

**SKBF**  
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**82-05**

**Migration of radionuclides in fissured  
rock –  
Results obtained from a model based  
on the concepts of hydrodynamic  
dispersion and matrix diffusion**

Anders Rasmuson  
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Royal Institute of Technology  
Department of Chemical Engineering  
Stockholm, Sweden, May 1982

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MIGRATION OF RADIONUCLIDES IN FISSURED ROCK -  
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OF HYDRODYNAMIC DISPERSION AND MATRIX DIFFUSION

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This report concerns a study which was conducted for SKBF/KBS. The conclusions and viewpoints presented in the report are those of the author(s) and do not necessarily coincide with those of the client.

A list of other reports published in this series during 1982, is attached at the end of this report. Information on KBS technical reports from 1977-1978 (TR 121), 1979 (TR 79-28), 1980 (TR 80-26) and 1981 (TR 81-17) is available through SKBF/KBS.

Migration of radionuclides in fissured rock -  
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## SUMMARY

The migration of individual radionuclides in a porous medium where hydrodynamic dispersion takes place and where the radionuclides migrate in the matrix of solid medium by diffusion has been calculated for a variety of cases. The cases center around the main case in the second KBS study on spent fuel. The main differences from the KBS study is the inclusion of matrix diffusion and the use of large dispersivities.

The effluent rates of 23 important nuclides are presented as functions of distance and time for various values of important parameters such as rock permeability, diffusion coefficients, release rates, time of first release, fissure spacing and longitudinal dispersion coefficients.

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## 1 INTRODUCTION

In the Swedish concept, the final repository for high level waste is to be in crystalline rock at 500 m depth (KBS 1978). To this end moderately fissured crystalline rocks such as Swedish granite and gneiss were investigated. The bedrock has a low hydraulic conductivity. Water flow occurs in fractures in the rock. Radionuclides may interact in several ways with the bedrock. Radionuclides may migrate into the micropores of the rock through the mechanism of molecular diffusion (Neretnieks, 1980). Many nuclides will sorb (e.g. adsorption, ion exchange) on the pore surfaces.

A one-dimensional transport model of this process was presented in Rasmuson and Neretnieks (1981). The model considers diffusion of nuclides into microfissures of the rock, linear sorption, and flow and longitudinal dispersion in the bedrock. Using this model, a number of simulations have been performed for estimated ranges of input parameters. The results of these calculations are presented in this report.

## 2 MATHEMATICAL MODEL

The mathematical model and its analytical solution are presented in detail in Rasmuson and Neretnieks (1980, 1981). A summary is given below.

In the analysis the rock is regarded as a double-porosity medium, consisting of porous blocks separated by fissures. Since the permeability of solid rock is very low, water flow is assumed to take place only in fissures. However, transport of dissolved constituents to the interior of the rock blocks takes place via the mechanism of molecular diffusion.

In mathematical terms, the process is governed by two coupled transport equations, one for the fissures and one for the blocks.

For flow and sorption from the water in the fissures we have:

$$\frac{\partial C_f}{\partial t} + U_f \frac{\partial C_f}{\partial z} - D_L \frac{\partial^2 C_f}{\partial z^2} = - \frac{1-\epsilon_f}{\epsilon_f} \left( \frac{\partial \bar{q}}{\partial t} \right) - \lambda_d C_f \quad (1)$$

The terms in this equation represent accumulation in water in the fissures, convective transport, transport by axial dispersion, accumulation in the blocks, and radioactive decay.



Diffusion into the matrix (assuming spherical blocks) is given by:

$$K \frac{\partial C_p}{\partial t} = \epsilon_p D_p \left( \frac{\partial^2 C_p}{\partial r^2} + \frac{2}{r} \frac{\partial C_p}{\partial r} \right) - K \lambda_d C_p \quad (2)$$

In this equation, the terms give sorption on the interior surfaces + accumulation in the pore fluid, radial diffusion in the pore fluid, and radioactive decay.

In a system which is initially free of nuclides, and in which the inlet ( $z=0$ ) nuclide concentration suddenly is increased to  $C_0$  at time  $t_0$ , and then decreased to 0 again at  $t_0 + \Delta t$ , the initial and boundary conditions are:

$$C_f(0, t) = \begin{cases} C_0 e^{-\lambda_d t} & t_0 \leq t \leq t_0 + \Delta t \\ 0 & t < t_0, t_0 + \Delta t < t \end{cases} \quad (3)$$

$$C_f(\infty, t) = 0 \quad (4)$$

$$C_f(z, 0) = 0 \quad (5)$$

$$\frac{\partial C_p}{\partial r}(0, z, t) = 0 \quad (6)$$

$$C_p(r_0, z, t) = C_p|_{r=r_0} \quad \text{given by} \quad \frac{\partial \bar{q}}{\partial t} = \frac{3k_f}{r_0} (C_f - C_p|_{r=r_0}) \quad (7)$$

$$C_p(r, z, 0) = 0 \quad (8)$$

The simultaneous solution for equations (1) and (2), with the boundary conditions indicated, has been obtained by the Laplace transform method and inversion in the complex plane (Rasmuson and Neretnieks, 1980).

In terms of the following dimensionless parameters:

$$\delta = \frac{3D_p \varepsilon_p}{r_o^2} \frac{z}{mU_f} \quad \text{bed length parameter}$$

$$R = \frac{K}{m} \quad \text{distribution ratio}$$

$$Pe = \frac{zU_f}{D_L} \quad \text{Peclet number}$$

$$y = \frac{2D_p \varepsilon_p}{Kr_o^2} t \quad \text{contact time parameter}$$

$$v = \frac{D_p \varepsilon_p}{k_f r_o} \quad \text{film resistance parameter}$$

the concentration in the fissures  $C_f$  is obtained as:

$$\frac{C_f}{C_o} = e^{-\lambda_d t} \left[ u(z, t - t_o) H(t - t_o) - u(z, t - (t_o + \Delta t)) H(t - (t_o + \Delta t)) \right] \quad (9)$$

where:

$$u(z, t) = \frac{1}{2} + \frac{2}{\pi} \int_0^{\infty} \exp\left(\frac{1}{2} \text{Pe} - \sqrt{\frac{(z^2_{x'})^2 + (z^2_{y'})^2}{2} + z^2_{x'}}\right) \sin\left(y \lambda^2 - \sqrt{\frac{(z^2_{x'})^2 + (z^2_{y'})^2}{2} - z^2_{x'}}\right) \frac{d\lambda}{\lambda} \quad (10)$$

and:

$$z^2_{x'} = \text{Pe} \left(\frac{1}{4} \text{Pe} + \delta H_1\right) \quad (11)$$

$$z^2_{y'} = \delta \text{Pe} \left(\frac{2}{3} \frac{\lambda^2}{R} + H_2\right) \quad (12)$$

$$H_1(\lambda, \nu) = \frac{H_{D1} + \nu(H_{D1}^2 + H_{D2}^2)}{(1 + \nu H_{D1})^2 + (\nu H_{D2})^2} \quad (13)$$

$$H_2(\lambda, \nu) = \frac{H_{D2}}{(1 + \nu H_{D1})^2 + (\nu H_{D2})^2} \quad (14)$$

$$H_{D1}(\lambda) = \lambda \left(\frac{\sinh 2\lambda + \sin 2\lambda}{\cosh 2\lambda - \cos 2\lambda}\right) - 1 \quad (15)$$

$$H_{D2}(\lambda) = \lambda \left(\frac{\sinh 2\lambda - \sin 2\lambda}{\cosh 2\lambda - \cos 2\lambda}\right) \quad (16)$$

It was shown by Rasmuson and Neretnieks (1981) that the film resistance may be neglected ( $\nu \sim 0$ ). Then the functions  $H_1$  and  $H_2$  may be simplified to:

$$H_1(\lambda, \nu) = H_{D_1}(\lambda) \quad (17)$$

$$H_2(\lambda, \nu) = H_{D_2}(\lambda) \quad (18)$$

Furthermore, for all radionuclides (except the non-sorbing I-129), the value of the capacity quotient  $R$  is so large that its influence is negligible. This is true, except for very short contact times, and is a consequence of the fact that accumulation in the fluid in the fissures may be neglected.

