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Authors
Ahn, J.
Chambre, P.L.
Pigford, T.H.

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Lawrence Berkeley Laboratory
UNIVERSITY OF CALIFORNIA

EARTH SCIENCES DIVISION

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J. Ahn, P. L. Chambré, T. H. Pigford

Earth Sciences Division, Lawrence Berkeley Laboratory

and

Department of Nuclear Engineering, University of California

Berkeley, California 94720

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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, California
94720

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REPORT OUTLINE

NUCLIDE MIGRATION THROUGH A PLANAR FISSURE WITH MATRIX DIFFUSION

1. Introduction and Summary

This report presents the first results of a new analytical study of the hydrological transport of a radioactive contaminant through a planar fracture in porous rock. The purpose is to predict the space-time dependent concentration of the contaminant in the groundwater, as affected by advective transport within the fracture and by molecular diffusion of the contaminant into and out of pores that intersect the fracture surfaces.

Previous analytical solutions of this problem have neglected dispersion and sorption within the fractures[1] or have presented results with untested approximations[1]. In the present report we formulate the transport problem for a sorbing radioactive contaminant with no decay precursors, assuming an exponentially decaying step and band functions source at the boundary.

Analytical solutions are obtained for zero-dispersion and non-zero dispersion in the fracture, and are compared with the solution for the one-dimensional transport through porous media. As the fracture retardation coefficient or the fracture width increases, or as the porosity of the rock matrix surrounding the fracture or the pore diffusion coefficient decreases, concentration profiles in the fracture approach those for the one-dimensional transport through porous media. A criterion for using porous media solutions instead of fractured media solutions is obtained by studies of numerical results.

Solutions for dispersive transport are also compared numerically with those for non-dispersive transport. The differences between the quantities calculated for non-zero fracture dispersion and for zero fracture dispersion become observable when a criterion is satisfied by the ratio, $\omega \equiv \frac{(v/R_f)^2}{2(D/R_f)} = \frac{v^2}{2DR_f}$

where v/R_f represents the contaminant velocity in the fracture and D/R_f the fracture dispersion coefficient divided by the fracture retardation coefficient, R_f. If ω becomes greater than some value, which is obtained by numerical results, the differences between these two cases become negligible, and one can use the zero dispersion solution with reasonable accuracy.

Future studies will be extended to include the effects of neighboring fractures, other source boundary conditions, and the effects of radioactive decay of migrating decay precursors.

2. Single Fissure Surrounded by Infinite Matrix, No Dispersion

2.1 Formulation of the Problem, Assumptions

Consider a rock matrix containing planar fissures extending in the z direction. Here the fissures are assumed to be parallel and widely separated, so that each fissure can be assumed to be surrounded by infinite porous rock. Within the fissure ground water flows at a constant velocity v in the z direction, but the water in the micropores in the rock is assumed to be at rest. The contaminant source at z = 0 is assumed to be uniformly distributed over the breadth of the fissure (normal to z). We seek to calculate:

a. the contaminant concentration N(z,t) in the water in the fissure at distance z along the fissure and at time t,

b. the contaminant concentration M(y,z,t) in water in the rock pores, at a distance y into the pore from the fissure surface,

c. the advective mass flux J(z,t) of the contaminant at position z in the fissure, and

d. the time-dependent cumulative release of the contaminant across a plane at z, and normal to z, in the fissure.

The concentration N(z,t) is the concentration averaged across the fissure thickness, and the concentration M(y,z,t) is averaged across the pore cross section. For the purpose of the first analysis, dispersion within the fissure is neglected. Additional assumptions are:

a. the contaminant source yields a specified exponentially decaying boundary concentration at z = 0, beginning step-wise at t = 0,

b. there is no decay precursor of the contaminant in the ground water.

c. the contaminant sorbs on the fissure walls and within the pores, and

d. sorption is governed by linear sorption isotherms.

2.2 Governing Equations

The transport terms and geometry are shown in Figure 2.1. Here, for completeness, dispersive transport is included. It will be later set equal to zero for the first analytical solutions. The terms that enter into the conservation equations, expressed as amount per unit time per unit area of fissure surface, are:

A. contaminant entering the control volume

$bvN(z)dt$ by convection

$-bD \frac{\partial N}{\partial z}\Big|_{z=z} dt$ by dispersion

B. contaminant leaving the control volume by fissure-water transport

$bvN(z+dz)dt = bv(N(z)+dN)dt$ by convection

$-bD \frac{\partial N}{\partial z}\Big|_{z=z+dz} dt = -bD\left(\frac{\partial N}{\partial z}\Big|_{z=z} + d(\frac{\partial N}{\partial z})\right) dt$ by dispersion

C. contaminant sorbed on the fissure surface

$\dot{r}_f dzdt$

D. contaminant diffusing into the rock pores

$qdzdt$

E. contaminant undergoing radioactive decay within the control volume

$\lambda N(z)bdzdt$

where

$N(z,t)$ = concentration of the radioactive contaminant in fissure water, kg/m^3

λ = radioactive decay constant, yr^{-1}

q = rate of diffusion from the fissure into pores, per unit area of fissure surface, kg/m^2yr

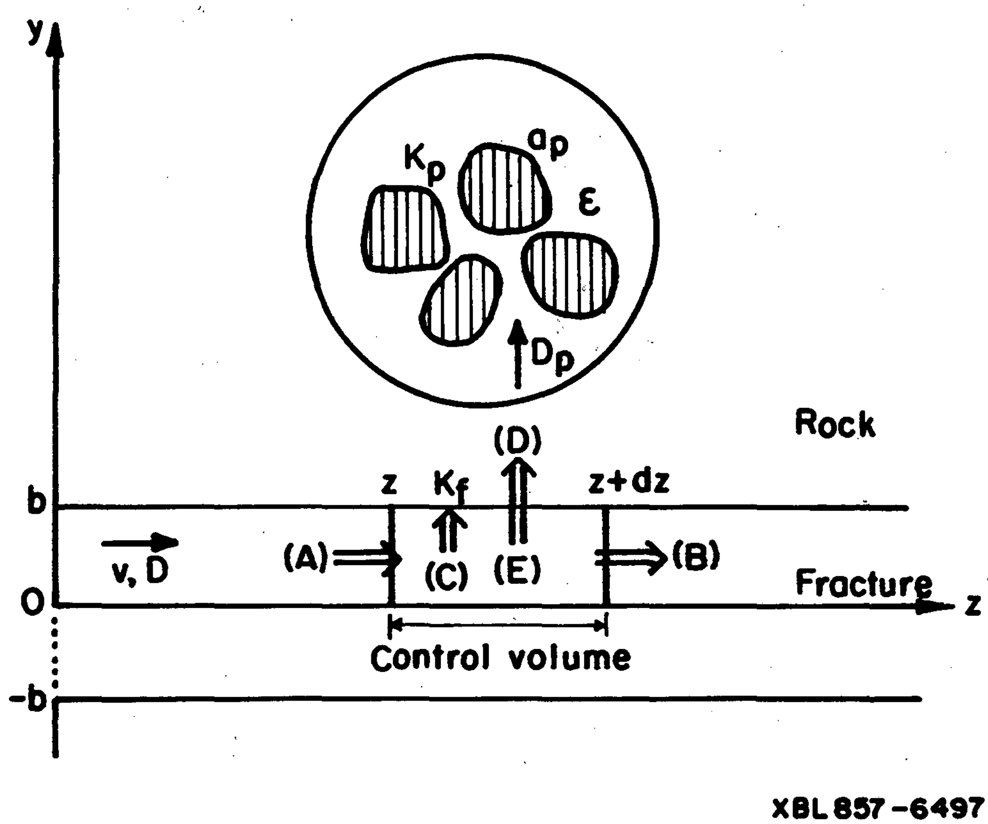

Fig. 2.1 A discrete fracture surrounded by a semi-infinite rock matrix. Quantities (A) - (E) are explained in the text.

$\dot{r}_f$ = rate of sorption from the fissure onto fissure surface, kg/m^2yr

b = half width of fissure, m

v = water velocity averaged across the fissure width, m/yr

D = coefficient for dispersive transport in fissure water, m^2/yr.

A mass balance on the control volume yields:

$$bdzdN = \left(bvNdt - bD\frac{\partial N}{\partial z}dt\right) - \left(bvNdt + bvdNdt\right.$$

$$\left. - bD\frac{\partial N}{\partial z}dt - bDd(\frac{\partial N}{\partial z})dt\right) + \dot{r}_f dzdt + qdzdt + \lambda Nbdzdt,$$

and so

$$\frac{\partial N}{\partial t} + v\frac{\partial N}{\partial z} - D\frac{\partial^2 N}{\partial z^2} + \lambda N + \frac{q}{b} + \frac{\dot{r}_f}{b} = 0. \tag{2.1}$$

Denoting the concentration of sorbed contaminant on the fissure surfaces as $N_s(z,t)$ (kg per m^2 of surface), and neglecting surface diffusion, the following rate equation applies:

$$\frac{\partial N_s}{\partial t} + \lambda Ns - \dot{r}_f = 0. \tag{2.2}$$

Assuming a linear sorption isotherm:

$$N_s(a,t) = K_f N(z,t), \tag{2.3}$$

where K_f is the sorption distribution coefficient for the fissure surface (m). Substituting (2.3) into (2.2), we obtain:

$$K_f\frac{\partial N}{\partial t} + \lambda K_f N - \dot{r}_f = 0, \tag{2.4}$$

and combining (2.4) and (2.1) yields:

$$R_f\frac{\partial N}{\partial t} + v\frac{\partial N}{\partial z} - D\frac{\partial^2 N}{\partial z^2} + R_f\lambda N + \frac{q}{b} = 0, \tag{2.5}$$

where R_f is the retardation coefficient for fissure transport:

$$R_f = 1 + \frac{K_f}{b}. \tag{2.6}$$

On the other hand, the governing equations for nuclides in the rock pores can be expressed by considering one-dimensional molecular diffusion in pore water, radioactive decay and sorption from pore water to pore surface and neglecting surface diffusion,

$$\varepsilon \frac{\partial M}{\partial t} - \varepsilon D_p \frac{\partial^2 M}{\partial y^2} + \varepsilon\lambda M + a_p \dot{r}_p = 0\,, \tag{2.7}$$

and

$$a_p \frac{\partial M_s}{\partial t} + a_p \lambda M_s - a_p \dot{r}_p = 0\,, \tag{2.8}$$

where (2.7) is for the water phase and (2.8) is for the sorbed contaminant on pore surfaces, and where

$M(y,z,t)$ = concentration of the radioactive contaminant in pore water, kg/m^3

$M_s(y,z,t)$ = concentration of sorbed contaminant on the pore surfaces, kg/m^2 of pore surface

ε = porosity of rock excluding the pores which are not connected to the fissure

a_p = pore surface area per unit volume of rock matrix, m^2 of surface/m^3 of rock

D_p = diffusion coefficient of contaminant in pores, m^2/yr

$\dot{r}_p$ = rate of sorption from pore water onto pore surfaces, $kg/m^2\ yr$.

Assuming a linear sorption isotherm:

$$M_s(y,z,t) = K_p M(y,z,t)\,, \tag{2.9}$$

where K_p is the sorption distribution coefficient for the pore surface (m). By (2.7), (2.8) and (2.9), we obtain

$$R_p \frac{\partial M}{\partial t} - D_p \frac{\partial^2 M}{\partial y^2} + R_p \lambda M = 0\,, \tag{2.10}$$

where R_p is the retardation coefficient for rock pore transport:

$$R_p = 1 + \frac{a_p}{\varepsilon} K_p . \tag{2.11}$$

By using the quantity, $M(y,z,t)$, we can evaluate the quantity, q, in (2.3) as follows:

$$q = - \varepsilon D_p \frac{\partial M}{\partial y} \bigg|_{y=b} . \tag{2.12}$$

2.3 <u>Analytical Solutions for No Dispersion</u>

By setting $D = 0$ in (2.5) we have the following governing equations for the case with no dispersion in the fracture:

$$R_f \frac{\partial N}{\partial t} + v \frac{\partial N}{\partial z} + R_f \lambda N + \frac{q}{b} = 0, \; t > 0, \; z > 0, \tag{2.13}$$

and

$$R_p \frac{\partial M}{\partial t} - D_p \frac{\partial^2 M}{\partial y^2} + R_p \lambda M = 0, \; t > 0, \; y > b, \; z > 0, \tag{2.10}$$

where

$$q = - \varepsilon D_p \frac{\partial M}{\partial y} \bigg|_{y=b}, \quad t > 0, \; z > 0, \tag{2.12}$$

$$R_f = 1 + \frac{K_f}{b} , \text{ and} \tag{2.6}$$

$$R_p = 1 + \frac{a_p}{\varepsilon} K_p . \tag{2.11}$$

The initial and boundary conditions are

$N(z,0) = 0,$	$z > 0$	(2.14a)
$M(y,z,0) = 0,$	$z > 0, \; y > b$	(2.14b)
$N(0,t) = \psi(t)$	$t > 0$	(2.14c)
$N(\infty,t) = 0,$	$t > 0$	(2.14d)
$M(b,z,t) = N(z,t),$	$t > 0, \; z > 0$	(2.14e)
$M(\infty,z,t) = 0,$	$t > 0, \; z > 0 .$	(2.14f)

We will first derive the solutions for a general release mode, $\psi(t)$, where $\psi(t)$ is any integrable function. By Laplace transformation of (2.10) we obtain

$$p\tilde{M} = \frac{D_p}{R_p} \frac{d^2\tilde{M}}{dy^2} - \lambda \tilde{M} , \tag{2.15}$$

where

$$\tilde{M}(y,z,p) \equiv \int_0^\infty e^{-pt} M(y,z,t) \, dt . \tag{2.16}$$

The solution which is physically admissible is

$$\tilde{M}(y,z,p) = c_1 \exp \{ -B(y-b) \sqrt{p+\lambda} \}, \tag{2.17}$$

where c_1 constant

$$B \equiv \sqrt{\frac{R_p}{D_p}} \quad , \; yr^{\frac{1}{2}}/m . \tag{2.18}$$

By Laplace transformation of the boundary condition (2.14e), we obtain

$$\tilde{M}(b,z,p) = \tilde{N}(z,p) = c_1 .$$

Therefore, (2.17) becomes

$$\tilde{M}(y,z,p) = \tilde{N}(z,p) \exp \{ - B(y-b) \sqrt{p+\lambda} \} . \tag{2.19}$$

From this, one can calculate the Laplace-transformed q as

$$\begin{aligned} \tilde{q} &= -\varepsilon D_p \frac{d\tilde{M}}{dy} \Bigg|_{y=b} \\ &= \varepsilon D_p B \sqrt{p+\lambda} \;\; \tilde{N}(z,p) . \end{aligned} \tag{2.20}$$

By Laplace transform of (2.13), we obtain

$$p\tilde{N} + \frac{v}{R_f} \frac{d\tilde{N}}{dz} + \lambda\tilde{N} + \frac{\tilde{q}}{b} = 0 . \tag{2.21}$$

On substitution of (2.20) into (2.21), we have

$$\frac{d\tilde{N}}{dz} + \frac{R_f}{v} \left(p + \lambda + \frac{\sqrt{p+\lambda}}{A} \right) \tilde{N} = 0 , \tag{2.22}$$

where

$$A \equiv \frac{bR_f}{\varepsilon\sqrt{D_pR_p}} \text{ , } yr^{\frac{1}{2}} \text{ .} \tag{2.23}$$

Then eq. (2.22) can be solved with respect to z;

$$\tilde{N}(z,p) = \tilde{\psi}(p)\exp\left\{-\frac{R_f}{v}(p+\lambda+\frac{1}{A}\sqrt{p+\lambda}\ )\,z\right\}, \tag{2.24}$$

using the Laplace-transformed boundary conditions:

$$\tilde{N}(o,p) = \tilde{\psi}(p), \tag{2.25}$$

$$\tilde{N}(\infty,p) = 0, \tag{2.26}$$

and

$$\tilde{\psi}(p) \equiv \int_o^\infty e^{-pt}\psi(t)dt. \tag{2.27}$$

Next we make the inverse transformation:

$$N(z,t) = e^{-\lambda ZA}\ L^{-1}\left[e^{-ZA\cdot p}e^{-Z\sqrt{p+\lambda}}\ \tilde{\psi}(p)\right] \tag{2.28}$$

where $Z \equiv \frac{R_f z}{vA}$, $yr^{\frac{1}{2}}$, and L^{-1} [ ] stands for inverse Laplace Transform. (2.29)

Making use of the formula,

$$L^{-1}\left[\tilde{\Phi}(p)e^{-pE}\right] = \Phi(t-E)h(t-E),\ E > 0 \tag{2.30}$$

where h(t) is Heaviside step function, (2.28) becomes

$$N(z,t) = e^{-\lambda ZA}\ h(t-ZA)L^{-1}[\tilde{\psi}(p)\exp\,(-Z\sqrt{p+\lambda}\ )]_{\ t\to t-ZA} \tag{2.31}$$

where the remaining inverse transform can be made by using the convolution rule:

$$L^{-1}\left[\tilde{\psi}(p)e^{-Z\sqrt{p+\lambda}}\right] = \int_o^t \psi(t-t')\ \frac{Z}{2\sqrt{\pi t'^3}}\ e^{-\frac{Z^2}{4t'} - \lambda t'}dt'. \tag{2.32}$$

Substituting (2.32) into (2.31) gives the analytical solution for N(z,t):

$$N(z,t) = e^{-\lambda ZA}\, h(t-ZA) \int_0^{t-ZA} \psi(t-ZA-t') \frac{Z}{2\sqrt{\pi t'^3}}\, e^{-\lambda t' - \frac{Z^2}{4t'}}\, dt',$$

$$t \geq 0,\ z \geq 0. \qquad (2.33)$$

By (2.24) and (2.19),

$$\tilde{M}(y,z,p) = \tilde{\psi}(p) e^{-\lambda ZA} \exp(-pZA) \exp\{-(Z+B(y-b))\sqrt{p+\lambda}\}. \qquad (2.34)$$

By a derivation similar to that for N(z,t), we obtain the analytical solution for M(y,z,t):

$$M(y,z,t) = e^{-\lambda ZA} h(t-ZA) \int_0^{t-ZA} \psi(t-ZA-t') \frac{Z'}{2\sqrt{\pi t'^3}}\, e^{-\lambda t' - \frac{Z'^2}{4t'}}\, dt'$$

$$t \geq 0,\ y \geq b,\ z \geq 0 \qquad (2.35)$$

where $Z' \equiv Z + B(y-b)$. (2.36)

The advective mass flux at position z in the fracture is defined as

$$J(z,t) \equiv vN(z,t) - D\frac{\partial N}{\partial z},\ t > 0,\ z > 0. \qquad (2.37)$$

By setting D = 0,

$$J(z,t) = vN(z,t),\ t \geq 0,\ z \geq 0. \qquad (2.38)$$

Finally, the time-dependent cumulative release across a plane at z in the fracture can be written as

$$\int_0^t J(z,t')\, dt' = ve^{-\lambda ZA} h(t-ZA) \int_0^{t-ZA} \int_0^{t-ZA-t'} \psi(\tau) d\tau \frac{Z}{2\sqrt{\pi t'^3}}\, e^{-\frac{Z^2}{4t'} - \lambda t'}\, dt',$$

$$t \geq 0,\ z \geq 0. \qquad (2.39)$$

For a step release,

$$\psi(t) = N^o h(t) e^{-\lambda t} \qquad (2.40)$$

the solutions are obtained by substituting (2.40) into (2.33), (2.35), (2.38) and (2.39):

$$\frac{N}{N^o} = F_1(z,t),\ t \geq 0,\ z \geq 0 \qquad (2.41)$$

$$\frac{M}{N^o} = F_2(y,z,t), \; t \geq 0, \; y \geq b, \; z \geq 0 \tag{2.42}$$

$$\frac{J}{N^o} = vF_1(z,t), \; t \geq 0, \; z \geq 0 \tag{2.43}$$

$$\int_o^t \frac{J(z,t')}{N^o} dt' = F_3(z,t), \; t \geq 0, \; z \geq 0 \tag{2.44}$$

where

$$F_1(z,t) = h(t-ZA)\; e^{-\lambda t} \text{erfc}\left(\frac{Z}{2\sqrt{t-ZA}}\right) \tag{2.45}$$

$$F_2(y,z,t) = h(t-ZA)\; e^{-\lambda t}\; \text{erfc}\left(\frac{Z+B(y-b)}{2\sqrt{t-ZA}}\right) \tag{2.46}$$

$$F_3(z,t) = \frac{v}{\lambda} h(t-ZA) \left[e^{-\lambda ZA} \cdot \frac{1}{2} \left\{ e^{\sqrt{\lambda}Z}\; \text{erfc}\left(\frac{Z}{2\sqrt{t-ZA}} + \sqrt{\lambda(t-ZA)}\right) + e^{-\sqrt{\lambda}Z} \text{erfc}\left(\frac{Z}{2\sqrt{t-ZA}} - \sqrt{\lambda(t-ZA)}\right)\right\} - e^{-\lambda t} \text{erfc}\left(\frac{Z}{2\sqrt{t-ZA}}\right)\right] \tag{2.47}$$

and N^o is the initial concentration of the contaminant at $z = 0$.

