrt{z D_T/u}$$

LAWRENCE BERKELEY LABORATORY
TECHNICAL INFORMATION DEPARTMENT
1 CYCLOTRON ROAD
BERKELEY, CALIFORNIA 94720