Thus the expression for  $z^2 y'$  may be simplified to:

$$z^2 y' = \delta Pe H_2 \quad (19)$$

Assuming known values of hydraulic conductivity, hydraulic gradient and fissure spacing, fissure width, fissure porosity and average fracture velocity are calculated according to a model proposed by Snow (1968):

$$(2b)^3 = \frac{1}{2} \frac{12\mu}{\rho g} \cdot SK_p \quad (20)$$

$$\epsilon_f = 3 (2b/S) \quad (21)$$

$$U_f \epsilon_f = K_p i \quad (22)$$

To model internal diffusion, the cubic blocks used in the hydraulic model (Snow, 1968) are approximated by spheres having the same surface-to-volume ratio as a cubic block. Then:

$$r_o = 0.5 S \quad (23)$$

A method for evaluating the infinite integral in equation (10) is given by Rasmuson and Neretnieks (1981).

### 3 INPUT PARAMETERS

Calculations were made for the 23 nuclides listed in Table 1.

The input parameters in the model are:

Hydraulic conductivity	$K_p$	L/T
Hydraulic gradient	$i$	L/L
Constant in equation (20)	$12\mu/\rho g$	LT
Effective diffusivity in pores	$D_p \epsilon_p$	$L^2/T$
Fissure spacing	$S$	L
Half Life	$T_{1/2}$	T
Volume equilibrium constant	$K$	$L^3/L^3$
Distance	$z$	L
Peclet number	$Pe$	-
Time of canister penetration	$t_o$	T
Time for dissolution of waste	$\Delta t$	T

L = length

T = time

Half-lives and mass sorption coefficients were taken from the Nuclear Fuel Safety Project study (KBS, 1978). Mass sorption coefficients are converted to volume sorption coefficients  $K$  by multiplying by the rock density  $\rho_p = 2700 \text{ kg/m}^3$ .

$D_p$  is the diffusivity in the water in the pores and is related to the diffusivity in pure water by  $D_p = D_v \delta_D / \tau^2$ . Here  $\delta_D / \tau^2$  is a geometric factor. The diffusivity of strong electrolytes in water at ambient temperature is  $D_v \approx 1.3 \cdot 10^{-9} \text{ m}^2/\text{s}$ . The ratio  $\delta_D / \tau^2$  is expected to be somewhere in the interval 0.15 to 0.6 (Neretnieks, 1980) and the porosity  $\epsilon_p$  has been found to be 0.003-0.005 for the granites in this study. Expected values for the effective pore diffusivity  $D_p \epsilon_p$  would then be from  $4 \cdot 10^{-13} \text{ m}^2/\text{s}$  to  $10 \cdot 10^{-12} \text{ m}^2/\text{s}$ . This was experimentally confirmed by Skagius et al (1981). In the present study we used  $D_p \epsilon_p = 10^{-12} \text{ m}^2/\text{s}$ .

The hydraulic conductivity used was in the range  $10^{-7}$ - $10^{-9} \text{ m/s}$ . The low permeability value was observed in several boreholes in granite and gneiss in south Sweden (KBS, 1979). The fissure

spacing was taken as 1-50 m. This is substantiated by the bore-hole investigations. In the calculations we used a hydraulic gradient of 0.001 - 0.01 m/m.

The Peclet numbers used in the examples were based on a recent compilation of about 50 field measurements by Lallemand - Barrès and Peaudecerf (1978). The data of Lallemand - Barrès and Peaudecerf have Peclet numbers ranging from 0.5 to 50, with most of the data around 5.

Times for canister penetration of 40, 5000 and 100,000 years have been used. The dissolution times were 30,000 and 500,000 years.

Using these data  $\sigma = \frac{2D_p \epsilon_p}{Kr_o^2}$  (coefficient in y) and the dimensionless quantities  $\delta$  and  $R$  may be computed.

The influence of  $R$  is in most cases negligible. (See discussion under "Mathematical model".) In these cases, there is no need to determine  $U_f$  and  $\epsilon_f$  separately, since  $mU_f \approx K_p i$ , giving:

$$\delta = \frac{3D_p \epsilon_p}{r_o^2} \frac{z}{K_p i} \quad (24)$$

It is in the nature of a dimensionless quantity that infinitely many combinations of the individual variables correspond to a specific value of e.g.  $\delta$ . All combinations of variables which result in a given value of  $\delta$  yield the same mathematical solution. For example,  $z = 100$  m and  $K_p = 10^{-9}$  m/s give the same solution as  $z = 1000$  m and  $K_p = 10^{-8}$  m/s. Dimensionless breakthrough curves for the approximate range of variation of  $\delta$ ,  $R$  and  $Pe$  are given in Rasmuson and Neretnieks (1981).

The time for canister penetration  $t_o$  is counted from an arbitrary starting time, for example, the time at which the fuel is taken from the reactor. At that time, the waste contains  $N_i^0$  Curies of nuclide  $i$ /ton of waste. Since this initial inventory decays with time, the inventory of this nuclide at time  $t$  is:

$$N^i = N_0^i e^{-\lambda_d^i t} \quad [Ci/ton] \quad (25)$$

In this single nuclide migration study, only the part of the nuclide inventory originally present in the waste is considered. The release of nuclides is taken to be proportional to the dissolution rate of the waste. The dissolution rate is assumed to be constant over the whole dissolution time  $\Delta t$ . Accordingly, the release of a nuclide during this dissolution time is:

$$n^i = \frac{N^i}{\Delta t} \quad [Ci/ton, year] \quad (26)$$

or, using equation (25),

$$n^i = \frac{N_0^i e^{-\lambda_d^i t}}{\Delta t} \quad (27)$$

This amount of nuclide corresponds to an initial concentration  $C_0^i e^{-\lambda_d^i t}$  (boundary condition (3)) in the water flowing through the bedrock. The nuclide transported with the water will be retarded by diffusion into the microfissures of the rock and by subsequent sorption on the intrapore surfaces.

The concentration in the flowing water is observed at a distance  $z$  downstream. This concentration is obtained from equation (9). The discharge rate of nuclide  $i$  at distance  $z$  is:



$$n_z^i = n^i \frac{C_f^i}{C_o^i e^{-\lambda_d^i t}} = \frac{N_o^i}{\Delta t} \cdot \frac{C_f^i}{C_o^i} \left[ \frac{C_i}{\text{ton, year}} \right] \quad (28)$$

The fraction of the original inventory of nuclide  $i$  arriving each year at distance  $z$  is:

$$\frac{n_z^i}{N_o^i} = \frac{C_f^i}{\Delta t C_o^i} \left[ \frac{\text{fraction}}{\text{year}} \right] \quad (29)$$

#### 4 COMPUTED CASES

Data for the different cases are given in Table 2. All (432) possible combinations of the parameters are treated. Actually, computations were made for  $t_0 = 0$  only. Breakthrough curves for different times of canister penetration are then obtained by multiplying by  $\exp(-\lambda_d t_0)$  and plotting the results as a function of  $t + t_0$ . Since the breakthrough calculations are done for 23 nuclides with 2 curves each (up at  $t_0$  and down at  $t_0 + \Delta t$ ) but for  $t_0 = 0$  only, this corresponds to 6 624 breakthrough curves.

The computer program for the model is presented in Appendix. The purpose of each SUBROUTINE is given, as well as a listing of INPUT parameters. A SOURCE listing is also provided.

## 5 RESULTS

In each case, breakthrough curves for the 23 nuclides at a given distance were calculated versus time. The results for  $z = 1000$  m were plotted (72 diagrams). Figures 1-10 give some typical examples. The resulting curves are shown for all nuclides which have  $C_f/C_o$  larger than  $10^{-9}$  at any time.