For a band release,

$$\psi(t) = N^o e^{-\lambda t}\; \{h(t) - h(t-T)\}, \tag{2.48}$$

the solutions are obtained by the superposition method:

$$\frac{N}{N^o} = F_1(z,t) - e^{-\lambda T} F_1(z,t-T), \; t \geq 0, \; z \geq 0 \tag{2.49}$$

$$\frac{M}{N^o} = F_2(y,z,t) - e^{-\lambda T} F_2(y,z,t-T), \; t \geq 0, \; y \geq b, \; z \geq 0 \tag{2.50}$$

$$\frac{J}{N^o} = v \left\{ F_1(z,t) - e^{-\lambda T} F_1(z,t-T) \right\}, \; t \geq 0, \; z \geq 0 \tag{2.51}$$

$$\int_o^t \frac{J(z,t')}{N^o}\, dt' = F_3(z,t) - e^{-\lambda T} F_3(z,t-T), \; t \geq 0, \; z \geq 0 \tag{2.52}$$

where T is the leach time.

2.4 Computer Code

2.4.1 Quantities Calculated

The following quantities can be calculated by FIS003 for the step release and by FIS007 for the band release:

a. the relative concentration, N/N^o, in fracture water, given by (2.41) or (2.49),

b. the relative concentration, M/N^o, in pore water in the surrounding rock, given by (2.42) or (2.50),

c. the normalized advective mass flux, J/N^o, in the fracture, given by (2.43) or (2.51), and

d. the normalized time-dependent cumulative release, $\int_o^t J/N^o dt'$, given by (2.44) or (2.52).

N/N^o is computed by the same subroutine for M/N^o by setting y=b, because (2.41) or (2.49) is a subcase of (2.42) or (2.50), respectively.

2.4.2 Algorithm

See Figure 2.2.

2.4.3 Input Data Format

See Table 2.1.

2.4.4 Parameter Ranges for Calculation

All the four quantities can be calculated for any (y,z,t) or (z,t) with reasonable accuracy.

3. Single Fissure Surrounded by Infinite Matrix, with Dispersion

3.1 Formulation of the Problem, Assumptions

The problem and assumptions are the same as stated in Section 2.1 except that dispersive transport in the fissure along the direction of z is now considered.

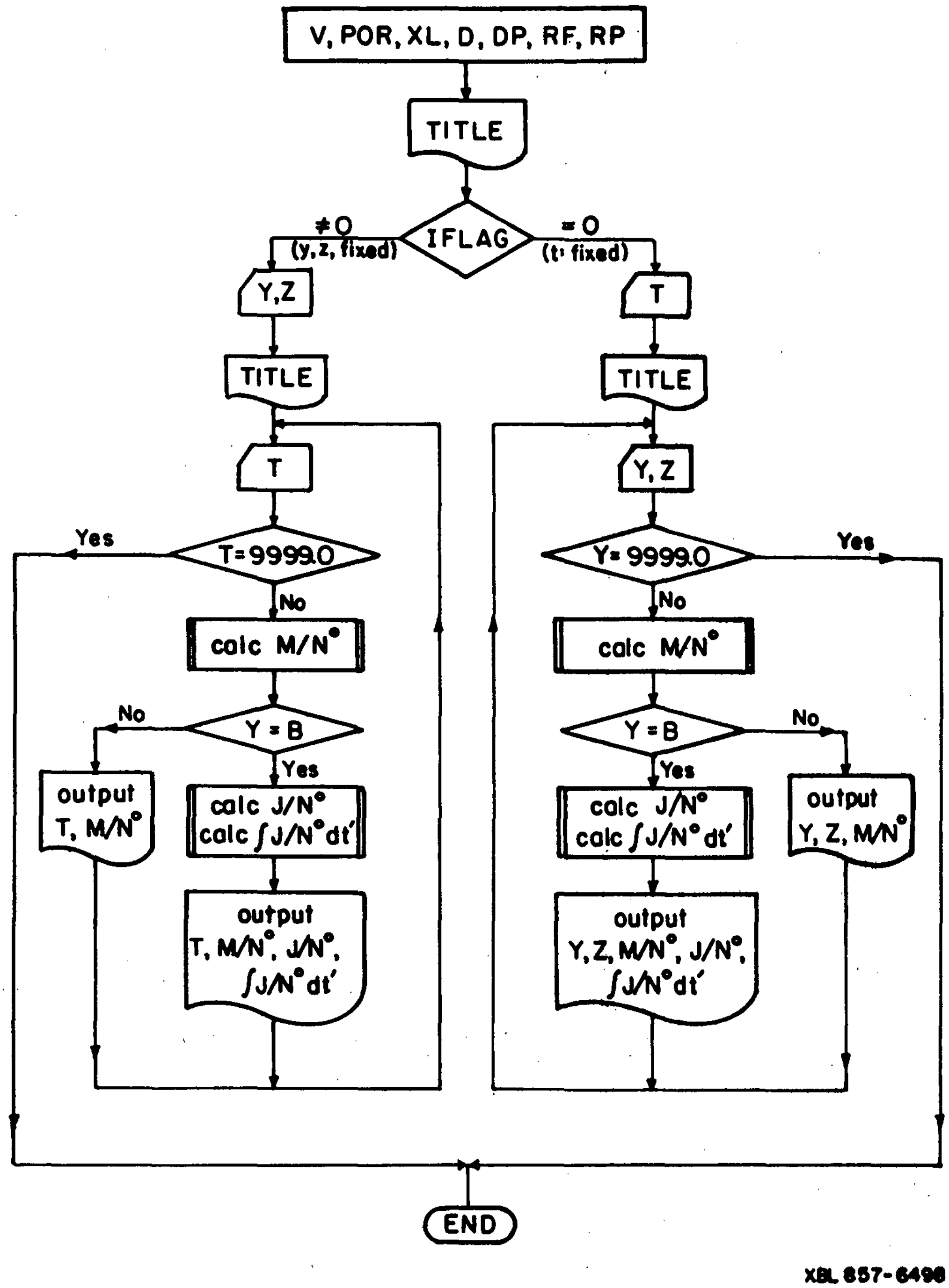

Fig. 2.2 Algorithm of the computer codes.

Table 2.1 Input Data Format

(a) For fixed time

	parameter	name in the codes	Format
1.	velocity	V	E10.3
2.	porosity	POR	E10.3
3.	half width of fracture	B	E10.3
4.	decay constant	XL	E10.3
5.	leach time(*)	TLEA	E10.3
6.	dispersion coeff.	D(**), DP	2E10.3
7.	retardation coeff.	RF, RP	2E10.3
8.		IFLAG(***)	I2
9.	time	T	E10.3
10.	location	Y,Z	2E10.3
	|		|
	|		|
	EOF		9.999E+3, 9.999E+3(****)

(b) For fixed location

	parameter	name in the codes	Format
1.	velocity	V	E10.3
2.	porosity	POR	E10.3
3.	half width of fracture	B	E10.3
4.	decay constant	XL	E10.3
5.	leach time(*)	TLEA	E10.3
6.	dispersion coeff.	D(**), DP	2E10.3
7.	retardation coeff.	RF, RP	2E10.3
8.		IFLAG(***)	I2
9.	location	Y,Z	2E10.3
10.	time	T	E10.3
	|		|
	|		|
	EOF		9.999E+3(****)

(*) only for the band release (FIS007, FIS017)
(**) must be input zero for zero dispersion (FIS003, FIS007)
(***) for fixed time, input 0; for fixed location, input 1.
(****) end-of-data mark.

3.2 Governing Equations

The complete derivation is shown in Section 2.2, but for further reference, we repeat the governing equations:

$$R_f \frac{\partial N}{\partial t} + v \frac{\partial N}{\partial z} - D \frac{\partial^2 N}{\partial z^2} + R_f \lambda N + \frac{q}{b} = 0, \; t > 0, \; z > 0 \tag{3.1}$$

$$R_p \frac{\partial M}{\partial t} - D_p \frac{\partial^2 M}{\partial y^2} + R_p \lambda M = 0, \; t > 0, \; y > b, \; z > 0 \tag{3.2}$$

with

$$R_f = 1 + \frac{K_f}{b} \tag{3.3}$$

$$R_p = 1 + \frac{a_p}{\varepsilon} K_p \tag{3.4}$$

$$q = - \varepsilon D_p \frac{\partial M}{\partial y}\bigg|_{y=b} , \; t > 0, \; z > 0 \tag{3.5}$$

and

$$J(z,t) \equiv vN(z,t) - D \frac{\partial N}{\partial z} , \; t > 0, \; z > 0 \tag{3.6}$$

subject to the same initial and boundary conditions as (2.14a) to (2.14f).

3.3 Analytical Solutions for Non-Zero Dispersion

First, we will solve these governing equations for the general release mode, $\psi(t)$, and then substitute (2.40) into those general solutions.

By Laplace transform of (3.2), we obtain the same equation as (2.15), and so we have, for $\tilde{M}(y,z,p)$,

$$\tilde{M}(y,z,p) = \tilde{N}(z,p) \exp \{- B(y-b) \sqrt{p+\lambda} \} \tag{3.7}$$

and for $\tilde{q}$,

$$\tilde{q} = \varepsilon D_p B \sqrt{p+\lambda} \; \tilde{N}(z,p), \tag{3.8}$$

both of which are obtained by the same derivation through (2.15) to (2.20). By Laplace transform of (3.1) and substitution of (3.8), we obtain

$$\frac{d^2\tilde{N}}{dz^2} - \frac{v}{D} \frac{d\tilde{N}}{dz} - \frac{R_f}{D} (p+\lambda+ \frac{1}{A} \sqrt{p+\lambda}) \tilde{N} = 0, \; z > 0. \tag{3.9}$$

The solution of (3.9) is generally expressed as

$$\tilde{N}(z,p) = C_2(p)e^{zr^+} + C_3(p)e^{zr^-} \tag{3.10}$$

where $C_2(p)$ and $C_3(p)$ are constants,

$$r^{\pm} \equiv \nu \left[1 \pm \left\{1+\beta^2(p+\lambda+ \frac{1}{A}\sqrt{p+\lambda}\ )\right\}^{\frac{1}{2}}\right] , \tag{3.11}$$

$$\nu \equiv v/2D \text{ and} \tag{3.12}$$

$$\beta^2 = \frac{4R_fD}{v^2} . \tag{3.13}$$

$C_2(p)$ and $C_3(p)$ are to be determined by the boundary conditions. $r^{\pm}$, ν, β^2 and A have been used for short-hand notation.

The Laplace transforms of the boundary conditions yield

$$\tilde{N}(0,p) = \tilde{\psi}(p) \qquad \therefore \quad C_2(p) + C_3cp) = \tilde{\psi}(p) \tag{3.14}$$

$$\tilde{N}(\infty,p) = 0 \qquad \therefore \quad C_2(p) = 0 . \tag{3.15}$$

Therefore, (3.10) can be written as

$$\tilde{N}(z,p) = \tilde{\psi}(p)e^{\nu z}\exp\left[-\nu z\left\{1+\beta^2\left(p+\lambda+ \frac{1}{A}\sqrt{p+\lambda}\right)\right\}^{\frac{1}{2}}\right] . \tag{3.16}$$

In order to avoid the difficulty of the double square root in (3.16), we apply the formula:

$$\int_0^{\infty} e^{-\xi^2 - \frac{X^2}{\xi^2}} d\xi = \frac{\sqrt{\pi}}{2} e^{-2X}, \ X > 0. \tag{3.17}$$

Then, (3.16) becomes

$$\tilde{N}(z,p) = \tilde{\psi}(p)e^{\nu z} \frac{2}{\sqrt{\pi}} \int_0^{\infty} e^{-\xi^2 - \frac{\nu^2 z^2}{4\xi^2}} \exp\left[-Y\sqrt{p+\lambda} - YA(p+\lambda)\right] d\xi \tag{3.18}$$

where

$$Y \equiv \frac{\nu^2\beta^2z^2}{4A\xi^2}. \tag{3.19}$$

Now we obtain the inverse Laplace transforms of (3.18):

$$N(z,t) = \frac{2}{\sqrt{\pi}} e^{\nu z} \int_0^{\infty} e^{-\xi^2 - \frac{\nu^2 z^2}{4\xi^2}} L^{-1}\left[\tilde{\psi}(p) e^{-Y\sqrt{p+\lambda}} e^{-YA(p+\lambda)} \right] d\xi. \tag{3.20}$$

Using the formulae:

$$L^{-1}\left[\tilde{\Phi}(p) e^{-pE} \right] = \Phi(t-E)h(t-E), \; E > 0 \tag{3.21}$$

and

$$L^{-1}\left[e^{-Y\sqrt{p+\lambda}} \right] = \frac{Y}{2\sqrt{\pi t^3}} e^{-\lambda t - \frac{Y^2}{4t}}, \tag{3.22}$$

we obtain the following as the solution to N(z,t) for the general release mode, $\psi(t)$:

$$N(z,t) = \frac{1}{\pi} e^{\nu z} \int_0^{\infty} e^{-\xi^2 - \frac{\nu^2 z^2}{4\xi^2}} e^{-\lambda YA} h(t-YA)Y$$

$$\cdot \int_0^{t-YA} \psi(t-YA-t') \frac{1}{\sqrt{t'^3}} e^{-\frac{Y^2}{4t'} - \lambda t'} dt' d\xi, \; t \geq 0, \; z \geq 0 \tag{3.23}$$

Substituting (3.18) into (3.7) yields

$$\tilde{M}(y,z,p) = \tilde{\psi}(p) e^{\nu z} \frac{2}{\sqrt{\pi}} \int_0^{\infty} e^{-\xi^2 - \frac{\nu^2 z^2}{4\xi^2}} \exp\{-Y'\sqrt{p+\lambda} - YA(p+\lambda)\} d\xi \tag{3.24}$$

where

$$Y' = Y + B(y-b). \tag{3.25}$$

Now we can obtain the inverse Laplace transform of (3.24) as the solution to M(y,z,t) for the general release mode, $\psi(t)$:

$$M(y,z,t) = \frac{1}{\pi} e^{\nu z} \int_0^{\infty} e^{-\xi^2 - \frac{\nu^2 z^2}{4\xi^2}} e^{-\lambda YA} h(t-YA) Y' \int_0^{t-YA} \psi(t-YA-t')$$

$$\cdot \frac{1}{\sqrt{t'^3}} e^{-\frac{Y'^2}{4t'} - \lambda t'} dt' d\xi, \; t \geq 0, \; y \geq b, \; z \geq 0. \tag{3.26}$$

In order to calculate J(z,t), we need $\frac{\partial N}{\partial z}$. Differentiating (3.18) with respect to z yields

$$\frac{\partial \tilde{N}}{\partial z} = \frac{2}{\sqrt{\pi}} \quad e^{\nu z}\left\{\int_o^\infty\left(\nu - \frac{\nu^2 z}{2\xi^2}\right) f(\xi;z) \ g \ (\xi,p;z)d\xi\right.$$

$$-\int_o^\infty \frac{\nu^2\beta^2 z}{2\xi^2 A} \ f(\xi;z) \ \sqrt{p+\lambda} \ g(\xi,p;z)d\xi$$

$$\left.-\int_o^\infty \frac{\nu^2\beta^2 z}{2\xi^2} \ f(\xi;z)(p+\lambda)g(\xi,p;z)d\xi\right\} \tag{3.27}$$

where

$$f(\xi;z) \equiv \exp\left(-\xi^2 - \frac{\nu^2 z^2}{4\xi^2}\right) \tag{3.28}$$

and

$$g(\xi,p;z) \equiv \tilde{\psi}(p) \ \exp \ [- \ \{\sqrt{p+\lambda} + A \ (p+\lambda)\}Y] \tag{3.29}$$

were used for short hand notation.

Now we will obtain the inverse Laplace transform of (3.27). Let

$$K_1 \equiv L^{-1}[g(\xi,p;z)] \tag{3.30}$$

$$K_2 \equiv L^{-1}[\sqrt{p+\lambda} \ \ g(\xi,p;z)], \text{ and} \tag{3.31}$$

$$K_3 \equiv L^{-1}[(p+\lambda)g(\xi,p;z)]. \tag{3.32}$$

K_1 can be obtained in the same way as (3.20) to (3.23), so that

$$K_1 = h(t-YA) \ e^{-\lambda YA} \int_o^{t-YA} \psi(t-YA-t') \ \frac{Y}{2\sqrt{\pi t'^3}} \ e^{-\frac{Y^2}{4t'} - \lambda t'} \ dt'. \tag{3.33}$$

Noticing that

$$L^{-1}\left[\sqrt{p} \ e^{-Y\sqrt{p}}\right] = \frac{e^{-\frac{Y^2}{4t}}}{4\sqrt{\pi t^3}} \quad H_2 \ \left(\frac{Y}{2\sqrt{t}}\right) \tag{3.34}$$

where

$$H_2 \ (X) \ = e^{X^2} \frac{d^2}{dX^2}\left(e^{-X^2}\right) = 4X^2 - 2 \tag{3.35}$$

and (3.21), we can write K_2 as follows:

$$K_2 = h(t-YA)e^{-\lambda YA}\int_o^{t-YA} \psi(t-YA-t') \ \frac{\frac{Y^2}{t'} - 2}{4\sqrt{\pi t'^3}} \ e^{-\frac{Y^2}{4t'} - \lambda t'} \ dt'. \tag{3.36}$$

Similarly, by using the identity

$$L^{-1}\left[pe^{-Y\sqrt{p}}\right] = \frac{1}{8\sqrt{\pi t^5}}\left(\frac{Y^3}{t} - 6Y\right) e^{-\frac{Y^2}{4t}} \tag{3.37}$$

and (3.21), we can write K_3 as follows

$$K_3 = h(t\text{-}YA)e^{-\lambda YA}\int_0^{t-YA} \psi(t\text{-}YA\text{-}t') \frac{1}{8\sqrt{\pi t'^5}}\left(\frac{Y^3}{t'} - 6Y\right)e^{-\frac{Y^2}{4t'} - \lambda t'} dt'. \tag{3.38}$$

Using (3.33), (3.36) and (3.38), we obtain the expression for $\frac{\partial N}{\partial z}$. Therefore $J(z,t)$ can be written as

$$J(z,t) = vN(z,t) - D\frac{\partial N}{\partial z}(z,t),$$

or

$$J(z,t) = \frac{e^{\nu z}}{2\pi}\int_0^{\infty} h(t\text{-}YA)e^{-\xi^2 - \frac{\nu^2 z^2}{4\xi^2}} e^{-\lambda YA}\int_0^{t-YA} \psi(t\text{-}YA\text{-}t')$$

$$\cdot \frac{1}{\sqrt{t'^3}} e^{-\frac{Y^2}{4t'} - \lambda t'}\left[vY\left(1+\frac{\nu z}{2\xi^2}\right) + \frac{\nu^2 D\beta^2 z}{2\xi^2}\left\{\left(\frac{Y^3}{2t'} + \frac{Y^2}{A} - 3Y\right)\frac{1}{t'}\right.\right.$$

$$\left.\left.- \frac{2}{A}\right\}\right] dt'd\xi, \quad t > 0,\ z > 0. \tag{3.39}$$

Then, the time-dependent cumulative release is

$$\int_0^t J(z,t')dt' = \frac{e^{\nu z}}{2\pi}\int_0^{\infty} h(t\text{-}YA)e^{-\xi^2 - \frac{\nu^2 z^2}{4\xi^2}} e^{-\lambda YA}\int_0^{t-YA}\int_0^{t-YA-t'} \psi(\tau)d\tau$$

$$\cdot \frac{1}{\sqrt{t'^3}} e^{-\frac{Y^2}{4t'} - \lambda t'}\left[vY\left(1+\frac{\nu z}{2\xi^2}\right) + \frac{\nu^2 D\beta^2 z}{2\xi^2}\left\{\left(\frac{Y^3}{2t'} + \frac{Y^2}{A} - 3Y\right)\frac{1}{t'}\right.\right.$$

$$\left.\left.- \frac{2}{A}\right\}\right] dt'd\xi, \quad t > 0,\ z > 0. \tag{3.40}$$

For a step release, $\psi(t) = N^o h(t)e^{-\lambda t}$, the solutions are obtained by substituting (2.40) into (3.23), (3.26), (3.39) and (3.40):

$$\frac{N}{N^o} = F_4(z,t), \quad t \geq 0,\ z \geq 0 \tag{3.41}$$

$$\frac{M}{N^o} = F_5(y,z,t), \quad t \geq 0,\ y \geq b,\ z \geq 0 \tag{3.42}$$

$$\frac{J}{N^o} = F_6\ (z,t),\ t > 0,\ z > 0 \tag{3.43}$$

$$\int_o^t \frac{J(z,t')}{N^o}\, dt' = F_7(z,t),\ t > 0,\ z > 0 \tag{3.44}$$

where

$$F_4(z,t) = \frac{2}{\pi}\, e^{\nu z} \int_o^\infty h(t\text{-}YA) e^{-\xi^2 - \frac{\nu^2 z^2}{4\xi^2}}\ e^{-\lambda t}\ \mathrm{erfc}\left(\frac{Y}{2\sqrt{t\text{-}YA}}\right) d\xi \tag{3.45}$$

$$F_5(y,z,t) = \frac{2}{\sqrt{\pi}}\, e^{\nu z} \int_o^\infty h(t\text{-}YA) e^{-\xi^2 - \frac{\nu^2 z^2}{4\xi^2}}\ e^{-\lambda t}\ \mathrm{erfc}\left(\frac{Y+B(y\text{-}b)}{2\sqrt{t\text{-}YA}}\right) d\xi, \tag{3.46}$$

$$F_6(z,t) = \frac{1}{\pi}\, e^{\nu z} \int_o^\infty h(t\text{-}YA) e^{-\xi^2 - \frac{\nu^2 z^2}{4\xi^2}}\ e^{-\lambda t} \left[\sqrt{\pi}\, v \left(1 + \frac{\nu z}{2\xi^2}\right) \right.$$

$$\left. \cdot\ \mathrm{erfc}\left(\frac{Y}{2\sqrt{t\text{-}YA}}\right) + \frac{R_f z}{2\xi^2}\ \frac{2t\text{-}YA}{A(t\text{-}YA)^{3/2}}\ \exp\left\{-\frac{Y^2}{4(t\text{-}YA)}\right\} \right] d\xi, \tag{3.47}$$

$$F_7(z,t) = -\frac{1}{\lambda}\ F_6(z,t) + \frac{1}{\lambda}\ \frac{1}{2\pi}\, e^{\nu z} \int_o^\infty h(t\text{-}YA) e^{-\xi^2 - \frac{\nu^2 z^2}{4\xi^2} - \lambda YA}$$

$$\cdot \left[v \left(1 + \frac{\nu z}{2\xi^2} + \frac{R_f z}{\xi^2 v}\ \lambda \right) \sqrt{\pi}\ P_+(\xi;z,t) \right.$$

$$+ \frac{R_f z}{2\xi^2}\ \frac{2t\text{-}YA}{A(t\text{-}YA)^{3/2}}\ \exp\left\{-\frac{Y^2}{4(t\text{-}YA)} - \lambda(t\text{-}YA)\right\}$$

$$\left. + \frac{R_f z}{\xi^2 A}\ \sqrt{\lambda\pi}\ P_-\ (\xi;z,t) \right] d\xi \tag{3.48}$$

$$P_\pm\ (\xi;z,t) = \pm\, e^{Y\sqrt{\lambda}}\ \mathrm{erfc}\left(\frac{Y}{2\sqrt{t\text{-}YA}} + \sqrt{\lambda(t\text{-}YA)}\right)$$

$$+ e^{-Y\sqrt{\lambda}}\ \mathrm{erfc}\left(\frac{Y}{2\sqrt{t\text{-}YA}} - \sqrt{\lambda(t\text{-}YA)}\right) \tag{3.49}$$

For a band release, one can obtain the solution by using the superposition method:

$$\frac{N}{N^o} = F_4(z,t) - e^{-\lambda T}F_4(z,t-T), \quad t \geq 0, \ z \geq 0 \tag{3.50}$$

$$\frac{M}{N^o} = F_5(y,z,t) - e^{-\lambda T}F_5(y,z,t-T), \quad t \geq 0, \ y \geq b, \ z \geq 0 \tag{3.51}$$

$$\frac{J}{N^o} = F_6(z,t) - e^{-\lambda T}F_6(z,t-T), \quad t > 0, \ z > 0 \tag{3.52}$$

$$\int_o^t \frac{J(z,t')}{N^o}\, dt' = F_7(z,t) - e^{-\lambda T}F_7(z,t-T), \quad t > 0, \ z > 0. \tag{3.53}$$

The verification for the solutions for the step release is given in the Appendix.

3.4 Computer Code

3.4.1 Quantities Calculated

To evaluate the integrals in the solutions, we introduce a variable transformation so that the integration interval becomes finite. By introducing

$$\mu = \frac{2}{z}\sqrt{\frac{Dt}{R_f}}\ \frac{1}{\xi}, \tag{3.54}$$

the interval, $\frac{z}{2}\sqrt{\frac{R_f}{Dt}} \leq \xi < \infty$ becomes $0 \leq \mu \leq 1$. To avoid computer overflow, we rewrite the exponential term as

$$e^{-\xi^2 - \frac{\nu^2 z^2}{4\xi^2} + \nu z} = e^{-\left(\nu\sqrt{\frac{Dt}{R_f}}\ \mu - \frac{z}{2}\sqrt{\frac{R_f}{Dt}}\ \frac{1}{\mu}\right)^2}, \tag{3.55}$$

otherwise, if z increases, $e^{\nu z}$ soon becomes too large for computers.

After changing the integration interval, one can use Gaussian quadrature to make numerical integrations. However, since each integrand function expressed with μ has such a sharp peak in $0 \leq \mu \leq 1$ that the function value exceeds the computer lower limit in a very small interval in $0 < \mu < 1$, one must compress the integration interval to the interval where the function is evaluated to be non-zero by computers.

For example, the magnitude of the integrand in N/N^o will be determined by the following 2 terms:

$$\exp\left\{-\left(\nu\sqrt{\frac{Dt}{R_f}}\ \mu - \frac{z}{2}\sqrt{\frac{R_f}{Dt}}\ \frac{1}{\mu}\right)^2\right\} \text{ and} \tag{3.56}$$

$$\operatorname{erfc}\left(\frac{t\mu^2+A\sqrt{\frac{R_p}{D_p}}\,(y-b)}{2A\sqrt{t(1-\mu^2)}}\right). \tag{3.57}$$

In case of

$$\left(\nu\sqrt{\frac{Dt}{R_f}}\ \mu - \frac{z}{2}\sqrt{\frac{R_f}{Dt}}\ \frac{1}{\mu}\right)^2 \geq 25.9^2,$$

(3.56) becomes smaller than 10^{-291}, which is the limit of the computation. When greater than 25.9, (3.56) is replaced by zero.

Considering the asymptotic expansion of erfc(X)[3],

$$\operatorname{erfc}(X) \cong \frac{1}{\sqrt{\pi}}\ \frac{1}{X^2}\ e^{-X^2} S$$

where

$$S = 1 + \sum_{m=1}^{\infty} (-1)^m \frac{1\cdot 3\cdots\cdots(2m-1)}{(2X^2)^m}\ ,\ |\arg X| < \frac{3}{4}\pi\ ,$$

the magnitude of erfc (X) at very large X depends upon e^{-X^2}. Therefore if this argument of (3.57) becomes 25.9, (3.57) is also replaced by zero. Therefore, the integration interval must be compressed to the range of the union of the following intervals:

$$\text{from (3.56)},\quad \mu_- \leq \mu \leq \mu_+ \quad \text{and} \tag{3.58}$$

$$\text{from (3.57)},\quad 0 \leq \mu \leq \mu_3 \tag{3.59}$$

where

$$\mu_{\pm} = \frac{\pm\ 25.9 + \sqrt{670.81 + 2\nu z}}{2\nu\sqrt{\frac{Dt}{R_f}}}\ ,$$

$$\mu_3 = \left(\frac{-670.81 - p/2A^2 + (670.81^2 + \frac{p+t}{A^2} \times 670.81)^{\frac{1}{2}}}{t/2A^2} \right)^{\frac{1}{2}} ,$$

and

$$p = A\sqrt{\frac{R_p}{D_p}}\,(y-b) \; .$$

In Figure 2.3, one can observe a few representative examples which illustrate the actual interval for numerical integration. As shown in the figure, the interval becomes smaller as t increases. In the Gaussian quadrature method, which is used in the codes FIS013 and FIS017, the abscissae are distributed in the compressed interval for accurate integration. Thus we integrate between μ- and μ+ instead of between 0 and 1.

In the same way, we obtain the same interval as (3.58) and (3.59) for N/N^o, J/N^o and $\int J/N^o dt'$ except that p is set to zero.

3.4.2 Algorithm

The algorithm for FIS013 and FIS017 is the same as that for FIS003 and FIS017. For the numerical integration, the package subroutine DØ1AJF of NAG library is called. The relative error of the numerical integration is set to less than 1×10^{-6}.

3.4.3 Input Data Format

Same as Table 2.1

3.4.4 Parameter Ranges for Calculation

For the values of

R_f: 1 to 10^4,

R_p: 1 to 10^4,

D : up to 100 (m^2/yr),

t : up to 10^9(yr), and

z : up to 10^6(m),

calculations were completed successfully.

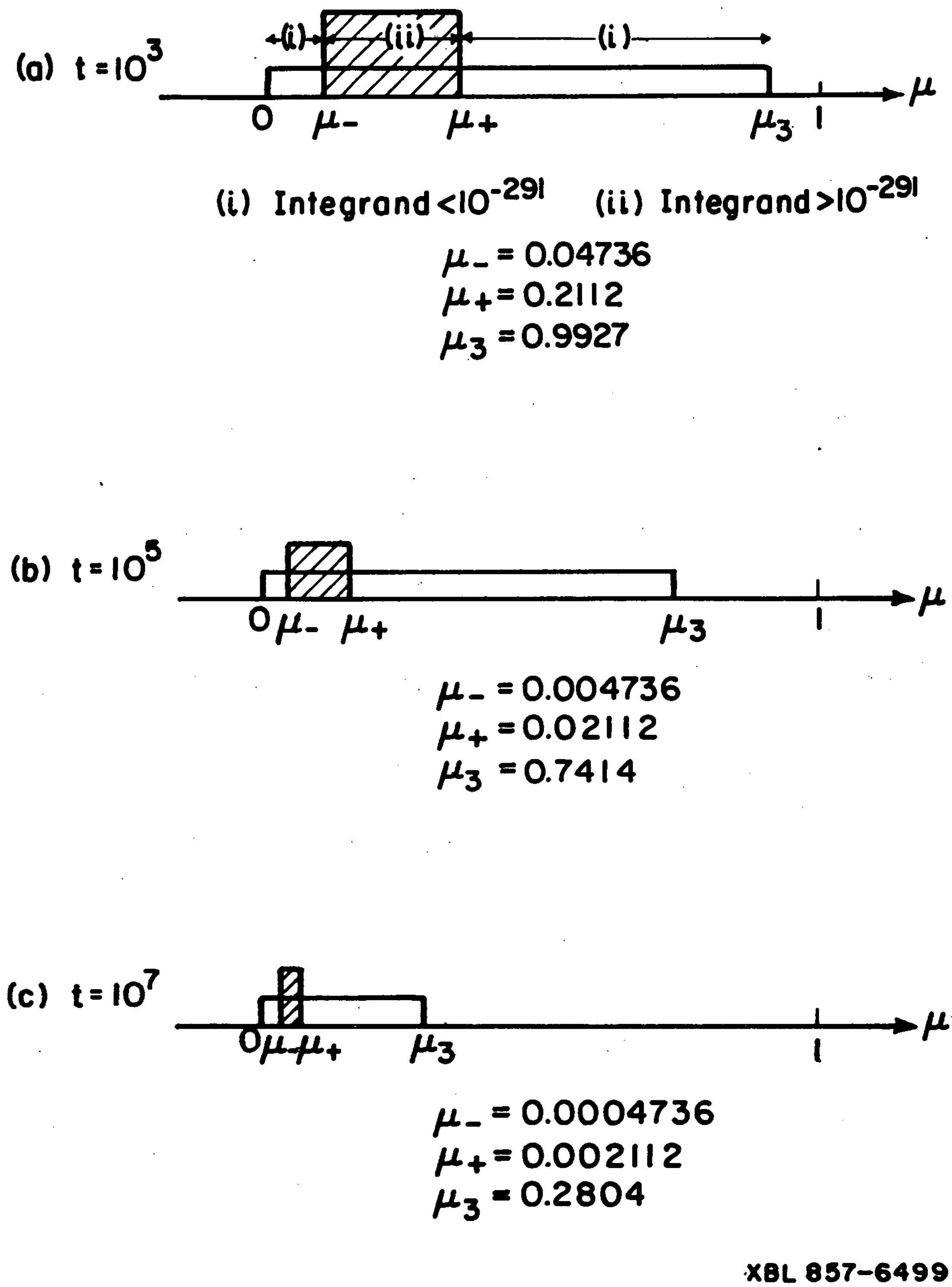

Fig. 2.3 Compressed integration intervals for several t values. Integration is made between μ- and μ+.

4. Examples of Numerical Evaluations

Here we will show some examples which illustrate the effects of the dispersive transport in the fracture (i.e., D) and the sorption in the rock pores (i.e, R_p) on the profiles of the concentrations, the advective mass flux and cululative release. The parameter values used in this report are obtained from our previous report[1].

In Figures from 4.1 to 4.4, one can observe the profiles at 10,000 years for a step release, of the relative concentration in the fracture (Fig. 4.1), the relative concentration in the rock pores at a distance of 100 m from the repository (Fig. 4.2), the advective mass flux in the fracture (Fig. 4.3), and the cumulative release in the fracture (Fig. 4.4), respectively. Effects of R_p are clearly observed in each figure. As R_p increases by a factor of 100, the distance from the repository, z, where the values of the vertical axes become 0.1 percent of the initial values at the repository, decreases by a factor of about 10. On the other hand, the differences between the values for D = 0 and D = 1 m^2/yr are so small that they cannot be distinguished on the figures, even though the values for D=1 m^2/yr are slightly greater than those for D = 0.

Figures 4.5, 4.6 and 4.7 depict the change of the quantities in time up to 10^9 years for a step release. Again the effect of D is very small. The relative concentration in the fracture at z = 100 m (Fig. 4.5) reaches a maximum of 0.9855 at 10000 years. This graph shows that the contaminant reaches the point, z = 100m, at t = 10 years, corresponding to the nuclide travel time $^z/(v/R_f)$ = 10 years. After the maximum, the concentration decreases because of the radioactive decay. After 10^7 years, the concentration becomes smaller than 1 x 10^{-140}. The advective mass flux in the fracture (Fig. 4.6) at z = 100 m has a very similar profile to Fig. 4.5. Figure 4.7 shows the change of the cumulative release in the fracture in time. This quantity has an upper limit because, in (2.44) as $t \to \infty$

$$\lim_{t\to\infty} \int_0^t \frac{J(z,t')}{N^o}\, dt' = \frac{v}{\lambda}\, e^{-\lambda ZA-\sqrt{\lambda}Z} \approx \frac{v}{\lambda}$$ for small λ. As shown in the figure, the cumulative release approaches $v/\lambda = 3.084 \times 10^7$(m).

In Figures 4.8 to 4.14 we show the profiles for a band release with a leach time of 5000 years. In Figures 4.8 to 4.11, one can observe the profiles at 10,000 years, when the leaching is finished, for the four quantities. Again effects of D are too slight to distinguish. Effects of R_p are very similar to those for a step release. Because of the band release, each profile has its peak except for Fig. 4.11. After the leaching has stopped, there is no contaminant flowing out of the repository, and uncontaminated water begins to flow in the fracture. However, there is still contaminant in the rock pores. Because the concentration in the rock pores is now higher than that in the fracture, the contaminant begins to diffuse back to the fracture. This situation is depicted in Fig. 4.9. In Fig. 4.9, the profiles for R_p = 1 and 100 show the concentration gradient from inside of the rock to the fracture. For R_p = 10,000, however, the opposite gradient still exists. For R_p = 1 and 100, the position, z = 100m, is located at the left hand side of the peak in the profile in Fig. 4.8, while for R_p = 10,000, at the right hand side of the peak.

Figures 4.12, 4.13 and 4.14 show the change of the quantities in time for a band release. Up to the end of leaching, the profiles are identical to the corresponding profiles for a step release. After the leach time, N/N^o and J/N^o suddenly decrease. Figure 4.14 shows the upper limit because in (2.52),

$$\lim_{t\to\infty} \int_0^t \frac{J(z,t')}{N^o}\, dt' = \frac{v}{\lambda}\,(1-e^{-\lambda T})e^{-\lambda ZA-\sqrt{\lambda}Z}$$

$\simeq \frac{v}{\lambda}(\lambda T) = vT$ for small λ. As shown in the figure, the cumulative release approach $vT = 5 \times 10^4$(m).

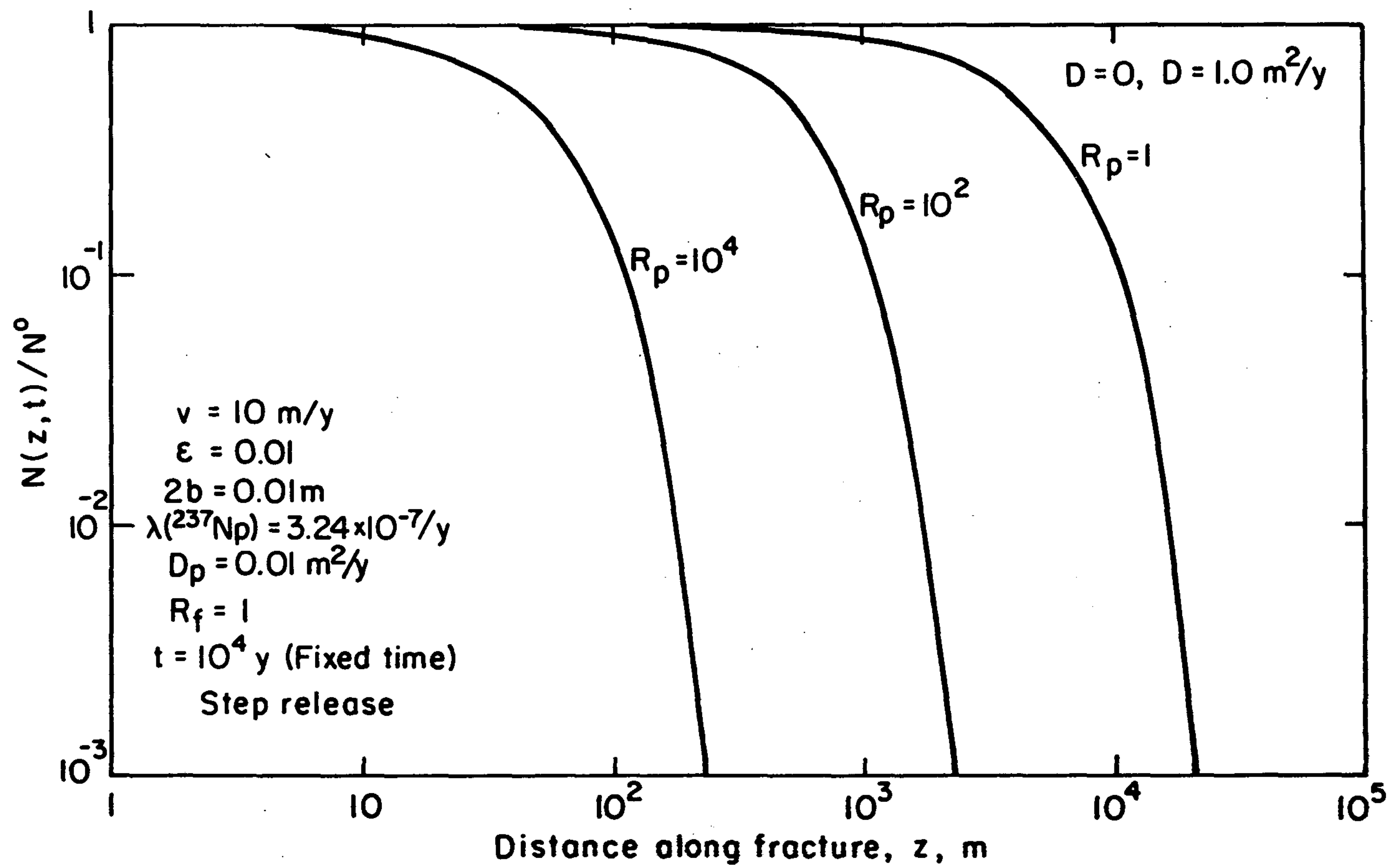

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Fig. 4.1 Concentration profiles of ^{237}Np in the fracture for a step release.

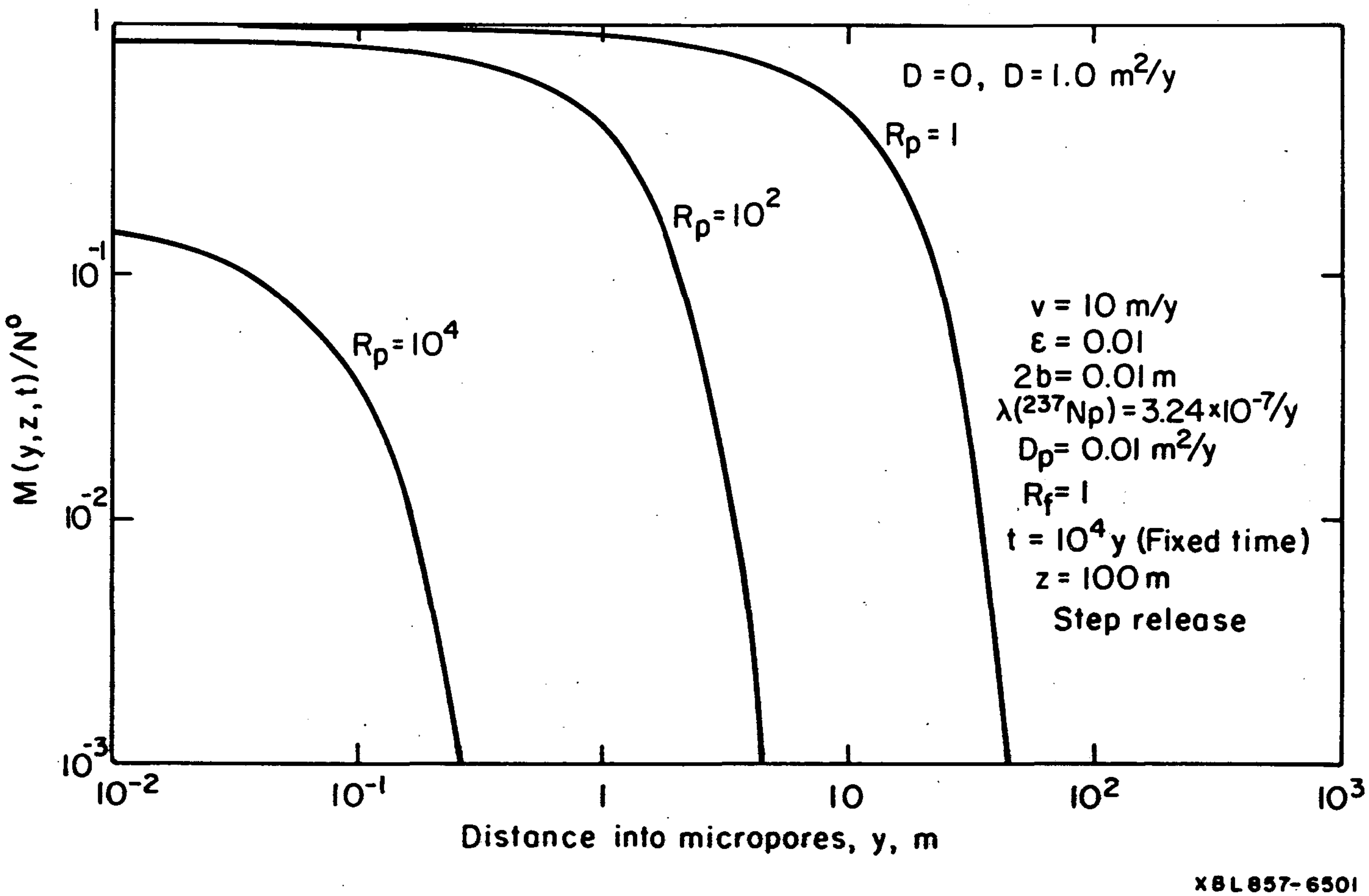

Fig. 4.2 Concentration profiles of ^{237}Np in the micropores, for a step release.