In Figures 11-34, the maximum points on the breakthrough curves are plotted versus distance. To limit the number of figures, the time of canister penetration is set to 0. The curves for other  $t_o$  are then obtained by multiplication by  $\exp(-\lambda_d^i t_o)$ . These factors are given in Table 3 for  $t_o = 40, 5000$  and 100 000 years. It may be inferred from the Table that some nuclides will decay to insignificant levels within the lifetime of the canister shielding. This is the case for

$t_o$	Nuclides
40	Cm-242
5000	+ Cs-137, Sr-90, Pu-241, Cm-244, Am-242m, Pu-238
100 000	+ Am-241, Ra-226

On the other hand, some radionuclides, notably Pu-242, Tc-99, Np-237, Cs-135, I-129, and U-238, will not decay to any substantial degree within even 100 000 years.

For these nuclides, the retardation capacity of the bedrock is essential.

Table 4 gives an overview of the cases computed and a reference to figures.

## 6 DISCUSSION AND CONCLUSIONS

The input parameters may be divided into two categories;

## I. Nuclide - independent

$$K_p, i, 12\mu/\rho g, S, z, Pe, t_0, \Delta t$$

(the last two terms affect only the source boundary condition)

## II. Nuclide - dependent

$$D_p \varepsilon_p (?), T_{1/2}, K$$

In most situations, the only significant term is the product  $K_p i$  (see discussion in the section "Input parameters"). Furthermore, the constant  $12\mu/\rho g$  (dependent on temperature) affects only the capacity ratio  $R$ . It was shown that (except for I-129)  $R$  may be taken as  $\infty$ . The influence of the input parameters are illustrated in Figures 1-10.

The influence of  $K_p$  (or  $i$ ). Calculations were made with  $K_p$  at two values  $10^{-9}$  and  $10^{-7}$  m/s. The latter case corresponds to a higher water velocity, and thus a shorter time for interaction with the solid rock. Except for I-129,  $K_p$  will affect only the dimensionless parameter  $\delta$  (equation (24)). An increase in  $K_p$

by two orders of magnitude will cause a decrease in  $\delta$  of the same order. The effect on the breakthrough curve is shown in diagrams given by Rasmuson and Neretnieks (1981). Since, for most cases, only the product  $K_p i$  is important, the same results are obtained for a variation in the hydraulic gradient  $i$ .

Different values of  $\delta$  produce breakthrough curves for various degrees of saturation of the solid rock. Low values of  $\delta$  imply that only the outer surface of the rock is utilized for sorption. For this situation ( $\delta \lesssim 10^{-2}$ ), it was shown that  $C_f/C_o$  is a function of  $y/\delta^2$ , and not of  $y$  and  $\delta$  independently. High values of  $\delta$ , on the other hand, indicate full penetration of the blocks and,  $C_f/C_o$  is a function of  $y/\delta$  ( $\delta \gtrsim 10^2$ ) (Rasmuson and Neretnieks, 1981).

Figures 3 and 10 differ only in the value used for the hydraulic conductivity  $K_p$ . We get  $\delta = 1.2 \cdot 10^3$  and  $1.2 \cdot 10^1$  respectively. The high value of  $\delta$  implies almost complete penetration of the rock matrix. The low value is an intermediate case. From the breakthrough calculations, referred to above, it may be inferred that the time scale for the highly sorbing nuclides will change by a factor of  $\approx 5000$ . For Cs-135 and U-238, the first arrival is roughly that much earlier in Figure 10. Note that the same reasoning does not hold for the non-sorbing I-129. Because of the earlier breakthrough, a large number of nuclides will not have time to decay for  $K_p = 10^{-7}$  m/s.

### The influence of S

Two values of S were used S = 1 and 50 m. The fracture spacing primarily affects the size of the rock blocks (equation (23)). In principal, it will also have an effect on the water velocity and the fracture porosity. From equations (20) - (22), we get  $U_f \propto S^{2/3}$  and  $\epsilon_f \propto S^{-2/3}$ . However, from equation (24), we see again that only the product  $U_f \epsilon_f = K_p i$  (independent of S) is important.

Thus a higher value of  $r_o$  gives less surface for contact with the moving water. In terms of the dimensionless quantities, we find that both  $\delta$  and  $y$  are proportional to  $r_o^{-2}$ .

In Figures 1-3 and 4-6, the cases differ only in values of S, 1 and 50 m. We have:

$$\text{Figures 1-3: } \delta = 1.2 \cdot 10^3, \quad \sigma = 8 \cdot 10^{-12}/K$$

$$\text{Figures 4-6: } \delta = 0.48, \quad \sigma = 3.2 \cdot 10^{-15}/K$$

The influence of Pe

As shown in Rasmuson and Neretnieks (1981), the impact of longitudinal dispersion is severe. This is further illustrated in Figures 1-3 and Figures 4-6, in which the Peclet number in each group decreases as  $\infty$ , 5.0 and 0.5.

The influence of  $t_0$  is shown in Figures 6-8, which are for the same case with three different values of canister penetration time: 40, 5000 and 100 000 years. The figures again illustrate that, for many radionuclides, the proposed engineering barriers are ineffective in preventing the arrival of significant concentrations at the site boundaries. Comparing Figure 6 and Figure 8, we find that only the Pu-240 peak has disappeared below the base-line.

The influence of  $\Delta t$  is illustrated in Figures 5 and 9. As  $\Delta t$  increases the breakthrough concentration usually decreases. This is not always true, since  $u(z,t) - u(z,t - \Delta t) H(t - \Delta t)$  (a function of  $\Delta t$ ) may increase faster than  $\Delta t$ .

For example, consider the curve for I-129 at  $t = 2.83 \cdot 10^5$  years. We have



Figure 5 ( $\Delta t = 3 \cdot 10^4$  years):  $2.13 \cdot 10^{-11}$   
fraction of inventory/year

Figure 9 ( $\Delta t = 5 \cdot 10^5$  years):  $1.98 \cdot 10^{-6}$   
fraction of inventory/year

However, as shown in Figures 11-34, the peak concentrations for all the calculated cases are lower for  $\Delta t = 5 \cdot 10^5$  years.

The points discussed above are further illustrated in Figures 11-34, in which the peak heights versus distance are given. The impacts of the nuclide-dependent quantities  $T_{1/2}$  and  $K$  are clearly shown. A good example of the influence of  $T_{1/2}$  for constant  $K$  is given by the isotopes of Pu: Pu-238, Pu-239, Pu-240, Pu-241 and Pu-242. For an example of the influence of  $K$  when  $T_{1/2}$  is (approximately) constant see Tc-99 and U-234.

Nuclide	Half life, years	K, m <sup>3</sup> /m <sup>3</sup>
Sr-90	28.1	43
Tc-99	2.12 x 10 <sup>5</sup>	135
I-129	1.7 x 10 <sup>7</sup>	0.005
Cs-135	3.0 x 10 <sup>6</sup>	170
Cs-137	30.2	170
Ra-226	1,600	1,350
Th-229	7,340	6,480
Th-230	80,000	6,480
U-233	1.62 x 10 <sup>5</sup>	3,240
U-234	2.47 x 10 <sup>5</sup>	3,240
U-238	4.51 x 10 <sup>9</sup>	3,240
Np-237	2.14 x 10 <sup>6</sup>	3,240
Pu-238	86	810
Pu-239	24,400	810
Pu-240	6,580	810
Pu-241	13.2	810
Pu-242	3.79 x 10 <sup>5</sup>	810
Am-241	458	86,000
Am-242m	152	86,000
Am-243	7,370	86,000
Cm-242	0.5	43,000
Cm-244	17.6	43,000
Cm-245	9,300	43,000

Table 1: Nuclides considered in this study. No decay chains are accounted for.