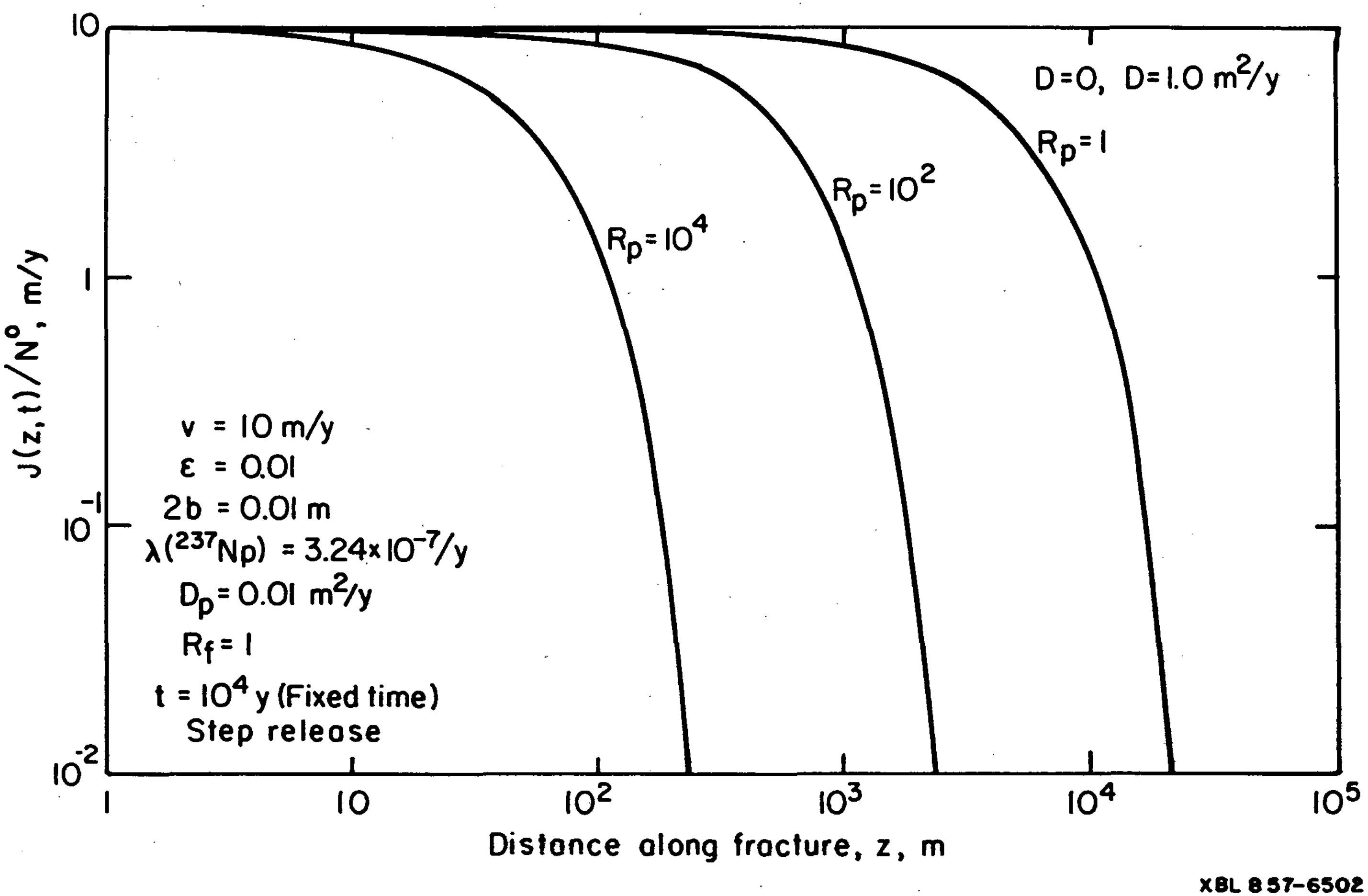

Fig. 4.3 Advective mass flux of ^{237}Np at position z in the fracture, for a step release.

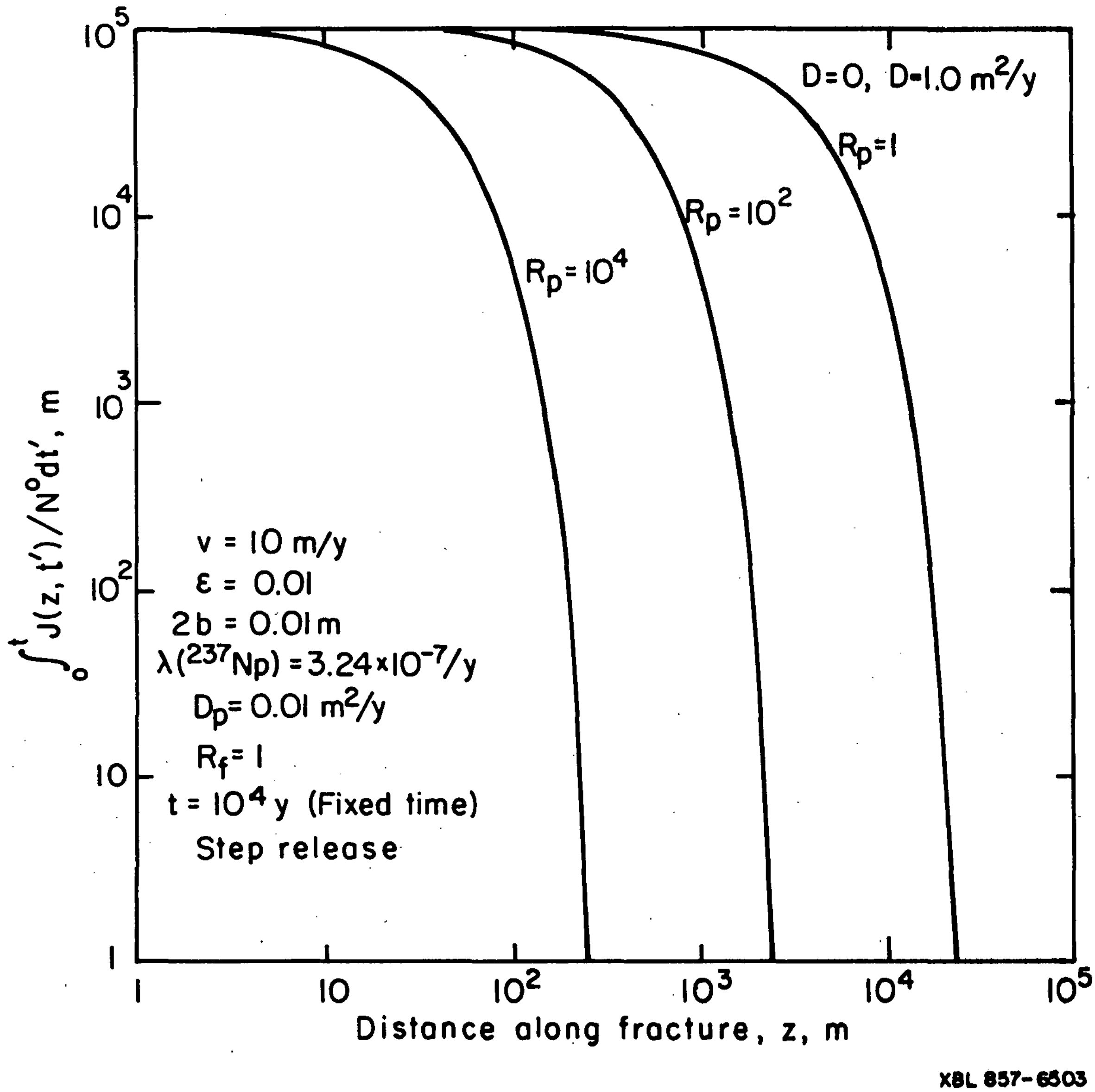

Fig. 4.4 Cumulative release of ^{237}Np across a plane at z and normal to z in the fracture, for a step release.

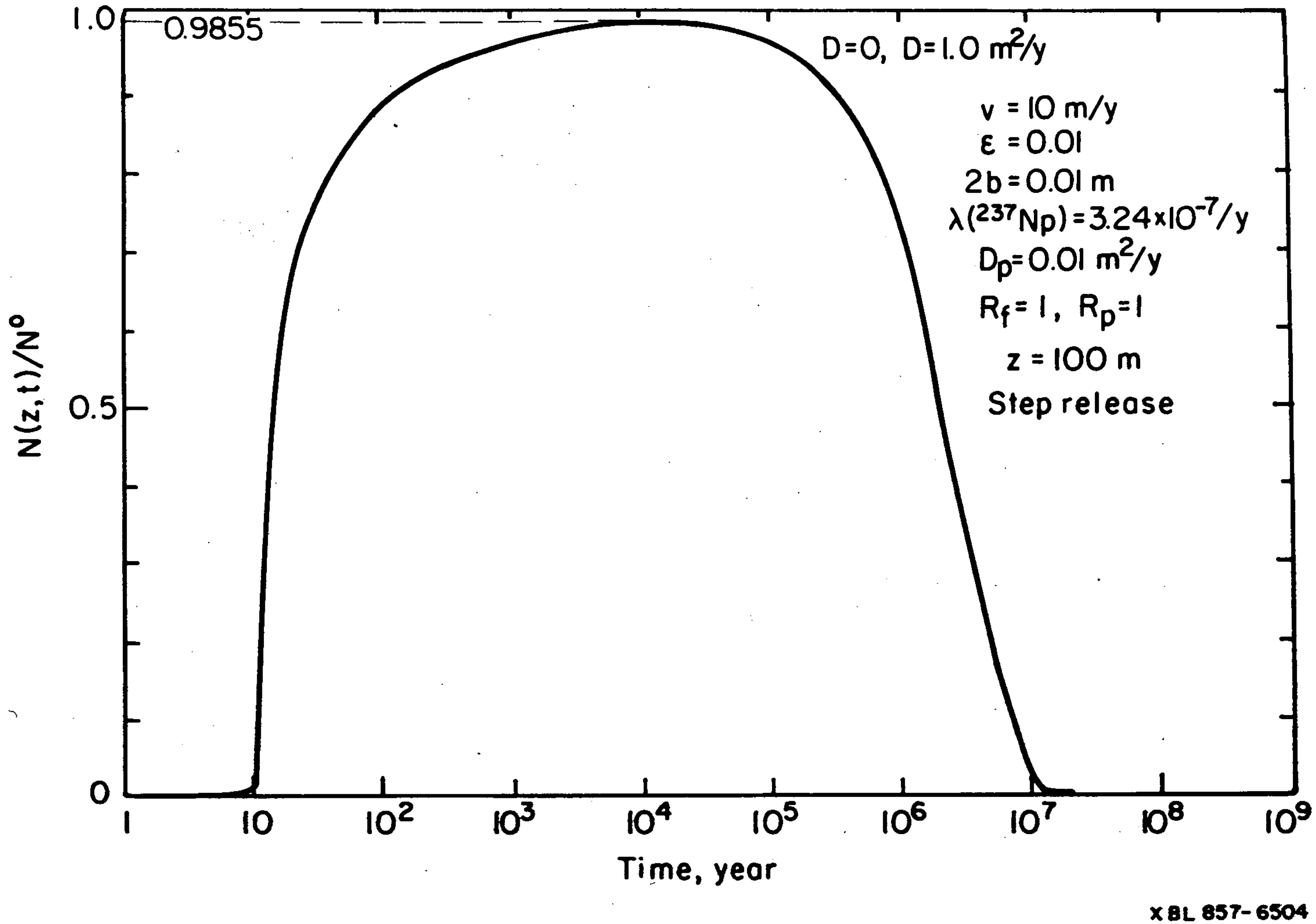

Fig. 4.5 Time dependent concentration of ^{237}Np at position z = 100 m in the fracture, a step release.

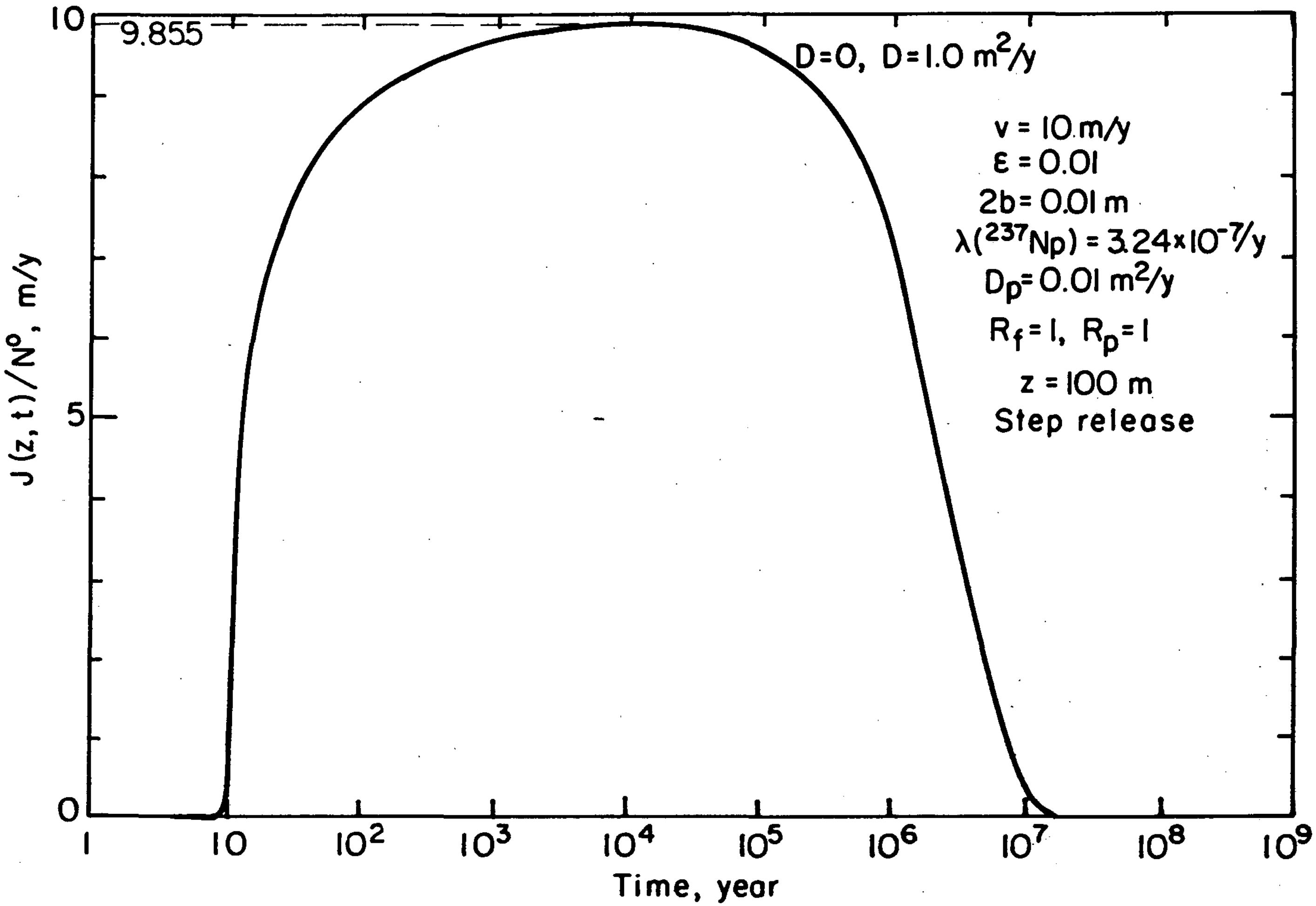

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Fig. 4.6 Time dependent advective mass flux of ^{237}Np at z = 100 m, step release.

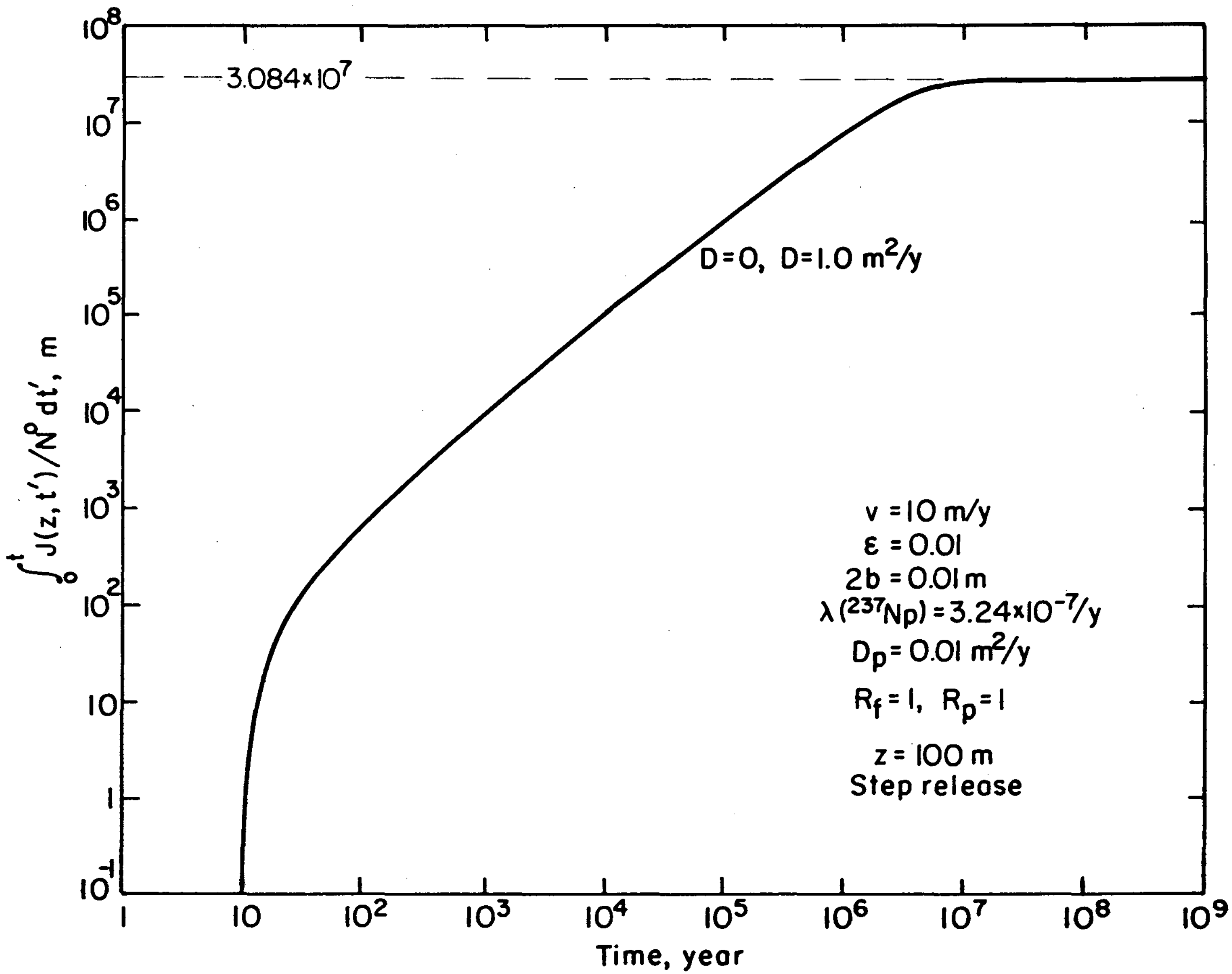

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Fig. 4.7 Time dependent cumulative release of ^{237}Np at z = 100 m, step release.