hydraulic conductivity	$K_p$	$10^{-9}; 10^{-7}$	m/s
hydraulic gradient	$i$	0.01	m/m
constant (kinematic viscosity $10^{-6}$ m <sup>2</sup> /s)	$12\mu/\rho g$	$1.223242 \times 10^{-6}$	ms
$D_p \epsilon_p$		$10^{-12}$	m <sup>2</sup> /s
fissure spacing	$S$	1; 50	m
Peclet number	$Pe$	$\infty; 5.0; 0.5$	-
distance from repository	$z$	30; 100; 300; 1000; 3000; 10,000	m
leach time	$\Delta t$	30,000; 500,000	years
time of canister breakdown	$t_o$	40; 5000; 100,000	years

Table 2: Values of the input parameters

Nuclide	Half life years	Time of canister breakdown (years)		
		40	5000	100,000
Sr-90	28.1	$3.7281 \cdot 10^{-1}$	0	
Tc-99	$2.12 \cdot 10^5$	$9.9987 \cdot 10^{-1}$	$9.8379 \cdot 10^{-1}$	$7.2112 \cdot 10^{-1}$
I-129	$1.7 \cdot 10^7$	1.0	$9.9980 \cdot 10^{-1}$	$9.9593 \cdot 10^{-1}$
Cs-135	$3.0 \cdot 10^6$	$9.9999 \cdot 10^{-1}$	$9.9885 \cdot 10^{-1}$	$9.7716 \cdot 10^{-1}$
Cs-137	30.2	$3.9929 \cdot 10^{-1}$	0	
Ra-226	$1.6 \cdot 10^3$	$9.8282 \cdot 10^{-1}$	$1.1463 \cdot 10^{-1}$	0
Th-229	$7.34 \cdot 10^3$	$9.9623 \cdot 10^{-1}$	$6.2365 \cdot 10^{-1}$	$7.9209 \cdot 10^{-5}$
Th-230	$8.0 \cdot 10^4$	$9.9965 \cdot 10^{-1}$	$9.5760 \cdot 10^{-1}$	$4.2045 \cdot 10^{-1}$
U-233	$1.62 \cdot 10^5$	$9.9983 \cdot 10^{-1}$	$9.7883 \cdot 10^{-1}$	$6.5190 \cdot 10^{-1}$
U-234	$2.47 \cdot 10^5$	$9.9989 \cdot 10^{-1}$	$9.8607 \cdot 10^{-1}$	$7.5531 \cdot 10^{-1}$
U-238	$4.51 \cdot 10^9$	1.0	1.0	$9.9998 \cdot 10^{-1}$
Np-237	$2.14 \cdot 10^6$	$9.9999 \cdot 10^{-1}$	$9.9838 \cdot 10^{-1}$	$9.6813 \cdot 10^{-1}$
Pu-238	86	$7.2441 \cdot 10^{-1}$	0	
Pu-239	$2.44 \cdot 10^4$	$9.9886 \cdot 10^{-1}$	$8.6759 \cdot 10^{-1}$	$5.8381 \cdot 10^{-2}$
Pu-240	$6.58 \cdot 10^3$	$9.9580 \cdot 10^{-1}$	$5.9055 \cdot 10^{-1}$	$2.6612 \cdot 10^{-5}$
Pu-241	13.2	$1.2240 \cdot 10^{-1}$	0	
Pu-242	$3.79 \cdot 10^5$	$9.9993 \cdot 10^{-1}$	$9.9090 \cdot 10^{-1}$	$8.3286 \cdot 10^{-1}$
Am-241	$4.58 \cdot 10^2$	$9.4126 \cdot 10^{-1}$	$5.1719 \cdot 10^{-4}$	0
Am-242m	$1.52 \cdot 10^2$	$8.3326 \cdot 10^{-1}$	$1.2523 \cdot 10^{-10}$	0
Am-243	$7.37 \cdot 10^3$	$9.9625 \cdot 10^{-1}$	$6.2485 \cdot 10^{-1}$	$8.2913 \cdot 10^{-5}$
Cm-242	0.5	0		
Cm-244	17.6	$2.0694 \cdot 10^{-1}$	0	
Cm-245	$9.3 \cdot 10^3$	$9.9702 \cdot 10^{-1}$	$6.8890 \cdot 10^{-1}$	$5.7959 \cdot 10^{-4}$

Table 3: The decay of original nuclide content (=1.0) for three different times of first canister penetration.

$t_o$ yrs	40	40	$5000/10^5$	40	40
$\Delta t$ yrs	$3 \cdot 10^4$	$3 \cdot 10^4$	$3 \cdot 10^4$	$5 \cdot 10^5$	$3 \cdot 10^4$
$K_p$ m/s	$10^{-9}$	$10^{-9}$	$10^{-9}$	$10^{-9}$	$10^{-7}$
S m	1	50	50	50	1
Pe -	$\infty/5/0.5$	$\infty/5/0.5$	0.5	5	5
Fig	1/2/3	4/5/6	7/8	9	10

$t_o$ yrs	0	0	0	0	0	0	0	0
$\Delta t$ yrs	$3 \cdot 10^4$	$5 \cdot 10^5$	$3 \cdot 10^4$	$5 \cdot 10^5$	$3 \cdot 10^4$	$5 \cdot 10^5$	$3 \cdot 10^4$	$5 \cdot 10^5$
$K_p$ m/s	$10^{-9}$	$10^{-9}$	$10^{-9}$	$10^{-9}$	$10^{-7}$	$10^{-7}$	$10^{-7}$	$10^{-7}$
S m	1	1	50	50	1	1	50	50
Pe -	$\infty/5/0.5$	$\infty/5/0.5$	$\infty/5/0.5$	$\infty/5/0.5$	$\infty/5/0.5$	$\infty/5/0.5$	$\infty/5/0.5$	$\infty/5/0.5$
Fig	11/12/13	14/15/16	17/18/19	20/21/22	23/24/25	26/27/28	29/30/31	32/33/34

Table 4. Overview of the cases computed with reference to the figures.

## NOTATION

b	half width of fissure	m
C	concentration in liquid	mol/m <sup>3</sup>
C <sub>f</sub>	concentration in liquid in fissures	mol/m <sup>3</sup>
C <sub>p</sub>	concentration in liquid in microfissures	mol/m <sup>3</sup>
C <sub>o</sub>	inlet concentration in the liquid	mol/m <sup>3</sup>
D <sub>L</sub>	longitudinal dispersion coefficient	m <sup>2</sup> /s
D <sub>p</sub>	diffusivity in water in pores	m <sup>2</sup> /s
D <sub>v</sub>	diffusivity in water	m <sup>2</sup> /s
g	gravitational constant	m/s <sup>2</sup>
H	Heaviside's step function	
H <sub>1</sub>	see equation (13)	
H <sub>2</sub>	see equation (14)	
H <sub>D1</sub>	see equation (15)	
H <sub>D2</sub>	see equation (16)	
i	hydraulic gradient	m/m
K	volume equilibrium constant	m <sup>3</sup> /m <sup>3</sup>
K <sub>p</sub>	hydraulic conductivity	m/s
k <sub>f</sub>	mass transfer coefficient	m/s
m	$= \frac{\epsilon_f}{1 - \epsilon_f}$	
N	inventory of nuclide	Ci/ton
N <sub>o</sub>	original inventory of nuclide	Ci/ton
n	release of nuclide	Ci/ton, year
n <sub>z</sub>	discharge rate of nuclide at distance z	Ci/ton, year
Pe	$= \frac{zU_f}{D_L}$ , Peclet number	
$\bar{q}$	volume averaged concentration in blocks	mol/m <sup>3</sup>

R	$= \frac{K}{m}$ , distribution ratio	
r	radial distance from center of spherical particle	m
r <sub>o</sub>	effective spherical radius	m
S	fissure spacing	m
T <sub>1/2</sub>	half life	s
t	time	s
t <sub>o</sub>	time of canister penetration	s
Δt	time for dissolution of waste	s
U <sub>f</sub>	average velocity of water in fissures	m/s
u	see equation (10)	
x'	see equation (11)	
y	$= \frac{2D_p \epsilon_p}{Kr_o^2} t$ , contact time parameter	
y'	see equation (12)	
z	distance in flow direction	m

Greek letters

δ	$= \frac{3D_p \epsilon_p}{r_o^2} \frac{z}{mU_f}$ , bed length parameter	
δ <sub>D</sub>	constrictivity for diffusion	
ε <sub>f</sub>	porosity of fissures	
ε <sub>p</sub>	porosity of rock matrix	
λ	variable of integration	
λ <sub>d</sub>	decay constant of radionuclide	s <sup>-1</sup>
μ	viscosity of water	Ns/m <sup>2</sup>
ν	$= \frac{D_p \epsilon_p}{k_f r_o}$	
ρ	density of water	kg/m <sup>3</sup>
σ	$= \frac{2D_p \epsilon_p}{Kr_o^2}$	s <sup>-1</sup>
τ	tortuosity	

Superscript

i nuclide i



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## APPENDIX

Computer program

PROGRAM NUCDIF1

FUNCTION F(LAM)

calculates the value of the integrand

$$f(\lambda) = \exp(\text{arg1}) \sin(\text{arg2}) / \lambda$$

$$\text{arg1} = \frac{1}{2} \text{Pe} - \sqrt{\frac{\sqrt{(z^2_{x'})^2 + (z^2_{y'})^2} + z^2_{x'}}{2}}$$

$$\text{arg2} = y\lambda^2 - \sqrt{\frac{\sqrt{(z^2_{x'})^2 + (z^2_{y'})^2} - z^2_{x'}}{2}}$$

$$z^2_{x'} = \text{Pe} \left( \frac{1}{4} \text{Pe} + \delta H_{D1} \right)$$

$$z^2_{y'} = \delta \text{Pe} \left( \frac{2}{3} \frac{\lambda^2}{R} + H_{D2} \right)$$

LAM variable of integration

SUBROUTINE HBOL (LAM, HD1, HD2)

evaluates:

$$H_{D1} = \lambda \left( \frac{\sinh 2\lambda + \sin 2\lambda}{\cosh 2\lambda - \cos 2\lambda} \right) - 1$$

$$H_{D2} = \lambda \left( \frac{\sinh 2\lambda - \sin 2\lambda}{\cosh 2\lambda - \cos 2\lambda} \right)$$

LAM = variable of integration

$$\text{HD1} = H_{D1} ; \text{HD2} = H_{D2}$$

SUBROUTINE DHBOL (LAM, DHD1, DHD2)

evaluates the derivatives of  $H_{D_1}$  and  $H_{D_2}$  :

LAM = variable of integration

$DHD1 = dH_{D_1} / d\lambda$

$DHD2 = dH_{D_2} / d\lambda$

SUBROUTINE ROOT (LAMROT, NROT)

calculates the n:th zero of  $\sin(\arg2)$

LAMROT = value of  $\lambda$  giving  $\arg2 = n \cdot \pi$

NROT = n

SUBROUTINE AVERAGE (LAMROT, NROT, SUM)

computation of integral by averaging of the partial sums.

LAMROT = value of  $\lambda$  giving  $\arg2 = n \cdot \pi$

NROT = n

SUM = value of integral

SUBROUTINE UPPER (B, TRUMAX)

calculates upper limit of infinite integral

B = upper limit

$e^{-TRUMAX} \sim$  truncation error

INPUT

PERM	hydraulic conductivity	m/s
GRADI	hydraulic gradient	m/m
CONST	constant $12\mu/\rho g$	ms
DPORE	$D_p \varepsilon_p$	$m^2/s$
SPACNG	fissure spacing	m
TLEAK	leach time	years
NAME	name of radionuclide e.g.	Cs-137
TNUCL	half life	years
KVOL	volume equilibrium constant	$m^3/m^3$
Z	distance	m
PECL	Peclet number	

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```
PROGRAM NUCDIF1(INPUT,OUTPUT,TAPE10,TAPE5=INPUT,TAPE6=OUTPUT)
*****
THIS PROGRAM CALCULATES 1-D MIGRATION OF SINGLE RADIONUCLIDES
IN FISSURED ROCK INCLUDING LONGITUDINAL DISPERSION AND DIFFU-
SION INTO SPHERICAL ROCK BLOCKS. AN ANALYTICAL SOLUTION BY
RASMUSON A. AND I. NERETNIEKS(J. GEOPHYSICAL RESEARCH
86,3749-3758(1981)) IS USED.
```

```
THE FILE TAPE10 IS CONCERNED WITH STORAGE OF OUTPUT DATA.
ACCORDINGLY ALL WRITE(10,X) STATEMENTS MAY BE OMITTED AS WELL
AS THE VECTORS UVEC,TVEC AND MAP. IN THE INTEGRATION THE
ROUTINE QNC7 FROM THE SANDIA MATHEMATICAL PROGRAM LIBRARY IS
USED. THIS LIBRARY ROUTINE MAY BE REPLACED BY ANY STANDARD
INTEGRATION ROUTINE.
```

```
*****
```

```
COMMON/COM1/DELTA,PECL,R,Y
DIMENSION UVEC(100),TVEC(100),MAP(2,30)
REAL KVOL,M,LAMROT
```

```
EXTERNAL F
DATA MAP/30*(10H ,0)/
```

```
CALL ERXSET(50,0)
```

```
IPRINT=-1
```

```
READ(5,*)PERM,GRADI,CONST,DPORE,SPACNG,TLEAK
```

```
READ(5,220)((MAP(I,J),I=1,2),J=1,23)
```

```
220 FORMAT(1X,10(A10,I3))
```

```
WRITE(10,200)PERM,GRADI,CONST,DPORE,SPACNG,TLEAK
```

```
WRITE(10,220)((MAP(I,J),I=1,2),J=1,30)
```

```
TLEAK=TLEAK*3.15E07
```

```
B1=0.5*SPACNG
```

```
B2=(0.5*CONST*SPACNG*PERM)**0.3333333333
```

```
FI=3.*(B2/SPACNG)
```

```
V=(PERM*GRADI)/FI
```

```
M=FI/(1.-FI)
```

```
DLPRIM=1.8*SPACNG*V
```

```
LOOP FOR DIFFERENT NUCLIDES
```

```
DO 4000 I4=1,23
```

```
READ(5,135)NAME
```

```
READ(5,*)TNUCL,KVOL
```

```
ALAM=0.69314718/TNUCL
```

```
DS=DPORE/KVOL
```

```
GAM=(3.*DS*KVOL)/(B1**2.)
```

```
SIG=(2.*DS)/(B1**2.)
```

```
R=KVOL/M
```

```
WRITE(6,105)
```

```
WRITE(6,105)
```

```
WRITE(6,100)PERM,GRADI,CONST,DPORE,SPACNG,TLEAK/3.15E07
```

```
WRITE(6,140)B1,V,FI,DS
```

```
WRITE(6,145)NAME,TNUCL,KVOL
```

```
WRITE(10,200)PERM,GRADI,CONST,DPORE,SPACNG,TLEAK/3.15E07
```

```
WRITE(10,205)NAME,TNUCL,KVOL
```

```
100 FORMAT(2X,*KP=*,E13.7,2X,*I=*,E13.7,2X,*CONST=*,
```

```
1E13.7,2X,*DPORE=*,E13.7,2X,*SPACNG=*,E13.7,
```

```
12X,*TLEAK=*,E13.7,2X,*YEARS*)
```

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```
135 FORMAT(A10)
140 FORMAT(2X,*RADIUS=*,E13.7,2X,*FRACTURE VELOCITY=*,
1E13.7,2X,*FRACTURE POROSITY=*,E13.7,2X,*APPARENT DIFFUSIVITY=*,
1E13.7)
145 FORMAT(2X,*NUCLIDE=*,A10,2X,*HALFLIFE=*,E13.7,2X,*YEARS*,
13X,*KVDL=*,E13.7)
200 FORMAT(6(1X,E13.7))
205 FORMAT(1X,A10,2(1X,E13.7))
```