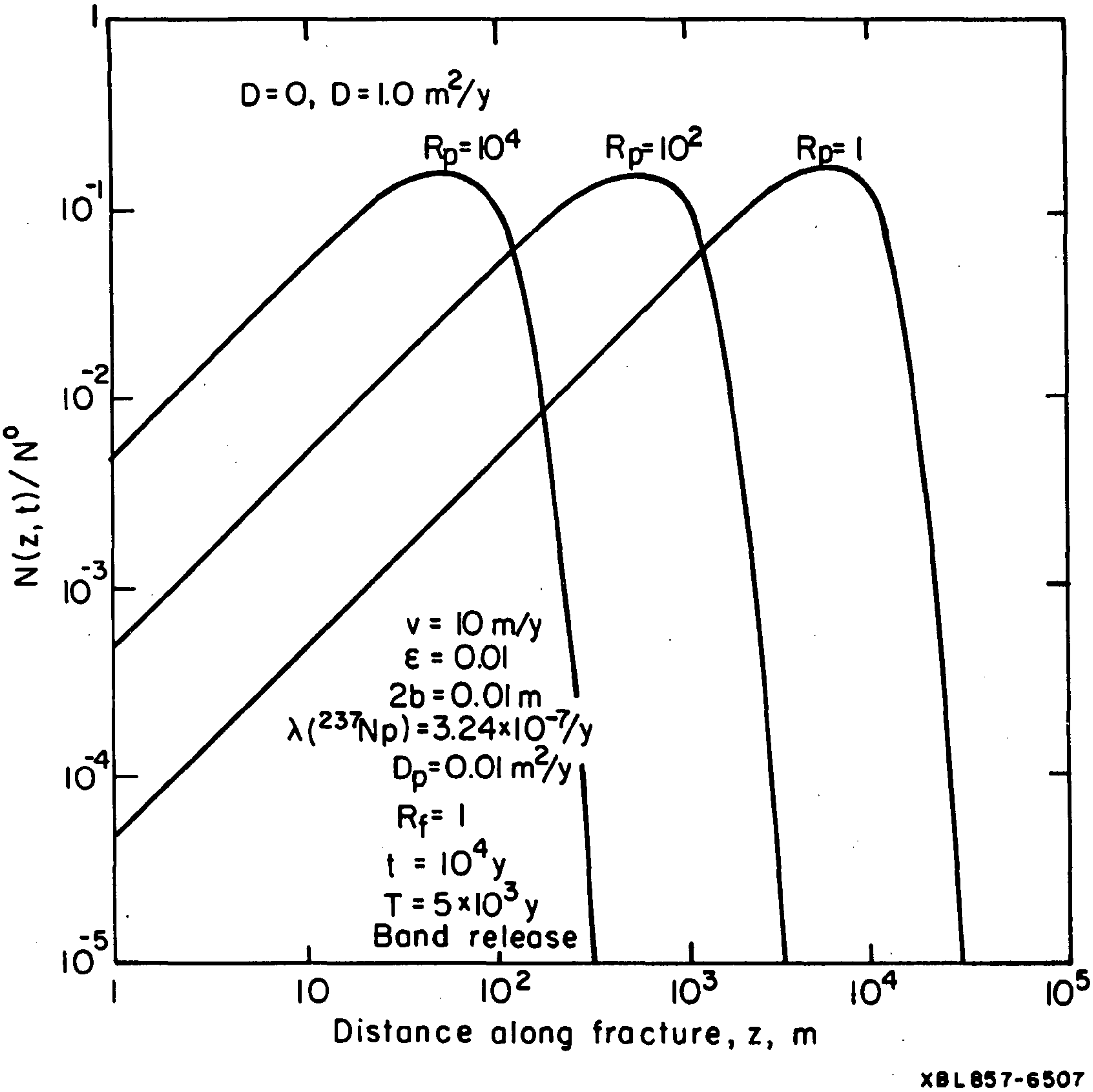

Fig. 4.8 Concentration profiles of ^{237}Np in the fracture, for a band release.

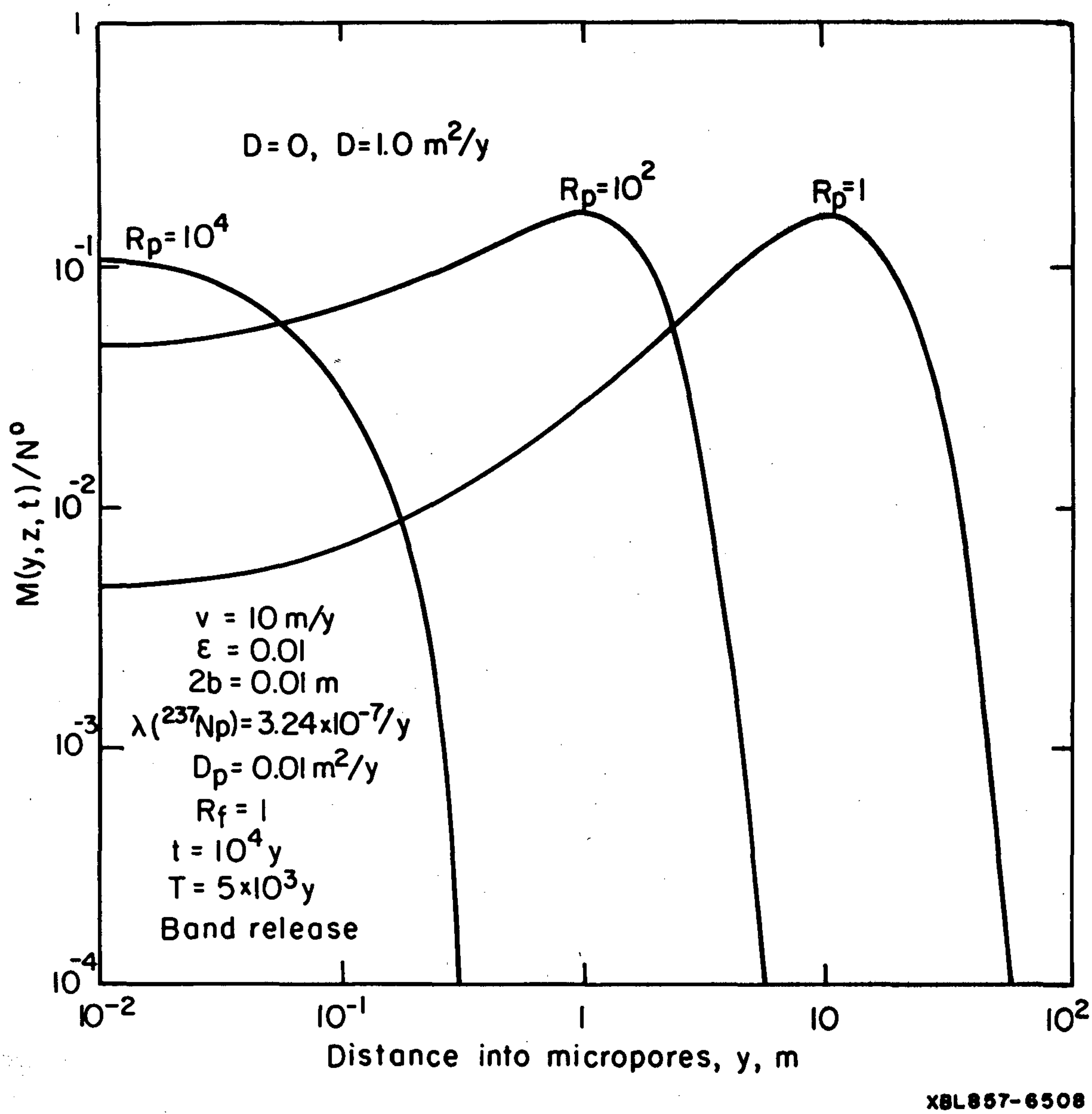

Fig. 4.9 Concentration profiles of ^{237}Np in the micropores, for a band release.

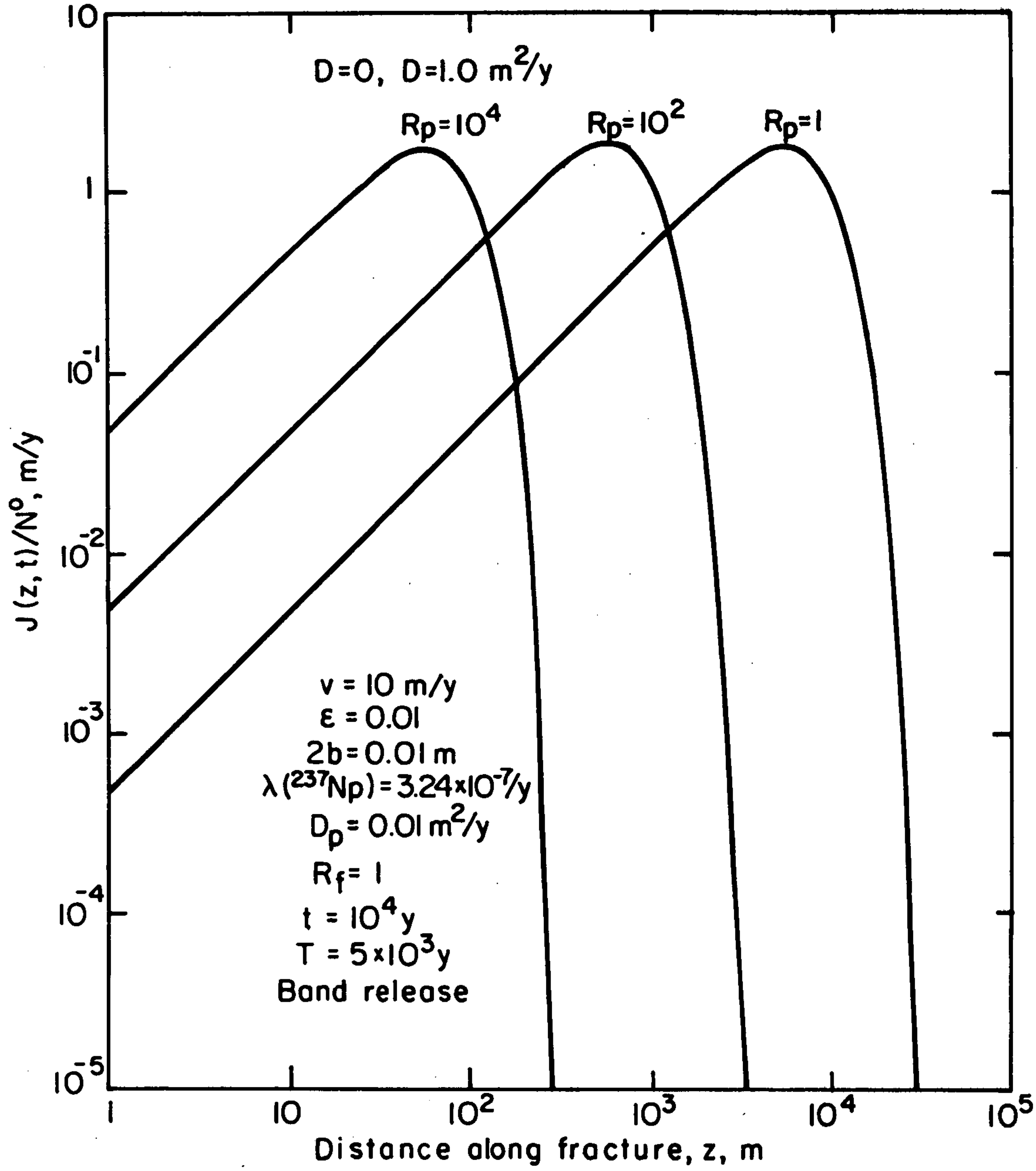

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Fig. 4.10 Advective mass flux of ^{237}Np at position z in the fracture, band release.

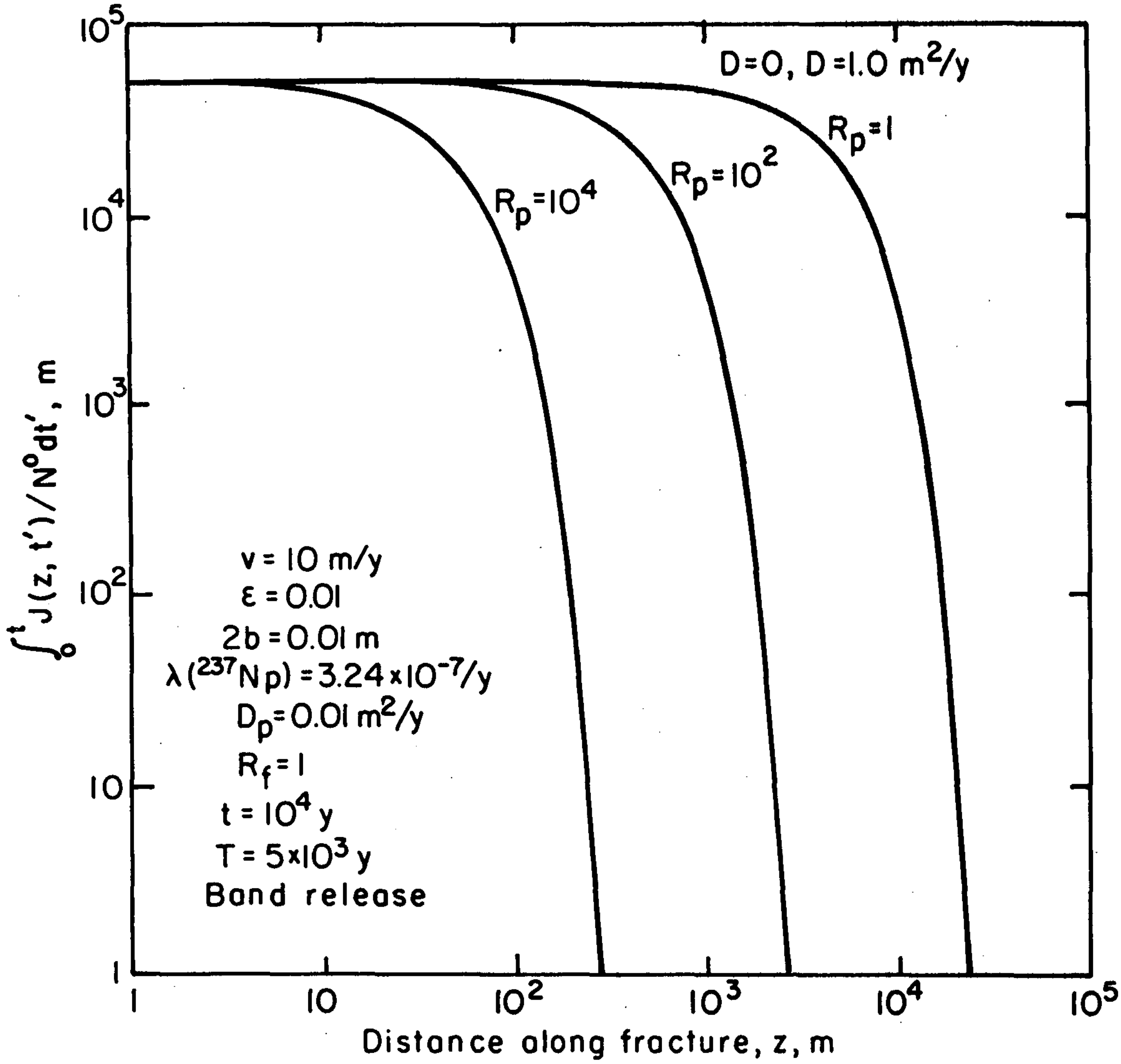

Fig. 4.11 Cumulative release of ^{237}Np across a plane at z and normal to z in the fracture, band release.

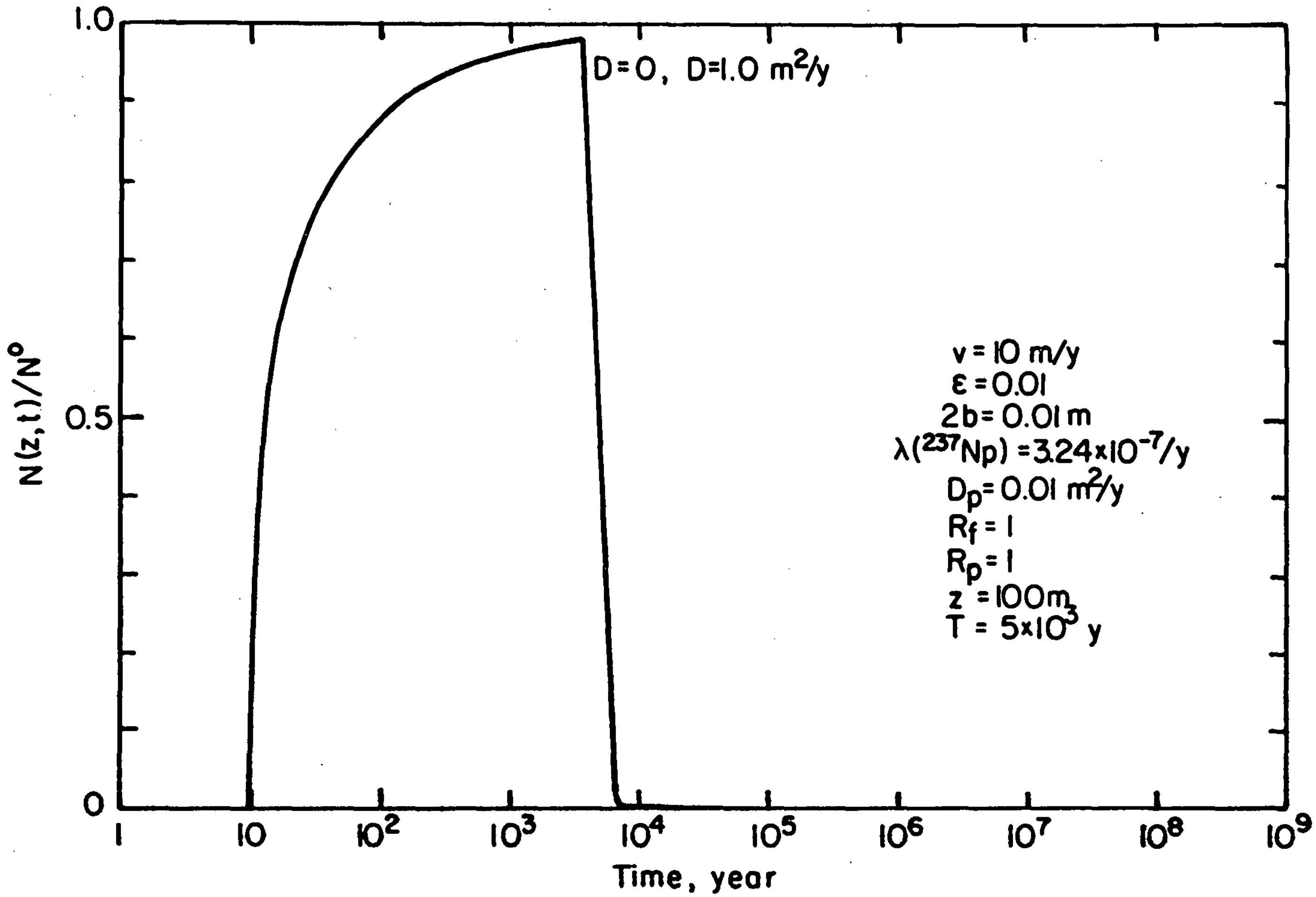

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Fig. 4.12 Time dependent concentration of ^{237}Np at position z = 100 m in the fracture, band release.

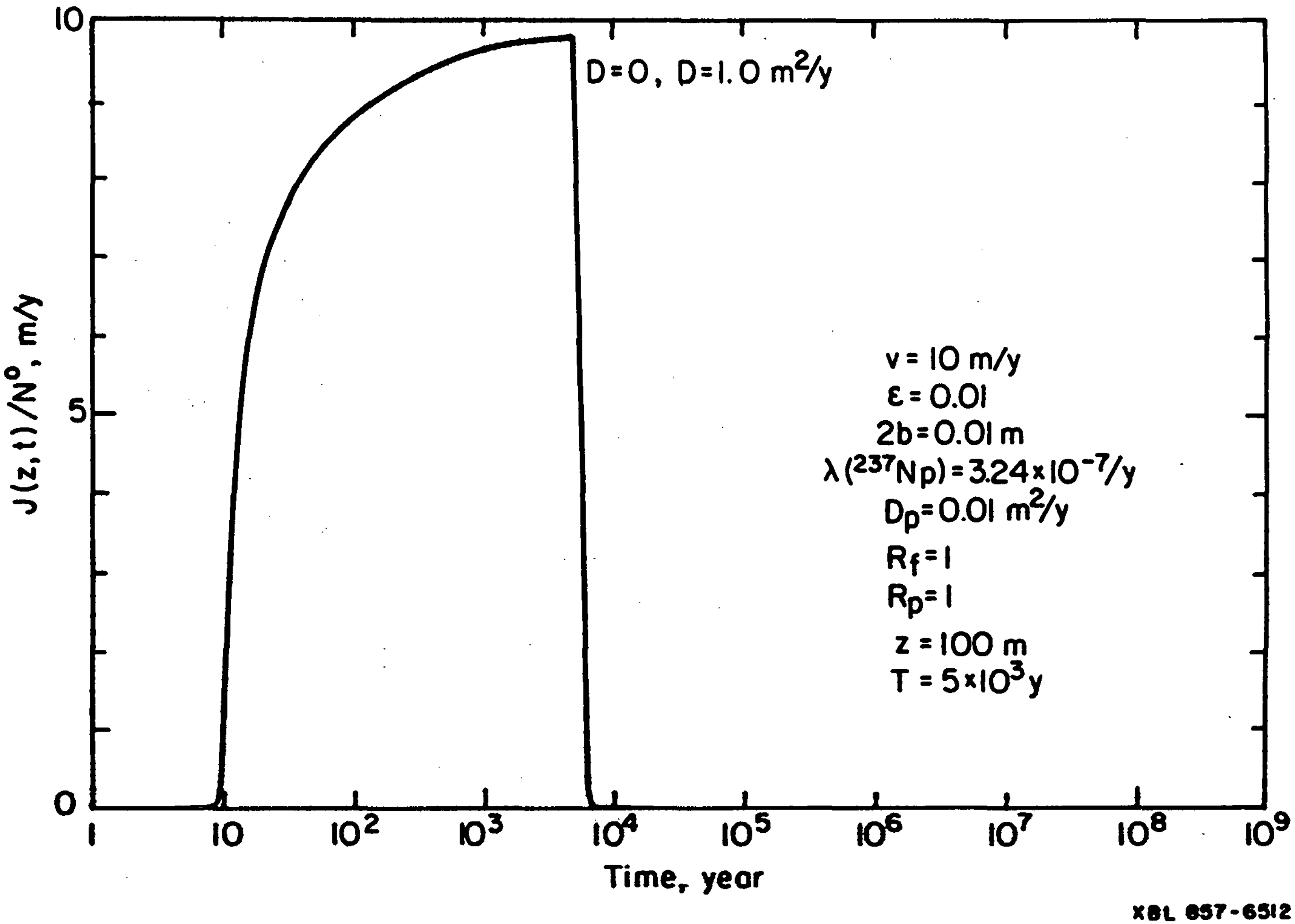

Fig. 4.13 Time dependent advective mass flux of ^{237}Np at z = 100 m, band release.