C  
C  
C  
C

LOOP FOR DIFFERENT DISTANCES

```
DO 3000 I1=1,6
  IF(I1.EQ.1)Z=30.
  IF(I1.EQ.2)Z=100.
  IF(I1.EQ.3)Z=300.
  IF(I1.EQ.4)Z=1000.
  IF(I1.EQ.5)Z=3000.
  IF(I1.EQ.6)Z=10000.
  DELTA=(GAM*Z)/(M*V)
  TW=Z/V
  PART=DS*KVDL**2.*TW/B2**2.
  RF=1.0+5.0*PART
  TMEAN=TW*RF
  R1PERC=1.0+PART/3.35
  T1PERC=TW*R1PERC
  WRITE(6,105)
  WRITE(6,105)
  WRITE(6,105)
105 FORMAT(2X)
  WRITE(6,110)TW/3.15E07,T1PERC/3.15E07,TMEAN/3.15E07
110 FORMAT(2X,*TW=*,E13.7,2X,*T1PERC=*,E13.7,2X,*TMEAN=*,E13.7,
13X,*YEARS*)
```

C  
C  
C  
C  
C

LOOP FOR DIFFERENT PECLET NUMBERS

```
DO 2000 I2=2,3
  NTIMES=0
  TRUMAX=40.
  L=-1
  L1=-1
  IF(I2.EQ.1)PECL=1.0E98
  IF(I2.EQ.2)PECL=5.0
  IF(I2.EQ.3)PECL=0.5
  IF(PECL.EQ.1.0E98)GOTO 40
  DL=(Z*V)/PECL
  GOTO 50
40 DL=0.0
50 WRITE(6,105)
  WRITE(6,105)
  WRITE(6,115)Z,DL,DELTA,PECL,R
  WRITE(6,105)
115 FORMAT(2X,*Z=*,E13.7,2X,*DL=*,E13.7,5X,*DELTA=*,E13.7,2X,
1*PECL=*,E13.7,2X,*R=*,E13.7)
```

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```

WRITE(6,120)
120 FORMAT(1H ,8X,*U*,13X,*T(YEARS)*,14X,*T(SEC)*,13X,*Y*,17X,
1*UPPER LIMIT*,6X,*ABS TRUNC ERR*,5X,*REL TRUNC ERR*)

```

C  
C  
C  
C  
C

LOOP FOR DIFFERENT TIMES

```

DO 1000 I3=1,50
ILEAK=-1
T=1.8**(I3-26.)*TMEAN/20.
IF(I3.GE.26)T=T+TW
TREL=(T/3.15E07)*ALAM
IF(TREL.GT.100.)GOTO 500
35 Y=SIG*T
IF(T.GT.TW)GOTO 60
IF(DL.GT.0.)GOTO 60
U=0.
TRUNC=0.
RELTRU=0.
B=0.
GOTO 20
60 CONTINUE

```

C  
C  
C  
C  
C

INTEGRATION

```

*****
IF(L.EQ.1)GOTO 10
IF(L1.EQ.1)GOTO 30
CALCULATION OF UPPER LIMIT OF INTEGRAL
IF(DL.EQ.0.)GOTO 70
AA1=0.5*PECL+TRUMAX
AA2=DELTA*PECL
B=(2.*AA1*(SQRT(2.*AA1**2.-0.25*PECL**2.+AA2)-AA1))/AA2
GOTO 85
70 B=(TRUMAX+DELTA)/DELTA
GOTO 90
85 IF(KVOL.GT.0.5)GOTO 90
CALL UPPER(B,TRUMAX)
GOTO 95
90 IF(B.LT.4.5)CALL UPPER(B,TRUMAX)
CALCULATION OF TRUNCATION ERROR
95 TRUNC=(2.*EXP(-TRUMAX))/3.1415926536
L1=1
30 ERR=1.0E-10
CALL QNC7(F,0.,B,ERR,ANS,IERR)
U=0.5+(2./3.1415926536)*ANS
IF(U.NE.0.)GOTO 5
RELTRU=0.
GOTO 15
5 RELTRU=TRUNC/U
15 CONTINUE
IF(IERR.EQ.1)GOTO 20

```

C  
C

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```
C      INTEGRATION BY SPECIAL TECHNIQUE
C
C
10  NROT=10
    CALL ROOT(LAMROT,NROT)
    B=LAMROT
    ERR=1.0E-08
C      EVALUATION OF INTEGRAL
    CALL QNC7(F,0.,B,ERR,ANS,IERR)
    IF(IPRINT.EQ.1)WRITE(6,130)ANS
130  FORMAT(2X,*ANS=*,E13.7)
    CALL AVERAGE(LAMROT,NROT,SUM)
    U=0.5+(2./3.1415926536)*(ANS+SUM)
    L=1
C      CALCULATION OF TRUNCATION ERROR
    TRUNC=(2./3.1415926536)*1.0E-08
    RELTRU=TRUNC/U
C      *****
C
C      FINITE LEACHING TIME
C
20  IF(ILEAK.EQ.1)GOTO 45
    IF(T.LT.TLEAK)GOTO 25
    U1=U
    T1=T
    Y1=Y
    B11=B
    TRUNC1=TRUNC
    RELTRU1=RELTRU
    T=T-TLEAK
    ILEAK=1
    GOTO 35
45  U=U1-U
    T=T1
    Y=Y1
    B=B11
    TRUNC=TRUNC1
    RELTRU=RELTRU1
C
C      OUTPUT
C
25  U=U*EXP(-TREL)
    UVEC(I3)=U
    TVEC(I3)=T/3.15E07
    NTIMES=I3
    WRITE(6,125)U,T/3.15E07,T,Y,B,TRUNC,RELTRU
125  FORMAT(2X,E13.7,5X,E13.7,8X,E13.7,5X,E13.7,
18X,E13.7,5X,E13.7,5X,E13.7)
1000 CONTINUE
500  WRITE(10,210)Z,PECL,NTIMES
    IF(NTIMES.EQ.0)GOTO 2000
    WRITE(10,215)(UVEC(I),TVEC(I),I=1,NTIMES)
210  FORMAT(2(1X,E13.7),1X,I5)
215  FORMAT(9(1X,E13.7))
2000 CONTINUE
```



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```
3000 CONTINUE
      ENDFILE 10
4000 CONTINUE
      END
```

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```
FUNCTION F(LAM)
COMMON/COM1/DELTA,PECL,R,Y
REAL LAM
IF(LAM.EQ.0.)GOTO 10
CALL HBOL(LAM,HD1,HD2)
IF(PECL.EQ.1.0E+98)GOTO 50
AA1=PECL*(0.25*PECL+DELTA*HD1)
AA2=DELTA*PECL*((2.*LAM**2.)/(3.*R)+HD2)
AA5=AA2/AA1
IF(AA5.LT.1.0E-03)GOTO 30
RR=SQRT(AA1**2.+AA2**2.)
AA3=RR+AA1
AA4=RR-AA1
GOTO 40
30 AA3=AA1*(2.+0.5*AA5**2.-0.125*AA5**4.)
AA4=AA1*(0.5*AA5**2.-0.125*AA5**4.)
40 ARG1=0.5*PECL-SQRT((AA3)/2.)
ARG2=Y*LAM**2.-SQRT((AA4)/2.)
GOTO 60
50 ARG1=-DELTA*HD1
ARG2=(Y-(2.*DELTA)/(3.*R))*LAM**2.-DELTA*HD2
60 F=(EXP(ARG1)*SIN(ARG2))/LAM
GOTO 20
10 F=0.0
20 RETURN
END
```

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```
SUBROUTINE HBOL(LAM,HD1,HD2)
REAL LAM
IF(LAM.LT.0.01)GOTO 10
IF(LAM.GT.15.)GOTO 20
HN=LAM/(COSH(Z.*LAM)-COS(Z.*LAM))
HD1=HN*(SINH(Z.*LAM)+SIN(Z.*LAM))-1.
HD2=HN*(SINH(Z.*LAM)-SIN(Z.*LAM))
GOTO 30
10 HD1=(4.*LAM**4.)/45.
   HD2=(2.*LAM**2.)/3.
   GOTO 30
20 HD1=LAM-1.
   HD2=LAM
30 RETURN
END
```

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```
SUBROUTINE DHDOL(LAM,DHD1,DHD2)
REAL LAM
IF(LAM.LT.0.01)GOTO 10
IF(LAM.GT.15.)GOTO 20
HN=LAM/(COSH(Z.*LAM)-COS(Z.*LAM))
HD1=HN*(SINH(Z.*LAM)+SIN(Z.*LAM))-1.
HD2=HN*(SINH(Z.*LAM)-SIN(Z.*LAM))
DHD1=(HD1+1.-4.*HN**2.*SINH(Z.*LAM)*SIN(Z.*LAM))/LAM
DHD2=(HD2+4.*HN**2.*(1.-COSH(Z.*LAM)*COS(Z.*LAM)))/LAM
GOTO 30
10 DHD1=(16.*LAM**3.)/45.
   DHD2=(4.*LAM)/3.
   GOTO 30
20 DHD1=1.
   DHD2=1.
30 RETURN
END
```

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```
SUBROUTINE ROOT(LAMROT,NROT)
COMMON/COM1/DELTA,PECL,R,Y
REAL LAMROT
IPRINT=-1
C INITIAL VALUE OF ITERATION
IF(PECL.EQ.1.0E+98)Y=Y-(2.*DELTA)/(3.*R)
AA1=DELTA/(2.*Y)
AA2=3.1415926536/Y
X0=AA1+SQRT(AA1**2.+NROT*AA2)
IF(X0.LT.4.5)X0=1.0
IF(X0.EQ.1.)GOTO 40
IF(PECL.NE.1.0E+98)GOTO 40
X1=X0
GOTO 30
40 CONTINUE
C NEWTON RAPHSON ITERATION
DO 1000 I=1,20
CALL HBOL(X0,HD1,HD2)
CALL DHBOL(X0,DHD1,DHD2)
IF(PECL.EQ.1.0E+98)GOTO 50
AA3=PECL*(0.25*PECL+DELTA*HD1)
AA4=DELTA*PECL*((2.*X0**2.)/(3.*R)+HD2)
AA5=AA4/AA3
RR=SQRT(AA3**2.+AA4**2.)
IF(AA5.LT.1.0E-03)GOTO 10
AA6=RR-AA3
GOTO 20
10 AA6=AA3*(0.5*AA5**2.-0.125*AA5**4.)
20 F=Y*X0**2.-SQRT(AA6/2.)-NROT*3.1415926536
DAA3=DELTA*PECL*DHD1
DAA4=DELTA*PECL*((4.*X0)/(3.*R)+DHD2)
FPRIM=2.*Y*X0-((AA3*DAA3+AA4*DAA4)/(RR-DAA3)/(4.*SQRT(AA6/2.))
GOTO 60
50 F=Y*X0**2.-DELTA*HD2-NROT*3.1415926536
FPRIM=2.*Y*X0-DELTA*DHD2
60 DELTA1=F/FPRIM
X1=X0-DELTA1
IF(IPRINT.EQ.1)WRITE(6,100)I,X0
100 FORMAT(2X,I2,3X,E13.7)
IF(ABS(X1-X0).LT.1.0E-05)GOTO 30
IF(I.EQ.20)WRITE(6,105)
105 FORMAT(2X,*THE ACCURACY OF LAMROT WAS NOT ACHIEVED*)
X0=X1
1000 CONTINUE
30 LAMROT=X1
IF(PECL.EQ.1.0E+98)Y=Y+(2.*DELTA)/(3.*R)
RETURN
END
```

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```
SUBROUTINE AVERAGE(LAMROT,NROT,SUM)
REAL LAMROT
EXTERNAL F
DIMENSION S(100)
IPRINT=-1
ERR=1.0E-08
IMAX=20
C CALCULATION OF PARTIAL SUMS
A=LAMROT
NROT=NROT+1
CALL ROOT(LAMROT,NROT)
B=LAMROT
IF(IPRINT.EQ.1)WRITE(6,100)A,B
100 FORMAT(2X,*A=*,E13.7,*B=*,E13.7)
CALL QNC7(F,A,B,ERR,ANS,IERR)
S(1)=ANS
DO 1000 I=2,IMAX
NROT=NROT+1
A=B
CALL ROOT(LAMROT,NROT)
B=LAMROT
ANS1=ANS
CALL QNC7(F,A,B,ERR,ANS,IERR)
S(I)=S(I-1)+ANS
IF(ANS1*ANS.GT.0.)WRITE(6,125)
IF(ABS(ANS)-ABS(ANS1).GT.0.)WRITE(6,130)
125 FORMAT(2X,*AVERAGE SUBSEQUENT TERMS IN SERIES *,
1*ARE NOT OF DIFFERENT SIGN*)
130 FORMAT(2X,*AVERAGE ABSOLUTE VALUES OF TERMS IN *,
1*SERIES ARE NOT DECREASING*)
IF(IPRINT.EQ.1)WRITE(6,105)A,B,ANS
105 FORMAT(2X,*A=*,E13.7,*B=*,E13.7,*ANS=*,E13.7)
1000 CONTINUE
IF(IPRINT.NE.1)GOTO 10
DO 2000 I=1,IMAX
WRITE(6,110)S(I)
110 FORMAT(2X,E13.7)
2000 CONTINUE
10 CONTINUE
C REPEATED AVERAGING
K=IMAX-1
50 DO 3000 I=1,K
S(I)=(S(I)+S(I+1))/2.
IF(ABS(S(I)-S(I+1)).LT.1.0E-08)GOTO 20
3000 CONTINUE
IF(IPRINT.NE.1)GOTO 30
WRITE(6,115)IMAX-K
115 FORMAT(2X,*ITER=*,I2)
DO 4000 I=1,K
WRITE(6,110)S(I)
4000 CONTINUE
30 K=K-1
IF(K.EQ.0)GOTO 40
GOTO 50
40 WRITE(6,120)
120 FORMAT(2X,*THE ACCURACY OF SUM WAS NOT ACHIEVED*)
```

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```
GOTO 60  
20 SUM=S(I)  
60 CONTINUE  
RETURN  
END
```

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```

SUBROUTINE UPPER(B,TRUMAX)
COMMON/COM1/DELTA,PECL,R,Y
X0=B
C NEWTON RAPHSON ITERATION
DO 1000 I=1,20
CALL HBOL(X0,HD1,HD2)
CALL DHBOL(X0,DHD1,DHD2)
IF(PECL.EQ.1.0E+98)GOTO 20
AA1=PECL*(0.25*PECL+DELTA*HD1)
AA2=DELTA*PECL*((2.*X0**2.)/(3.*R)+HD2)
RR=SQRT(AA1**2.+AA2**2.)
AA3=RR+AA1
F=0.5*PECL+TRUMAX-SQRT(AA3/2.)
DAA1=DELTA*PECL*DHD1
DAA2=DELTA*PECL*((4.*X0)/(3.*R)+DHD2)
FPRIM=-((AA1*DAA1+AA2*DAA2)/RR+DAA1)/(4.*SQRT(AA3/2.))
GOTO 30
20 F=DELTA*HD1-TRUMAX
FPRIM=DELTA*DHD1
30 DELTA1=F/FPRIM
X1=X0-DELTA1
IF(ABS(DELTA1/X1).LT.1.0E-05)GOTO 10
IF(I.EQ.20)WRITE(6,100)
100 FORMAT(2X,
1*THE ACCURACY OF UPPER INTEGRATION LIMIT WAS NOT ACHIEVED*)
X0=X1
1000 CONTINUE
10 B=X1
RETURN
END
```