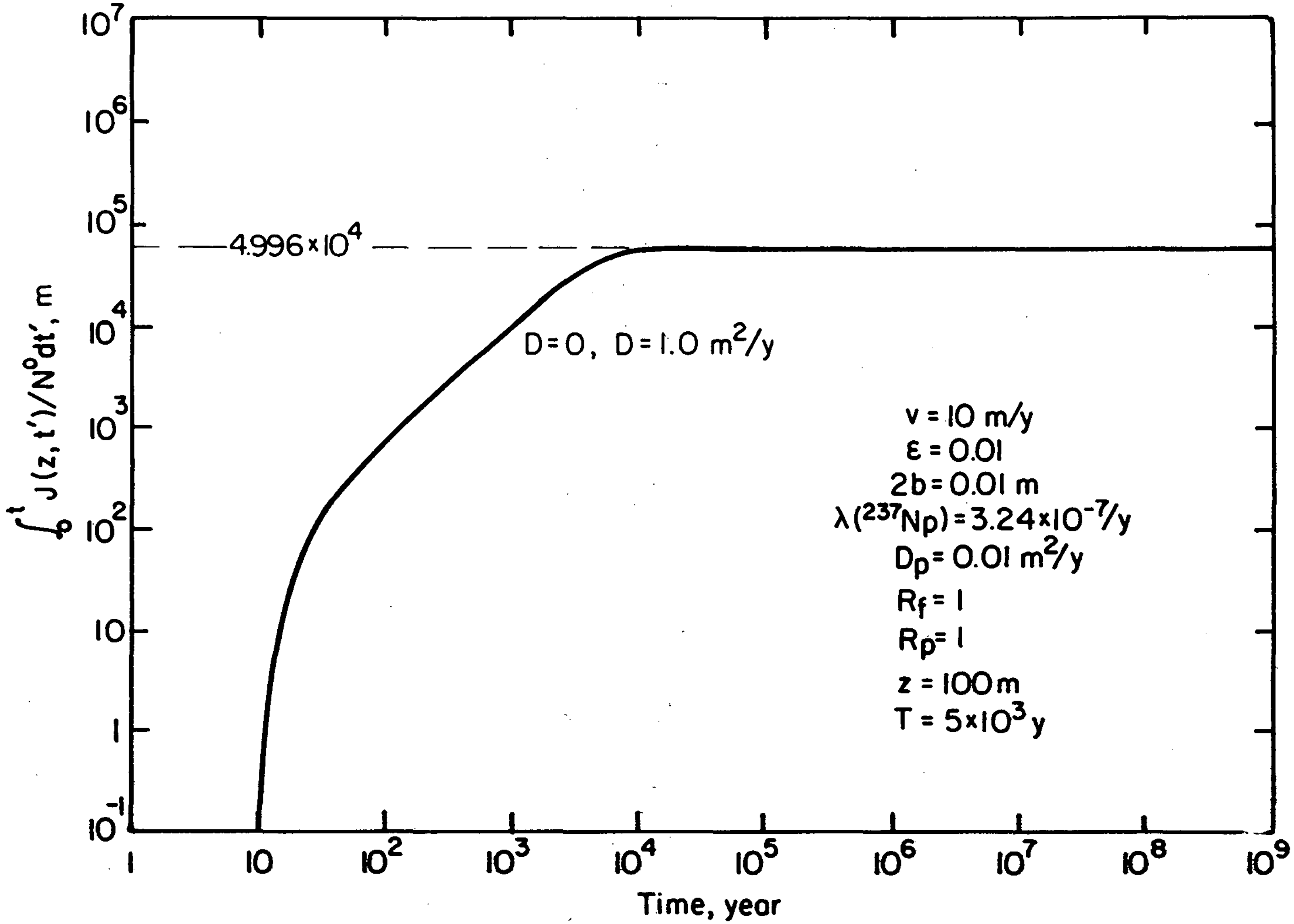

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Fig. 4.14 Time dependent cumulative release of ^{237}Np at z = 100 m, band release.

5. Effects of the Retardation and Dispersion in the Fracture

As was shown in the previous chapters, the solutions for $D \neq 0$ (non-zero dispersion in the fracture) are more complicated than those for $D = 0$. However, from the computed numerical values for $D = 1\ m^2/yr$ and $D = 0$, we find that the differences are so small that we cannot distinguish two cases in the graphs.

Several questions then arise:

(i) At what value of D will these two profiles be separated?

(ii) Are there any other factors which affect the shape of the profiles?

(iii) What are these effects?

Next, we will study the relation between the fractured-media solution and the porous-media solution for a step release, and the effects of fracture dispersion.

5.1 Consideration of the Solutions for Fractured Media with No Dispersion

Analytical solutions to the concentration in the fracture, eq. (2.33), the advective mass flux, (2.38), and the time-dependent cumulative release, (2.39) for a general release, $\psi(t)$, at the repository are rewritten as, by setting a new variable,

$$Tn = \frac{z}{\left(v/R_f\right)} , \tag{5.1}$$

$$N(Tn,t) = e^{-Tn\lambda} h(t-Tn) \int_0^{t-Tn} \psi(t-Tn-t') \frac{Tn/A}{2\sqrt{\pi t'^3}} \exp\left\{- \frac{(Tn/A)^2}{4t'} - \lambda t'\right\} dt', \tag{5.2a}$$

$$J(Tn,t) = vN(Tn,t), \tag{5.2b}$$

and

$$\int_0^t J(Tn,t')dt' = ve^{-Tn\lambda} h(t-Tn) \int_0^{t-Tn} \int_0^{t-Tn-t'} \psi(\tau)d\tau \frac{Tn/A}{2\sqrt{\pi t'^3}} \cdot \exp\left\{- \frac{(Tn/A)^2}{4t'} - \lambda t'\right\} dt', \tag{5.2c}$$

respectively. These equations show that profiles will be the same for the same value of parameter A for a fixed time t if one draws profiles in the domains of N vs Tn, J vs Tn or $\int$ Jdt' vs Tn. The variable Tn is the nuclide travel time (yr) when nuclides are transported through a medium where water is flowing with velocity v and nuclides are retarded by the factor of R_f.

Considering the governing equation (2.13) for the transport in the fracture, if the rate q/bR_f of diffusion into rock pores across the y = b plane is negligible, this equation becomes that for transport in a one-dimensional porous medium, i.e.,

$$\frac{\partial N}{\partial t} + \frac{v}{R_f}\frac{\partial N}{\partial z} + \lambda N = 0, \quad 0 < z < \infty \tag{5.3}$$

subject to the side conditions:

$$N(0,t) = \psi(t), \quad t > 0 \tag{5.3a}$$

$$N(\infty,t) = 0, \quad t > 0 \tag{5.3b}$$

$$N(z,0) = 0, \quad z > 0. \tag{5.3c}$$

Hence one can expect that one of the extreme cases of (2.13) is (5.3), so it will be useful to compare the solutions of (2.13) with those of (5.3). The solutions to (5.3) are, by using Tn,

$$N(Tn,t) = e^{-Tn\lambda}h(t-Tn)\psi(t-Tn) \tag{5.4a}$$

$$J(Tn,t) = vN(Tn,t) \text{ and} \tag{5.4b}$$

$$\int_0^t J(Tn,t')dt' = ve^{-Tn\lambda}h(t-Tn)\int_0^{t-Tn}\psi(\tau)d\tau. \tag{5.4c}$$

Comparing (5.2a), (5.2b), and (5.2c) with (5.4a), (5.4b), and (5.4c), one can say that, if A tends to infinity, (5.2) becomes (5.4). For illustration, let us derive the solutions for a step release. For the fractured media,

$$N(Tn,t) = N^o e^{-\lambda t}h(t-Tn)\ \text{erfc}\left(\frac{Tn/A}{2\sqrt{t-Tn}}\right), \tag{5.5a}$$

$$J(Tn,t) = vN(Tn,t), \text{ and} \tag{5.5b}$$

$$\int_0^t J(Tn,t')dt' = \frac{v}{\lambda} N^o h(t-Tn) \left[e^{-\lambda Tn} \frac{1}{2} \left\{ e^{\sqrt{\lambda}\frac{Tn}{A}} \operatorname{erfc}\left(\frac{Tn/A}{2\sqrt{t-Tn}} + \sqrt{\lambda(t-Tn)} \right) \right.\right.$$

$$\left. + e^{-\sqrt{\lambda}\, Tn/A} \operatorname{erfc}\left(\frac{Tn/A}{2\sqrt{t-Tn}} - \sqrt{\lambda(t-Tn)} \right) \right\}$$

$$\left. -e^{-\lambda t} \operatorname{erfc}\left(\frac{Tn/A}{2\sqrt{t-Tn}} \right) \right] . \qquad (5.5c)$$

For the porous media,

$$N(Tn,t) = N^o e^{-\lambda t} h(t-Tn), \qquad (5.6a)$$

$$J(Tn,t) = vN(Tn,t), \text{ and} \qquad (5.6b)$$

$$\int_0^t J(Tn,t')dt' = \frac{v}{\lambda} N^o h(t-Tn) \left[e^{-\lambda Tn} - e^{-\lambda t} \right] . \qquad (5.6c)$$

Again if A tends to infinity (5.5) becomes (5.6), as is illustreted in Fig. 5.1.

5.2 Consideration of the Solutions for Fractured Media with Non-Zero Dispersion

With non-zero dispersion, we find results similar to those described for D = 0. Let us compare the fractured media solutions with the solutions for one-dimensional porous media. The governing equation for porous media is obtained by neglecting the q/bR_f term in the fractured media governing equation:

$$\frac{\partial N}{\partial t} + \frac{v}{R_f} \frac{\partial N}{\partial z} - \frac{D}{R_f} \frac{\partial^2 N}{\partial Z^2} + \lambda N = 0, \quad 0 < z < \infty \qquad (5.7)$$

subject to the same side conditions as (5.3a,b,c). By using the variables, Tn, and

$$\omega = \frac{(v/R_f)^2}{2(D/R_f)} = \frac{v^2}{2DR_f} , \qquad (5.8)$$

the solutions for a step release in fractured media can be rewritten as

$$N(Tn,t) = \frac{2N^o}{\sqrt{\pi}} e^{\omega Tn} e^{-\lambda t} \int_{\sqrt{\frac{\omega}{2t}}\, Tn}^{\infty} e^{-\xi^2 - \frac{\omega^2 Tn^2}{4\xi^2}} \operatorname{erfc}\left(\frac{\frac{\omega Tn^2}{2\xi^2} \cdot \frac{1}{A}}{2\sqrt{t - \frac{\omega Tn^2}{2\xi^2}}} \right) d\xi, \qquad (5.9a)$$

$$J(Tn,t) = v \cdot \frac{N^o}{\pi} e^{\omega Tn} e^{-\lambda t} \int_{\sqrt{\frac{\omega}{2t}}\,Tn}^{\infty} e^{-\xi^2 - \frac{\omega^2 Tn^2}{4\xi^2}} \left[\sqrt{\pi}\left(1+\frac{\omega Tn}{2\xi^2}\right) \mathrm{erfc}\left(\frac{\frac{\omega Tn^2}{2\xi^2} \cdot \frac{1}{A}}{2\sqrt{t - \frac{\omega Tn^2}{2\xi^2}}} \right) \right.$$

$$\left. + \frac{Tn}{2\xi^2} \frac{2t - \omega Tn^2/2\xi^2}{A\left(t - \frac{\omega Tn^2}{2\xi^2}\right)^{3/2}} \exp\left\{ - \frac{\left(\frac{\omega Tn^2}{2\xi^2 A}\right)}{4\left(t - \frac{\omega Tn^2}{2\xi^2}\right)} \right\} \right] d\xi , \qquad (5.9b)$$

$$\int_0^t J(Tn,t')dt' = - \frac{J(Tn,t)}{\lambda} + \frac{N^o}{\lambda} \frac{1}{2\pi} e^{\omega Tn} \int_{\sqrt{\frac{\omega}{2t}}\,Tn}^{\infty} e^{-\xi^2 - \frac{\omega^2 Tn^2}{4\xi^2} - \lambda \frac{\omega Tn^2}{2\xi^2}}$$

$$\cdot \left[\sqrt{\pi}\, v \left(1+\frac{\omega Tn}{2\xi^2} + \frac{\lambda Tn}{\xi^2}\right) P'_{+}(\xi;Tn,t) \right.$$

$$+ \frac{vTn}{\xi^2} \frac{\sqrt{\lambda\pi}}{A} P'_{-}(\xi;Tn,t) + \frac{vTn}{2\xi^2} \frac{2t - \frac{\omega Tn^2}{2\xi^2}}{A\left(t - \frac{\omega Tn^2}{2\xi^2}\right)^{3/2}}$$

$$\left. \cdot \exp\left\{ - \frac{1}{4}\left(\frac{\omega Tn^2}{2\xi^2 A}\right)^2 \frac{1}{t - \frac{\omega Tn^2}{2\xi^2}} - \lambda\left(t - \frac{\omega Tn^2}{2\xi^2}\right) \right\} \right] d\xi , \qquad (5.9c)$$

where

$$P'_{\pm}(\xi;Tn,t) = \pm \exp\left(\frac{\omega Tn^2}{2\xi^2}\sqrt{\lambda}\right) \mathrm{erfc}\left(\frac{\frac{\omega Tn^2}{2\xi^2} \frac{1}{A}}{2\sqrt{t - \frac{\omega Tn^2}{2\xi^2}}} + \sqrt{\lambda\left(t - \frac{\omega Tn^2}{2\xi^2}\right)} \right)$$

$$+ \exp\left(-\frac{\omega Tn^2}{2\xi^2}\sqrt{\lambda}\right) \mathrm{erfc}\left(\frac{\frac{\omega Tn^2}{2\xi^2} \frac{1}{A}}{2\sqrt{t - \frac{\omega Tn^2}{2\xi^2}}} - \sqrt{\lambda\left(t - \frac{\omega Tn^2}{2\xi^2}\right)} \right) .$$

And the solutions to (5.7) for a step release in porous media are

$$N(Tn,t) = \frac{2N^o}{\sqrt{\pi}} e^{\omega Tn} e^{-\lambda t} \int_{\sqrt{\frac{\omega}{2t}}Tn}^{\infty} e^{-\xi^2 - \frac{\omega^2 Tn^2}{4\xi^2}} d\xi , \qquad (5.10a)$$

$$J(Tn,t) = v\frac{N^o}{\sqrt{\pi}} e^{\omega Tn} e^{-\lambda t} \int_{\sqrt{\frac{\omega}{2t}}Tn}^{\infty} e^{-\xi^2 - \frac{\omega^2 Tn^2}{4\xi^2}} \left(1+ \frac{\omega Tn}{2\xi^2}\right) d\xi , \qquad (5.10b)$$

and

$$\int_0^t J(Tn,t')dt' = -\frac{J}{\lambda} + \frac{v}{\lambda} \frac{N^o}{\sqrt{\pi}} e^{\omega Tn} \int_{\sqrt{\frac{\omega}{2t}}Tn}^{\infty} e^{-\xi^2 - \frac{\omega^2 Tn^2}{4\xi^2} - \lambda \frac{\omega Tn^2}{2\xi^2}}$$

$$\cdot \left(1+ \frac{\omega Tn}{2\xi^2} + \frac{\lambda Tn}{\xi^2}\right) d\xi . \qquad (5.10c)$$

Again if A tends to infinity, (5.9a,b,c) becomes (5.10 a,b,c).

Another comparison can be made between (5.5 a,b,c) and (5.9 a,b,c), namely, between zero dispersion and non-zero dispersion. As can be seen after some mathematical manipulation, if ω tends to infinity, (5.9 a,b,c) can be reduced to (5.5 a,b,c), corresponding to taking $D \to 0$. This situation is illustrated in Fig. 5.1.

Knowing the criteria at which more complicated solutions can be approximated by simpler solutions can save computation time. In the next section we seek numerical values of these criteria.

5.3 Computational Results and Discussions

The sets of parameter values which were taken for numerical study are listed in Table 5.1.

For relatively small values of A and large values of D, the computation could not be completed with the present code, because the integrand functions dealt with in the computer code have very sharp peaks and numerical errors are significant. However, one of the consequences derived from the discussion

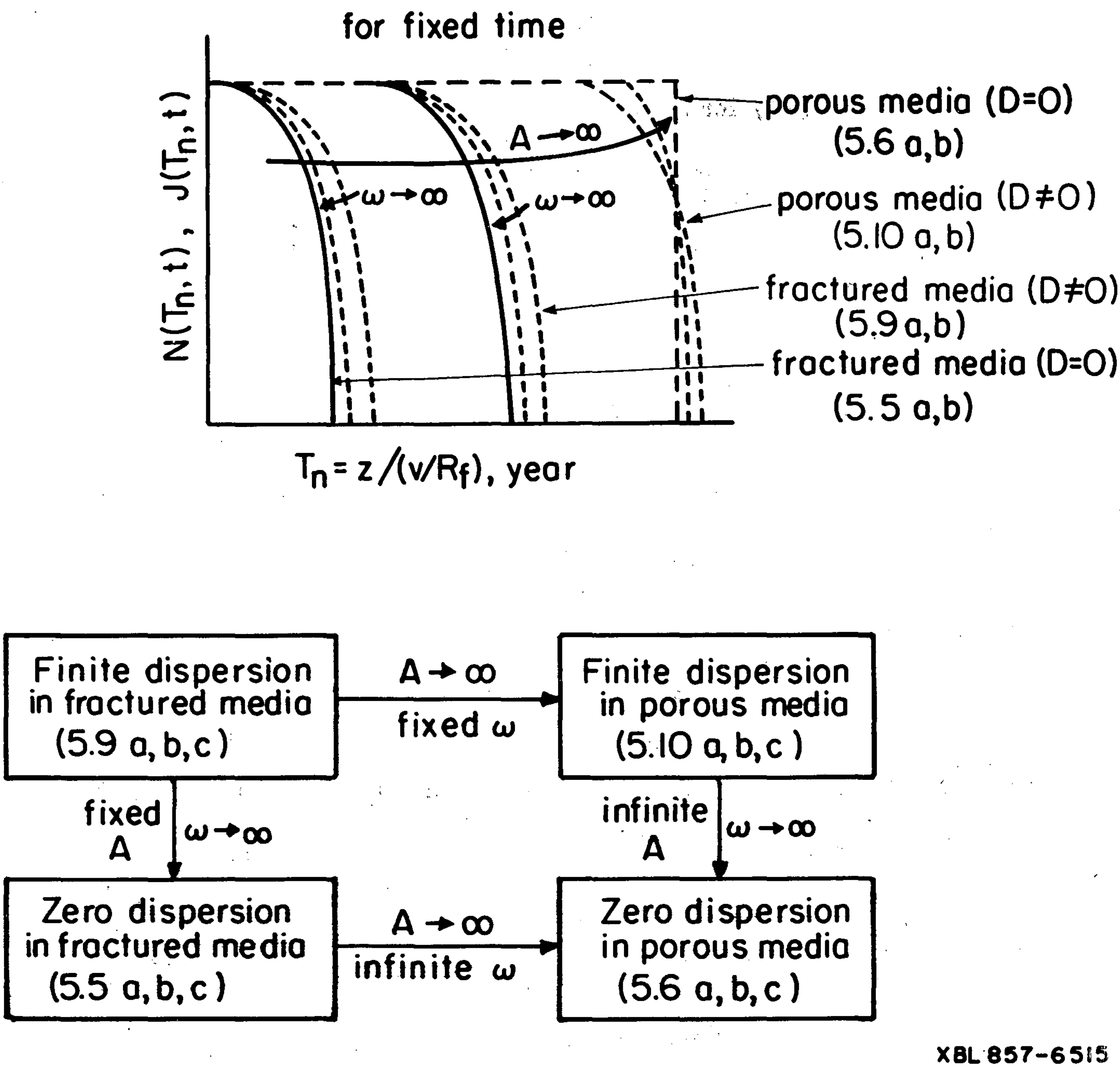

Fig. 5.1 Relations among the solutions for a porous medium and for a fractured medium; for zero dispersion and non-zero dispersion.

Table 5.1

$[R_p = 1]$

$D \backslash R_f$	1(A=5)	10(A=50)	100(A=500)	1000(A=500)
0	$\omega = \infty$	$\omega = \infty$	$\omega = \infty$	$\omega = \infty$
1	$\omega = 50$	$\omega = 5$	$\omega = 0.5$	$\omega = 0.05$
10	$\omega = 5$	$\omega = 0.05$	$\omega = 0.05$	$\omega = 0.005$
100	$\omega = 0.5$ O	$\omega = 0.005$ O	$\omega = 0.005$	$\omega = 0.0005$

v=10m/y
ε=0.01
2b=0.01m
$\lambda=3.24\text{x}10\text{x}10^{-7}/y$
$D_p=0.01m^2/y$
t=10000 y

$[R_p = 100]$

$D \backslash R_f$	1(A=0.5)	10(A=5)	100(A=50)	1000(A=500)
0	$\omega = \infty$	$\omega = \infty$	$\omega = \infty$	$\omega = \infty$
1	$\omega = 50$	$\omega = 5$	$\omega = 0.5$	$\omega = 0.05$
10	$\omega = 5$	$\omega = 0.5$	$\omega = 0.05$	$\omega = 0.005$
100	$\omega = 0.5$ O	$\omega = 0.05$ O	$\omega = 0.005$	$\omega = 0.0005$

$\psi = N^o h(t) e^{-\lambda t}$

$$A = \frac{bR_f}{\varepsilon\sqrt{D_p R_p}} = \frac{5R_f}{\sqrt{R_p}}$$

$[R_p = 10000]$

$D \backslash R_f$	1(A=0.05)	10(A=0.05)	100(A=5)	1000(A=50)
0	$\omega = \infty$	$\omega = \infty$	$\omega = \infty$	$\omega = \infty$
1	$\omega = 50$	$\omega = 5$	$\omega = 0.5$	$\omega = 0.05$
10	$\omega = 5$ O	$\omega = 0.5$ O	$\omega = 0.05$	$\omega = 0.005$
100	$\omega = 0.5$	$\omega = 0.05$	$\omega = 0.005$	$\omega = 0.0005$

$$\omega = \frac{v^2}{2DR_f} = \frac{50}{DR_f}$$

Note: "O" indicates that the computation could not be completed.

in the previous sections is that, for the same values of A and ω, the profiles become identical with respect to Tn. Therefore, even if the computation cannot be made for some set of values of the parameters, one may try another set of values, keeping A and ω the same. For example, for $(R_p, R_f, D) = (100,10,100)$, computation was not completed, while for $(R_p, R_f, D) = (10000,100,10)$ we could obtain the answer.

Figure 5.2 shows the profiles of N vs Tn. There are curves for different values of A and ω. From this figure, one can tentatively say that if

$$A = \frac{bR_f}{\varepsilon\sqrt{D_p R_p}} \gtrsim 500, \ \mathrm{yr}^{1/2}, \tag{5.11}$$

the solutions can be approximated with those of a porous medium. If we observe the factor A, the numerator bR_f consists of the parameter relevant to the fracture; bR_f is a kind of "capacity" of the fracture for contaminant transport. The denominator $\varepsilon\sqrt{D_p R_p}$ is a parameter of the porous matrix surrounding the fracture. The fact that the medium can be regarded as a one-dimensional porous medium when A becomes very large means that, if the relative significance of the fracture transport compared with the matrix diffusion becomes large, one can ignore the diffusive transport into the rock matrix.

In order to confirm this, let us consider the flux of contaminant diffusing into the rock matrix from the fracture, q, which is defined by eq. (2.12). For a step release and D = 0, for simplicity, $^q/R_f b$ can be calculated as

$$\frac{q}{R_f b} = \frac{N^o}{\sqrt{\pi}\, A} e^{-\lambda t} h(t-Tn) \frac{1}{\sqrt{t-Tn}} e^{-\frac{(Tn/_A)^2}{4(t-Tn)}} . \tag{5.12}$$

This shows that as A becomes large, $^q/R_f b$ becomes negligible. This means that the flux diffusing into the rock matrix becomes smaller because:

- the amount sorbed on the fracture wall becomes large, and the relative amount diffusing into the rock is reduced, or

- the capacity of the rock matrix for contaminant is reduced and the relative importance of fracture transport becomes large.

Thus, if the amount of contaminant in the fracture and that sorbed on the fracture wall is considerably larger than that diffusing out of the fracture, the fractured medium can be regarded as a porous medium.

The criterion for using the solutions with zero dispersion instead of those with non-zero dispersion can be obtained from the numerical results. From Fig. 5.2, the values of ω_{crit}, at which the $D \neq 0$ curves start to deviate from the $D = 0$ curve, depends upon the value of A:.

A	0.05	0.5	5	50
ω_{crit}	~ 1	~ 0.1	~ 0.01	~ 0.001

, $A\,\omega_{crit} \simeq 0.05\ yr^{-1/2}$

A increases, ω_{crit} decreases. If $A\,\omega$ is greater than $A\,\omega_{crit}$, then one can use the solutions for zero dispersion with reasonable accuracy instead of those for non-zero dispersion.

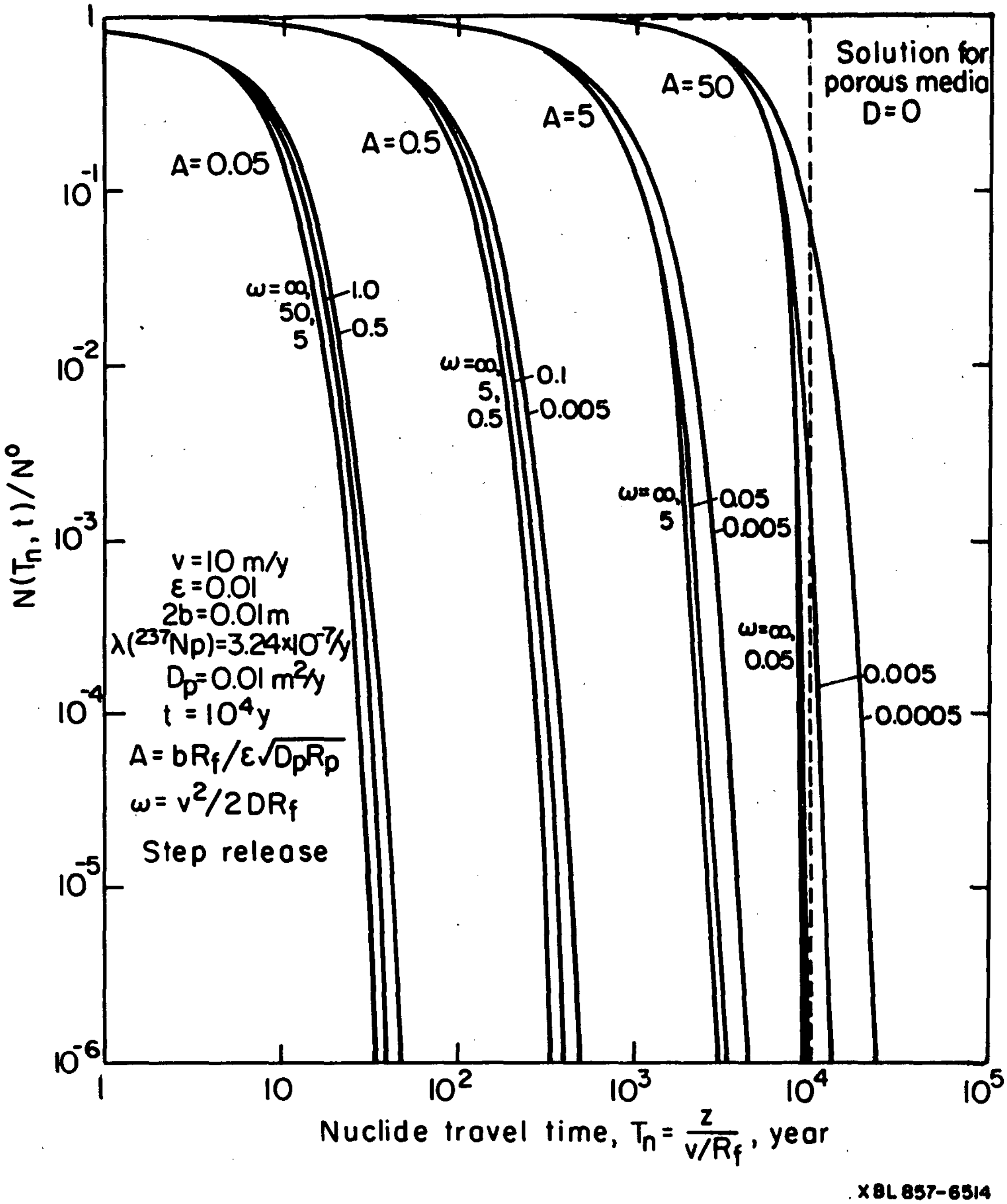

Fig. 5.2 Concentration profiles of ^{237}Np in the N-Tn domain, step release.

6. References

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Appendix

Verification of the Solutions for the Single Fractured Media with Finite Fracture Dispersion.

We will verify that

$$N(z,t) = \frac{2}{\sqrt{\pi}} N^o e^{\nu z-\lambda t} \int_{\frac{\nu z\beta}{2\sqrt{t}}}^{\infty} e^{-\xi^2 - \frac{\nu^2 z^2}{4\xi^2}} \text{erfc}\left(\frac{Y}{2\sqrt{t-YA}}\right) d\xi, \; t \geq 0, \; z \geq 0 \quad (3.41)$$

and

$$M(y,z,t) = \frac{2}{\sqrt{\pi}} N^o e^{\nu z-\lambda t} \int_{\frac{\nu\beta z}{2\sqrt{t}}}^{\infty} e^{-\xi^2 - \frac{\nu^2 z^2}{4\xi^2}} \text{erfc}\left(\frac{Y+B(y-b)}{2\sqrt{t-YA}}\right) d\xi, \; t \geq 0, \; y \geq b, \; z \geq 0 \quad (3.42)$$

are the solutions to the problem:

$$\frac{\partial^2 N}{\partial z^2} - 2\nu \frac{\partial N}{\partial t} - \frac{R_f}{D} \lambda N - \frac{q}{bD} = 0, \; t > 0, \; z > 0 \quad (3.1)$$

$$\frac{\partial^2 M}{\partial y^2} - B^2 \frac{\partial M}{\partial t} - \lambda B^2 M = 0, \; t > 0, \; y > b, \; z > 0 \quad (3.2)$$

subject to the side conditions:

$N(z,o) = 0$	$z > 0$	(a)
$M(y,z,o) = 0$	$y > b, \; z > 0$	(b)
$N(0,t) = N^o e^{-\lambda t}$	$t > 0$	(c)
$N(\infty,t) = 0$	$t > 0$	(d)
$M(b,z,t) = N(z,t)$	$z > 0, \; t > 0$	(e)
$M(\infty,z,t) = 0$	$z > 0, \; t > 0$	(f)

where

$$q \equiv - \varepsilon D_p \frac{\partial M}{\partial y}\bigg|_{y=b}, \; z > 0, \; t > 0 \quad (g)$$

$$Y = \frac{\nu^2\beta^2 z^2}{4A\xi^2}, \; B = \sqrt{\frac{R_p}{D_p}}, \; \nu = \frac{v}{2D}, \; \beta^2 = \frac{4DR_f}{v^2}, \; A = \frac{bR_f}{\varepsilon\sqrt{D_p R_p}}.$$

[1] Side Conditions

(a) $N(z,0) = 0, \; z > 0$

For $z > 0$, the integration interval in (3.41) becomes from ∞ to ∞. If the value of the integrand evaluated at $\xi = \infty$ is bounded, the integral itself becomes zero. That value of integrand becomes zero because

$$\lim_{\xi \to \infty} e^{-\xi^2 - \frac{\nu^2 z^2}{4\xi^2}} = 0$$

and by letting $P = \dfrac{Y}{2\sqrt{t-YA}}$,

$$\lim_{\substack{\xi \to \infty \\ t \to 0}} P = \lim_{\substack{\xi \to \infty \\ t \to 0}} \left(\frac{\frac{\nu^2 \beta^2 z^2}{4A}}{\sqrt{\xi^4 t - \frac{\nu^2 \beta^2 z^2}{4} \xi^2}} \right) = 0.$$

The last manipulation is possible because $\xi^4 t$ goes to infinity faster than ξ^2 and so the denominator goes to infinity, where as the numerator is a positive constant. Therefore, we have

$$\lim_{\substack{\xi \to \infty \\ t \to 0}} \operatorname{erfc}(P) = \operatorname{erfc}(0) = 1.$$

Therefore at the limit of $\xi \to \infty$, the integrand becomes zero and so bounded. Therefore

$$N(z,0) = 0, \; z > 0.$$

(b) $M(y,z,0) = 0, \; y > b, \; z > 0$

By setting $P' = \dfrac{Y+B(y-b)}{2\sqrt{t-YA}}$, we consider the following limit operation:

$$\lim_{\substack{\xi \to \infty \\ t \to 0}} P' = \lim_{\substack{\xi \to \infty \\ t \to 0}} \frac{\frac{\nu^2 \beta^2 z^2}{4A\xi^2} + B(y-b)}{\sqrt{t - \frac{\nu^2 \beta^2 z^2}{4A\xi^2}}} \to \infty .$$

Therefore, $\lim_{\substack{\xi \to \infty \\ t \to 0}} \text{erfc}\,(P') = 0$

By the same argument, $M(y,z,0) = 0$ for $y > b$, $z > 0$.

(c) $N(0,t) = N^o e^{-\lambda t}$, $t > 0$.

Considering the integrand in $N(z,t)$, the integrand function is integrable in ξ over every finite subinterval of $C \equiv \left\{\xi \geq {}^{\nu\beta z}/2\sqrt{t}\right\}$ for any (z,t) in $S \equiv \{z \geq 0,\ t \geq 0\}$. The integrand function is also continuous in (z,t), ξ for (z,t), ξ on S, C. The integrand is bounded by

$$\left| e^{-\xi^2 - \frac{\nu^2 z^2}{4\xi^2}} \text{erfc}\left(\frac{Y}{2\sqrt{t-YA}}\right) \right| \leq e^{-\xi^2} \text{ for all } (z,t)\in S \text{ and } \xi\in C.$$

Therefore, the integral converges absolutely and uniformly and is continuous in (z,t) for $(z,t)\in S$. Therefore, we can exchange the order of $\lim_{z\to 0}$ and $\int$, obtaining

$$\lim_{z\to 0} N(z,t) = \frac{2}{\sqrt{\pi}} N^o e^{-\lambda t} \int_o^\infty \lim_{z\to 0} \left\{ e^{-\xi^2 - \frac{\nu^2 z^2}{4\xi^2}} \text{erfc}\left(\frac{Y}{2\sqrt{t-YA}}\right) \right\} d\xi$$

$$= \frac{2}{\sqrt{\pi}} N^o e^{-\lambda t} \int_o^\infty e^{-\xi^2} d\xi,\ t > 0$$

$$= N^o e^{-\lambda t},\ t > 0$$

by using $\int_o^\infty e^{-\xi^2} d\xi = {}^{\sqrt{\pi}}/2$.

Therefore $N(o,t) = N^o e^{-\lambda t}$, $t > 0$.

(d) $N(\infty,t) = 0$, $t > 0$.

As shown in (c), the integrand is continuous in (z,t), ξ for (z,t), ξ on S, C, and the integral converges uniformly and absolutely in $(z,t)\in S$. Therefore we can exchange the order of $\lim_{z\to\infty}$ and $\int$, obtaining

$$\lim_{z\to\infty} N(z,t) = \frac{2}{\sqrt{\pi}} N^o e^{-\lambda t} \lim_{z\to\infty} \left\{ \int_{\frac{\nu\beta z}{2\sqrt{t}}}^{\infty} e^{-\left(\xi - \frac{\nu z}{2\xi}\right)^2} \operatorname{erfc}\left(\frac{Y}{2\sqrt{t-YA}}\right) d\xi \right\}$$

$$= \frac{2}{\sqrt{\pi}} N^o e^{-\lambda t} \int_{\infty}^{\infty} \lim_{z\to\infty} \left[e^{-\left(\xi - \frac{\nu z}{2\xi}\right)^2} \operatorname{erfc}\left(\frac{Y}{2\sqrt{t-YA}}\right)\right] d\xi \, .$$

The exponential term in the integrand becomes zero as $z \to \infty$. The argument of "erfc" function tends to zero, and so "erfc" function to unity. Thus, the integrand becomes zero as $z \to \infty$. Hence

$N(\infty,t) = 0$ for $t > 0$.

(e) $M(b,z,t) = N(z,t), \quad z > 0, \; t > 0$

This is easily shown from (3.41) and (3.42) by setting $y = b$ in (3.42).

(f) $M(\infty,z,t) = 0, \; z > 0, \; t > 0$.

The integrand in $M(y,z,t)$ is integrable in ξ over every finite subinterval of C for any (y,z,t) in $S' \equiv \{y \geq b, \; z \geq 0, \; t \geq 0\}$. The integrand is also continuous in (y,z,t), ξ for $(y,z,t),\xi$ on S', C. The integrand is bounded by

$$\left| e^{-\xi^2 - \frac{\nu^2 z^2}{4\xi^2}} \operatorname{erfc}\left(\frac{Y+B(y-b)}{2\sqrt{t-YA}}\right) \right| \leq e^{-\xi^2} \text{ for all } (y,z,t) \in S' \text{ and } \xi \in C,$$

where

$\int_C e^{-\xi^2} d\xi \leq \frac{\sqrt{\pi}}{2}$. Therefore the integral converges absolutely and uniformly and is continuous in (y,z,t) for $(y,z,t) \in S'$. Then the order of $\lim_{y\to\infty}$ and $\int$ can be exchanged. Since

$$\lim_{y\to\infty} \operatorname{erfc}\left(\frac{Y+B(y-b)}{2\sqrt{t-YA}}\right) = 0, \; z > 0, \; t > 0$$

the integral becomes zero as $y \to \infty$. Therefore

$$\lim_{y\to\infty} M(y,z,t) = 0, \; z > 0, \; t > 0.$$

[2] Equation (3.2)

Next we will show that the proposed solution for M(y,z,t), i.e., (3.42) satisfies the governing equation (3.2). Instead of substituting (3.42) directly into (3.2), we assume the solution of (3.2) to be of the form of

$$M(y,z,t) = \frac{2}{\sqrt{\pi}} N^o e^{\nu z-\lambda t} K(y,t;z) . \tag{A}$$

On substitution of (A) into (3.2), we obtain an equation which K(y,t;z) should satisfy:

$$\frac{\partial^2 K}{\partial y^2} = B^2 \frac{\partial K}{\partial t}, \; t > 0, \; y > b \tag{B}$$

subject to $\quad K(y,o;z) = 0 \qquad y > b, \; z > 0$

$\quad K(\infty,t;z) = 0 \qquad t > 0, \; z > 0$

and $\quad K(b,t;z) = \frac{\sqrt{\pi}}{2N^o} \; e^{\lambda t-\nu z} N(z,t), \; t > 0, \; z > 0$

where the side conditions for K(y,t;z) have been checked as shown in [1].

Comparing (3.42) and (A), we must show that

$$K(y,t;z) = \int_{\frac{\nu\beta z}{2\sqrt{t}}}^{\infty} e^{-\xi^2 - \frac{\nu^2 z^2}{4\xi^2}} \operatorname{erfc}\left(\frac{Y+B(y-b)}{2\sqrt{t-YA}}\right) d\xi, \; t > 0, \; y \geq b, \; z \geq 0 \tag{C}$$

satisfies (B). First we must show the validity of the differentiation operations of the improper integral (C), so we must establish that

(i) the integral (C) converges in $S' = \{t \geq 0, \; y \geq b, \; z \geq 0\}$

and

(ii) $\frac{\partial K}{\partial t}$, $\frac{\partial K}{\partial y}$ and $\frac{\partial^2 K}{\partial y^2}$ converge uniformly in S'.

For (i), as shown in [1](f), the integral in M(y,z,t) which is identical to K(y,z,t) is uniformly convergent and continuous in (y,z,t) for $(y,z,t) \in S'$.

For (ii),

$$\frac{\partial K}{\partial t} = -f\left(y,z,t; \frac{\nu\beta z}{2\sqrt{t}}\right) \cdot \frac{\partial}{\partial t}\left(\frac{\nu\beta z}{2\sqrt{t}}\right) + \int_{\frac{\nu\beta z}{2\sqrt{t}}}^{\infty} \frac{\partial f}{\partial t} \, d\xi ,$$

where $f(y,z,t;\xi)$ is the integrand of $K(y,t;z)$.

The first term becomes zero because

$$f\left(y,z,t;\frac{\nu\beta z}{2\sqrt{t}}\right) = e^{-\left(\frac{\nu^2\beta^2 z^2}{4t}\right) - \frac{t}{\beta^2}} \operatorname{erfc}(\infty) = 0.$$

Hence we have

$$\frac{\partial K}{\partial t} = \int_{\frac{\nu\beta z}{2\sqrt{t}}}^{\infty} \frac{\partial f}{\partial t}\, d\xi = \int_{\frac{\nu\beta z}{2\sqrt{t}}}^{\infty} e^{-\xi^2 - \frac{\nu^2 z^2}{4\xi^2}}\, \bar{f}(\xi;y,z,t)\, d\xi, \qquad \text{(D)}$$

where $$\bar{f}(\xi;y,z,t) = \frac{2}{\sqrt{\pi}} \frac{Y+B(y-b)}{4(t-YA)^{3/2}}\, e^{-\frac{\{Y+B(y-b)\}^2}{4(t-YA)}}.$$

For $\xi = \frac{\nu\beta z}{2\sqrt{t}}$, $\bar{f}\left(\frac{\nu\beta z}{2\sqrt{t}}; y,z,t\right) = 0$.

For $\xi \geq \frac{\nu\beta z}{2\sqrt{t}} + \varepsilon$, $\varepsilon > 0$, $t - YA \geq \delta > 0$.

$$\therefore \left| e^{-\xi^2 - \frac{\nu^2 z^2}{4\xi^2}}\, \bar{f}(\xi;y,z,t) \right| \leq \frac{2}{\sqrt{\pi}} \frac{1}{2\delta} \left[\frac{Y-B(y-b)}{2\sqrt{t-YA}}\, e^{-\left\{\frac{Y+B(y-b)}{2\sqrt{t-YA}}\right\}^2} \right] e^{-\xi^2}$$

$$\leq \frac{1}{\sqrt{\pi}} \left(\frac{1}{\delta} \sqrt{\frac{1}{2}}\, e^{-1/2} \right) e^{-\xi^2}$$

for all $\xi \in C$ and $(y,z,t) \in S'$,

because by setting $P' = \frac{Y+B(y-b)}{2\sqrt{t-YA}}$, the function of $p'e^{-p'^2}$ has the maximum at $P' = \frac{1}{\sqrt{2}}$. Hence the integrand is bounded and also continuous in $(y,z,t) \in S'$ and $\xi \in C$. Therefore, by expressing $M = \frac{1}{2\delta}\sqrt{\frac{1}{2}}\, e^{-1/2}$

$$\left| \frac{\partial K}{\partial t} \right| \leq \frac{2}{\sqrt{\pi}} M \int_{\frac{\nu\beta z}{2\sqrt{t}}}^{\infty} e^{-\xi^2}\, d\xi \leq \frac{2}{\sqrt{\pi}} M \int_{0}^{\infty} e^{-\xi^2}\, d\xi = M,$$

which shows $\frac{\partial K}{\partial t}$ is uniformly convergent and continuous in $(y,z,t) \in S'$.

Similarly, for $\frac{\partial K}{\partial y}$ and $\frac{\partial^2 K}{\partial y^2}$, where

$$\frac{\partial K}{\partial y} = -\int_{\frac{\nu\beta z}{2\sqrt{t}}}^{\infty} e^{-\xi^2 - \frac{\nu^2 z^2}{4\xi^2}} \frac{2}{\sqrt{\pi}} \frac{B}{2\sqrt{t-YA}} e^{-\frac{\{Y+B(y-b)\}^2}{4(t-YA)}} d\xi, \quad (y,z,t) \in S', \tag{E}$$

and

$$\frac{\partial^2 K}{\partial y^2} = B^2 \int_{\frac{\nu\beta z}{2\sqrt{t}}}^{\infty} e^{-\xi^2 - \frac{\nu^2 z^2}{4\xi^2}} \frac{2}{\sqrt{\pi}} \frac{Y+B(y-b)}{4(t-YA)^{3/2}} e^{-\frac{\{Y+B(y-b)\}^2}{4(t-YA)}} d\xi, \quad (y,z,t) \in S', \tag{F}$$

the integrands are continuous and bounded in (y,z,t) and ξ for $(y,z,t) \in S'$ and $\xi \in C$. Hence both $\frac{\partial K}{\partial y}$ and $\frac{\partial^2 K}{\partial y^2}$ are uniformly convergent and continuous in $(y,z,t) \in S'$. Thus, we showed the validity of the differentiation operation for the improper integral (C).

By comparing (D) and (F), one can immediately say that (C) satisfies (B), which verifies that (3.42) satisfies (3.2).

[3] Equation (3.1)

Thirdly, we will show that (3.41) satisfies (3.1). Instead of substituting (3.41) into (3.1), we assume the solution of (3.1) to be of the form of

$$N(z,t) = \frac{2}{\sqrt{\pi}} N^o e^{\nu z-\lambda t} I(z,t). \tag{G}$$

On substitution of (G) into (3.1), we obtain an equation which I(z,t) should satisfy:

$$-\nu^2 I + \frac{\partial^2 I}{\partial z^2} - \frac{R_f}{D}\frac{\partial I}{\partial t} - \frac{q}{bD} e^{-\nu z+\lambda t} \frac{\sqrt{\pi}}{2N^o} = 0, \; t > 0, \; z > 0 \tag{H}$$

subject to
$$I(z,0) = 0, \qquad z > 0$$
$$I(o,t) = \sqrt{\pi}/2, \qquad t > 0$$
$$I(\infty,t) = 0, \qquad t > 0$$

where the side conditions for I(z,t) are already shown to be satisfied by I(z,t) as shown in [1]. Therefore we must show that

$$I(z,t) = \int_{\frac{\nu\beta z}{2\sqrt{t}}}^{\infty} e^{-\xi^2 - \frac{\nu^2 z^2}{4\xi^2}} \operatorname{erfc}\left(\frac{Y}{2\sqrt{t-YA}}\right) d\xi, \; (z,t)\in S \tag{J}$$

satisfies (H). By using (E), we obtain

$$\left.\frac{\partial K}{\partial y}\right|_{y=b} = -\int_{\frac{\nu\beta z}{2\sqrt{t}}}^{\infty} e^{-\xi^2 - \frac{\nu^2 z^2}{4\xi^2}} \frac{2}{\sqrt{\pi}} \frac{1}{2\sqrt{t-YA}} e^{-\frac{Y^2}{4(t-YA)}} d\xi .$$

Therefore, $\frac{q}{bD}$ can be written as, from the definition of q,

$$\frac{q}{bD} = \frac{R_f}{D}\frac{N^o}{A}\frac{2}{\sqrt{\pi}} e^{\nu z-\lambda t} \int_{\frac{\nu\beta z}{2\sqrt{t}}}^{\infty} e^{-\xi^2 - \frac{\nu^2 z^2}{4\xi^2}} \frac{2}{\sqrt{\pi}} \frac{1}{2\sqrt{t-YA}} \exp\left(-\frac{Y^2}{4(t-YA)}\right) d\xi,$$

$$z > 0, \; t > 0.$$

But considering

$$\frac{\partial}{\partial t}\operatorname{erfc}\left(\frac{Y}{2\sqrt{t-YA}}\right) = \frac{2}{\sqrt{\pi}}\frac{Y}{4}\frac{1}{(t-YA)^{3/2}} e^{-\frac{Y^2}{4(t-YA)}},$$

$$t > 0, \; z > 0, \; z > \frac{\nu\beta z}{2\sqrt{t}}, \tag{K}$$

one can rewrite $\frac{q}{bD}$ as

$$\frac{q}{bD}\ \frac{\sqrt{\pi}}{2N^o}\ e^{-\nu z+\lambda t} = \frac{R_f}{D}\int_{\frac{\nu\beta z}{2\sqrt{t}}}^{\infty} e^{-\xi^2-\frac{\nu^2 z^2}{4\xi^2}}\ \frac{2(t-YA)}{YA}\ \frac{\partial}{\partial t}\,\mathrm{erfc}\left(\frac{Y}{2\sqrt{t-YA}}\right) d\xi,$$

$$t > 0,\ z > 0\ .$$

By substituting this into (H), (H) becomes

$$-\nu^2 I + \frac{\partial^2 I}{\partial z^2} - \frac{R_f}{D}\frac{\partial I}{\partial t} - \frac{R_f}{D}\int_{\frac{\nu\beta z}{2\sqrt{t}}}^{\infty} e^{-\xi^2-\frac{\nu^2 z^2}{4\xi^2}}\ \frac{2(t-YA)}{YA}\ \frac{\partial}{\partial t}\,\mathrm{erfc}\left(\frac{Y}{2\sqrt{t-YA}}\right) d\xi = 0,$$

$$t > 0,\ z > 0. \qquad \text{(H')}$$

Next, let us check the validity of the differentiation operations of the improper integral (J). We follow the same procedure as in the previous section.

For the convergence of $I(z,t)$, we have already shown in [1](C) that the integral in $N(z,t)$, which is identical to $I(z,t)$, is uniformly convergent and continuous in (z,t) for $(z,t)\in S = \{z \geq 0,\ t > 0\}$.

For $\frac{\partial I}{\partial t}$, we have

$$\frac{\partial I}{\partial t} = \int_{\frac{\nu\beta z}{2\sqrt{t}}}^{\infty} e^{-\xi^2-\frac{\nu^2 z^2}{4\xi^2}}\ \frac{2}{\sqrt{\pi}}\ \frac{1}{4}\ \frac{Y}{(t-YA)^{3/2}}\ e^{-\frac{Y^2}{4(t-YA)}}\ d\xi\ .$$

The integrand is continuous in $(z,t)\in S$ and $\xi\in C$. By the same argument as for $\frac{\partial K}{\partial t}$, except that here $P' = \frac{Y}{2\sqrt{t-YA}}$, the integrand is bounded by $\frac{2}{\sqrt{\pi}}\ Me^{-\xi^2}$ for all $\xi\in C$ and $(z,t)\in S$. Therefore

$$\left|\frac{\partial I}{\partial t}\right| \leq \frac{2}{\sqrt{\pi}}\ M\int_0^{\infty} e^{-\xi^2}\ d\xi = M,$$

which shows the uniform convergence and the continuity of $\frac{\partial K}{\partial t}$ in $(z,t)\in S$.

For $\frac{\partial I}{\partial z}$, we have

$$\frac{\partial I}{\partial z} = \lim_{\eta \to \frac{\nu\beta z}{2\sqrt{t}}} \int_{\eta}^{\infty} \left(- \frac{\nu^2 z^2}{2\xi^2} \right) e^{-\xi^2 - \frac{\nu^2 z^2}{4\xi^2}} \operatorname{erfc}\left(\frac{Y}{2\sqrt{t-YA}} \right) d\xi$$

$$+ \int_{\frac{\nu\beta z}{2\sqrt{t}}}^{\infty} e^{-\xi^2 - \frac{\nu^2 z^2}{4\xi^2}} \frac{\partial}{\partial z} \operatorname{erfc}\left(\frac{Y}{2\sqrt{t-YA}} \right) d\xi, \; z > 0, \; t > 0. \qquad \text{(L)}$$

Noting that

$$\frac{\partial Y}{\partial z} = \frac{\beta^2 \nu^2 z}{2A\xi^2}, \; \frac{\partial Y}{\partial \xi} = - \frac{\beta^2 \nu^2 z^2}{2A\xi^3}, \; z > 0, \; t > 0, \; \xi > \frac{\nu\beta z}{z\sqrt{t}} ,$$

$\frac{\partial}{\partial z} \operatorname{erfc}\left(\frac{Y}{2\sqrt{t-YA}} \right)$ can be expressed as

$$\frac{\partial}{\partial z} \operatorname{erfc}\left(\frac{Y}{2\sqrt{t-YA}} \right) = - \frac{\xi}{z} \frac{\partial}{\partial \xi} \operatorname{erfc}\left(\frac{Y}{2\sqrt{t-YA}} \right) , \; z > 0, \; t > 0, \; \xi > \frac{\nu\beta z}{2\sqrt{t}} \qquad \text{(M)}$$

Since $e^{-\xi^2 - \frac{\nu^2 z^2}{4\xi^2}}$ and $\operatorname{erfc}\left(\frac{Y}{2\sqrt{t-YA}} \right)$ have continuous derivatives with respect to ξ in $\xi \in \overline{C} \equiv \left\{ \xi > {}^{\nu\beta z}/2\sqrt{t} \right\}$, and the resultant integral is uniformly convergent in (z,r) for $(z,t) \in \overline{S} \equiv \left\{ z > 0, \; t > 0 \right\}$ as shown below, one can make the integration by parts for the second term of (L), resulting in

$$\frac{\partial I}{\partial z} = \lim_{\eta \to \frac{\nu\beta z}{2\sqrt{\tau}}} \int_{\eta}^{\infty} \left(\frac{1}{z} - \frac{2\xi^2}{z} \right) e^{-\xi^2 - \frac{\nu^2 z^2}{4\xi^2}} \operatorname{erfc}\left(\frac{Y}{2\sqrt{t-YA}} \right) d\xi, \text{ for all } (z,t) \in \overline{S} . \qquad \text{(L')}$$

By using this

$$\left|\frac{\partial I}{\partial z}\right| \leq \int_0^\infty \left| \left(\frac{1}{z} - \frac{2\xi^2}{z}\right) e^{-\xi^2 - \frac{\nu^2 z^2}{4\xi^2}} \right| d\xi, \text{ for all } (z,t)\in S'$$

By setting $\mu = \frac{\nu z}{2\xi}$,

$$\left|\frac{\partial I}{\partial z}\right| \leq \frac{\nu}{2} \int_0^\infty \left| \left(-\frac{1}{2\mu^2} + \frac{\nu^2 z^2}{4}\right) e^{-\mu^2 - \frac{\nu^2 z^2}{4\mu^2}} \right| d\mu . \qquad (*)$$

Considering the identity(1):

$$\int_0^\infty e^{-\xi^2 - \frac{X^2}{\xi^2}} d\xi = \frac{\sqrt{\pi}}{2} e^{-2X}, \; X > 0 \qquad (**)$$

and its second derivative with respect to X,

$$\int_0^\infty \left(-\frac{1}{2\xi^2} + \frac{X^2}{\xi^4}\right) e^{-\xi^2 - \frac{X^2}{\xi^2}} d\xi = \frac{\sqrt{\pi}}{2} e^{-2X}, \; X > 0,$$

(this differentiation is justified since these improper integrals are bounded by $\frac{\sqrt{\pi}}{2}$, independent of X and have continuous integrands in $\xi > 0$, which means they are continuous and uniformly convergent for all $X > 0$), the integral (*) becomes

$$\left|\frac{\partial I}{\partial z}\right| \leq \frac{\nu}{2} \int_0^\infty e^{-\mu^2 - \frac{\nu^2 z^2}{4\mu^2}} d\mu \leq \frac{\nu}{2} \int_0^\infty e^{-\mu^2} d\mu = \frac{\nu\sqrt{\pi}}{4} .$$

And the integrand of (L') is continuous in (z,t) and ξ for $(z,t)\in\bar{S}$, $\xi\in\bar{C}$. Therefore $\frac{\partial I}{\partial z}$ is continuous and uniformly convergent in $(z,t)\in\bar{S}$.

Differentiating (L') once more with respect to z, we obtain

$$\frac{\partial^2 I}{\partial z^2} = \int_{\frac{\nu\beta z}{2\sqrt{t}}}^{\infty} \left(-\frac{1}{z^2} - \frac{\nu^2}{2\xi^2}\right) (1-2\xi^2)\, e^{-\xi^2 - \frac{\nu^2 z^2}{4\xi^2}} \operatorname{erfc}\left(\frac{Y}{2\sqrt{t-YA}}\right) d\xi$$

$$+ \int_{\frac{\nu\beta z}{2\sqrt{t}}}^{\infty} (1-2\xi^2)\, \frac{1}{z}\, e^{-\xi^2 - \frac{\nu^2 z^2}{4\xi^2}} \frac{\partial}{\partial z} \operatorname{erfc}\left(\frac{Y}{2\sqrt{t-YA}}\right) d\xi,$$

for all $(z,t)\in\overline{S}$. (N)

Since $\frac{1}{z}(1-2\xi^2)e^{-\xi^2 - \frac{\nu^2 z^2}{4\xi^2}}$ and $\operatorname{erfc}\left(\frac{Y}{2\sqrt{t-YA}}\right)$ have continuous derivatives with respect to ξ in $(z,t)\in\overline{S}$ and $\xi\in\overline{C}$, one can make the integration by parts for the second term in (N) as was done for (L), resulting in

$$\frac{\partial^2 I}{\partial z^2} = \int_{\frac{\nu\beta z}{2\sqrt{t}}}^{\infty} \frac{1}{z^2} \left(-6\xi^2 + 4\xi^4\right) e^{-\xi^2 - \frac{\nu^2 z^2}{4\xi^2}} \operatorname{erfc}\left(\frac{Y}{2\sqrt{t-YA}}\right) d\xi, \qquad \text{(N')}$$

for all $(z,t)\in\overline{S}$.

By using this,

$$\left|\frac{\partial^2 I}{\partial z^2}\right| \leq \int_0^{\infty} \left|\frac{1}{z^2}\left(-6\xi^2 + 4\xi^4\right) e^{-\xi^2 - \frac{\nu^2 z^2}{4\xi^2}}\right| d\xi.$$

By differentiating (**) three times with respect to X,

$$\int_0^{\infty} \left(\frac{X^3}{\xi^6} - \frac{3X}{2\xi^4}\right) e^{-\xi^2 - \frac{X^2}{\xi^2}} d\xi = \frac{\sqrt{\pi}}{2} e^{-2X}.$$

Therefore

$$\left|\frac{\partial^2 I}{\partial z^2}\right| \leq \nu^2 \int_0^{\infty} \left(\frac{\nu^3 z^3}{8\mu^6} - \frac{3}{2}\frac{\nu z}{\mu^4}\right) e^{-\mu^2 - \frac{\nu^2 z^2}{4\mu^2}} d\mu$$

$$= \nu^2 \int_0^\infty e^{-\mu^2 - \frac{\nu^2 z^2}{4\mu^2}} d\mu \leq \nu^2 \frac{\sqrt{\pi}}{2} .$$

And the integrand of (N') is continuous in (z,t) and ξ for $(z,t)\in\bar{S}$ and $\xi\in\bar{C}$. Therefore $\frac{\partial^2 I}{\partial z^2}$ is continuous and uniformly convergent in $(z,t)\in\bar{S}$.

By substituting (L') and (M') into the left hand side of (H'), we obtain

$$(\text{l.h.s.}) = \int_{\frac{\nu\beta z}{2\sqrt{t}}}^{\infty} \left(-\nu^2 - \frac{6\xi^2}{z^2} + \frac{4\xi^4}{z^2}\right) e^{-\xi^2 - \frac{\nu^2 z^2}{4\xi^2}} \operatorname{erfc}\left(\frac{Y}{2\sqrt{t-YA}}\right) d\xi$$

$$- \frac{R_f}{D} \int_{\frac{\nu\beta z}{2\sqrt{t}}}^{\infty} e^{-\xi^2 - \frac{\nu^2 z^2}{4\xi^2}} \frac{(2t-YA)}{YA} \frac{\partial}{\partial t} \operatorname{erfc}\left(\frac{Y}{2\sqrt{t-YA}}\right) d\xi \qquad \text{(P)}$$

for $(z,t)\in\bar{S}$.

But from (K) and (M), we have

$$\frac{\partial}{\partial t} \operatorname{erfc}\left(\frac{Y}{2\sqrt{t-YA}}\right) = \frac{\xi}{2(2t-YA)} \frac{\partial}{\partial \xi} \operatorname{erfc}\left(\frac{Y}{2\sqrt{t-YA}}\right), \qquad \text{(Q)}$$

for $(z,t)\in\bar{S}$, $\xi\in\bar{C}$.

Substituting (Q) into the second term of (P) yields

$$(\text{2nd term}) = \int_{\frac{\nu\beta z}{2\sqrt{t}}}^{\infty} \left[e^{-\xi^2 - \frac{\nu^2 z^2}{4\xi^2}} \frac{2\xi^3}{z^2}\right] \frac{\partial}{\partial \xi} \operatorname{erfc}\left(\frac{Y}{2\sqrt{t-YA}}\right) d\xi, \quad (z,t)\in\bar{S}.$$

Since both $\left[e^{-\xi^2 - \frac{\nu^2 z^2}{4\xi^2}} \frac{2\xi^3}{z^2}\right]$ term and $\operatorname{erfc}\left(\frac{Y}{2\sqrt{t-YA}}\right)$ have continuous derivatives with respect to ξ in $\xi\in C$, $(z,t)\in\bar{S}$, one can make the integration by parts and obtain

$$(\text{2nd term}) = -\int_{\frac{\nu\beta z}{2\sqrt{t}}}^{\infty} \left(\frac{6\xi^2}{z^2} - \frac{4\xi^4}{z^2} + \nu^2\right) e^{-\xi^2 - \frac{\nu^2 z^2}{4\xi^2}} \operatorname{erfc}\left(\frac{Y}{2\sqrt{t-YA}}\right) d\xi$$

$(z,t)\in\bar{S}$.

Therefore (1.h.s.) = 0 .

Hence it is verified that (J) satisfies (H), and so that (3.41) satisfies (3.1).

Hence (3.41) and (3.42) are the solutions for this problem.

Reference

(1) Abramowitz and Stegun, Handbook of Mathematical Functions, Dover, New York.

(2) Theorems used here were referred from:

P. L. Chambré and E. L. Pinney, "Notes for Mathematics 120," Department of Mathematics, University of California, Berkeley, 1984,

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LAWRENCE BERKELEY LABORATORY
TECHNICAL INFORMATION DEPARTMENT
UNIVERSITY OF CALIFORNIA
BERKELEY, CALIFORNIA 94720