Fraction of inventory to reach 1000 m, year<sup>-1</sup>

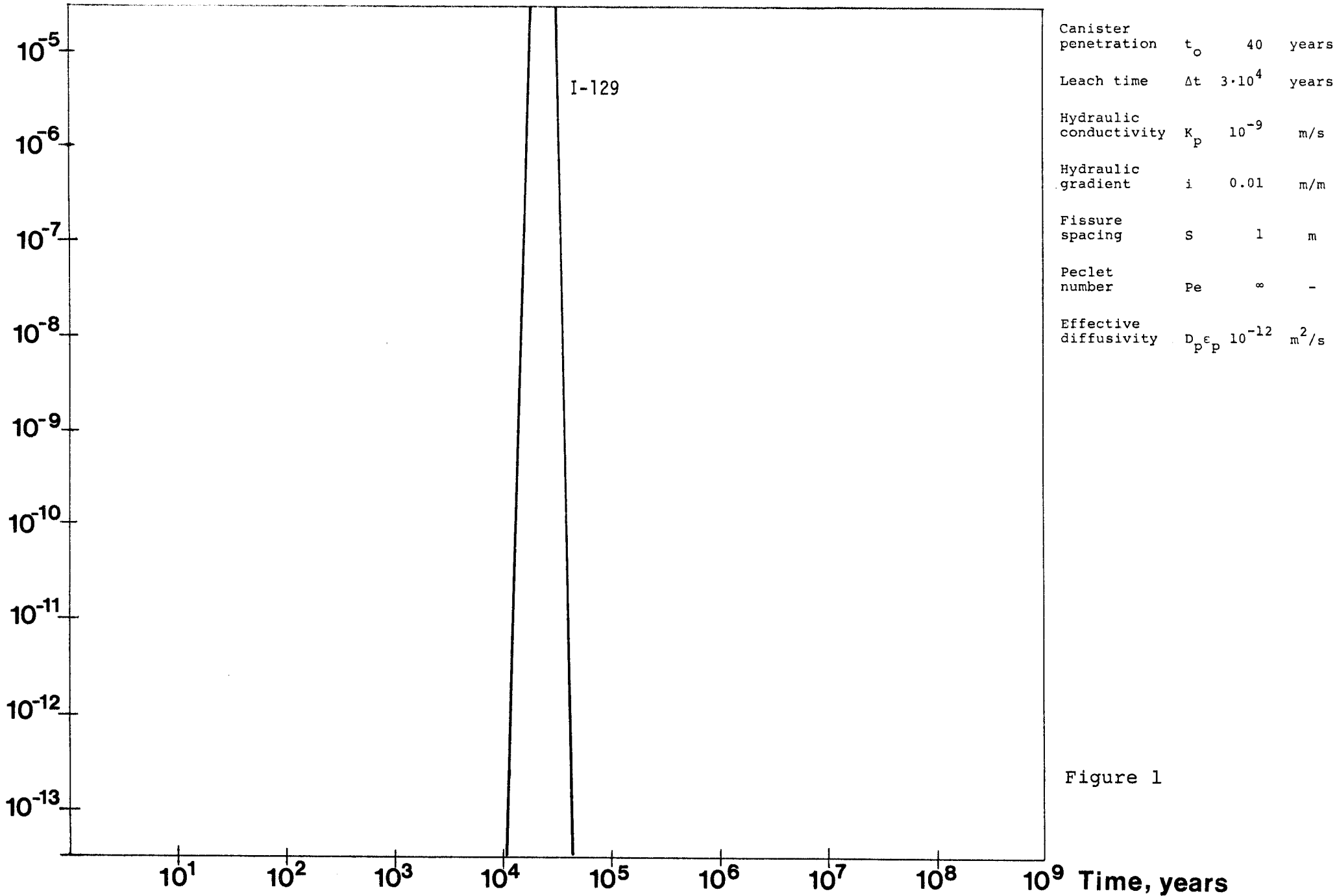
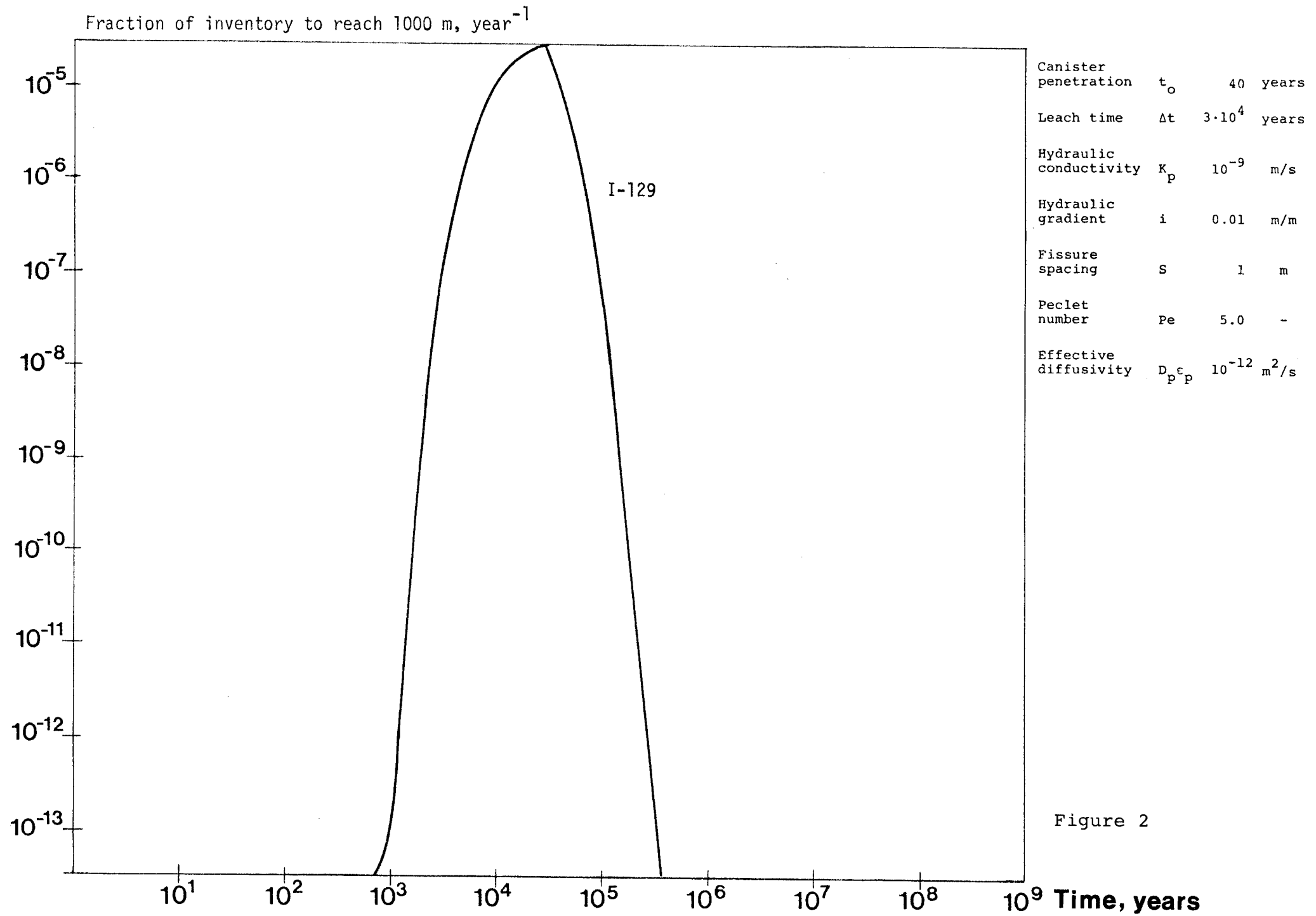


Figure 1



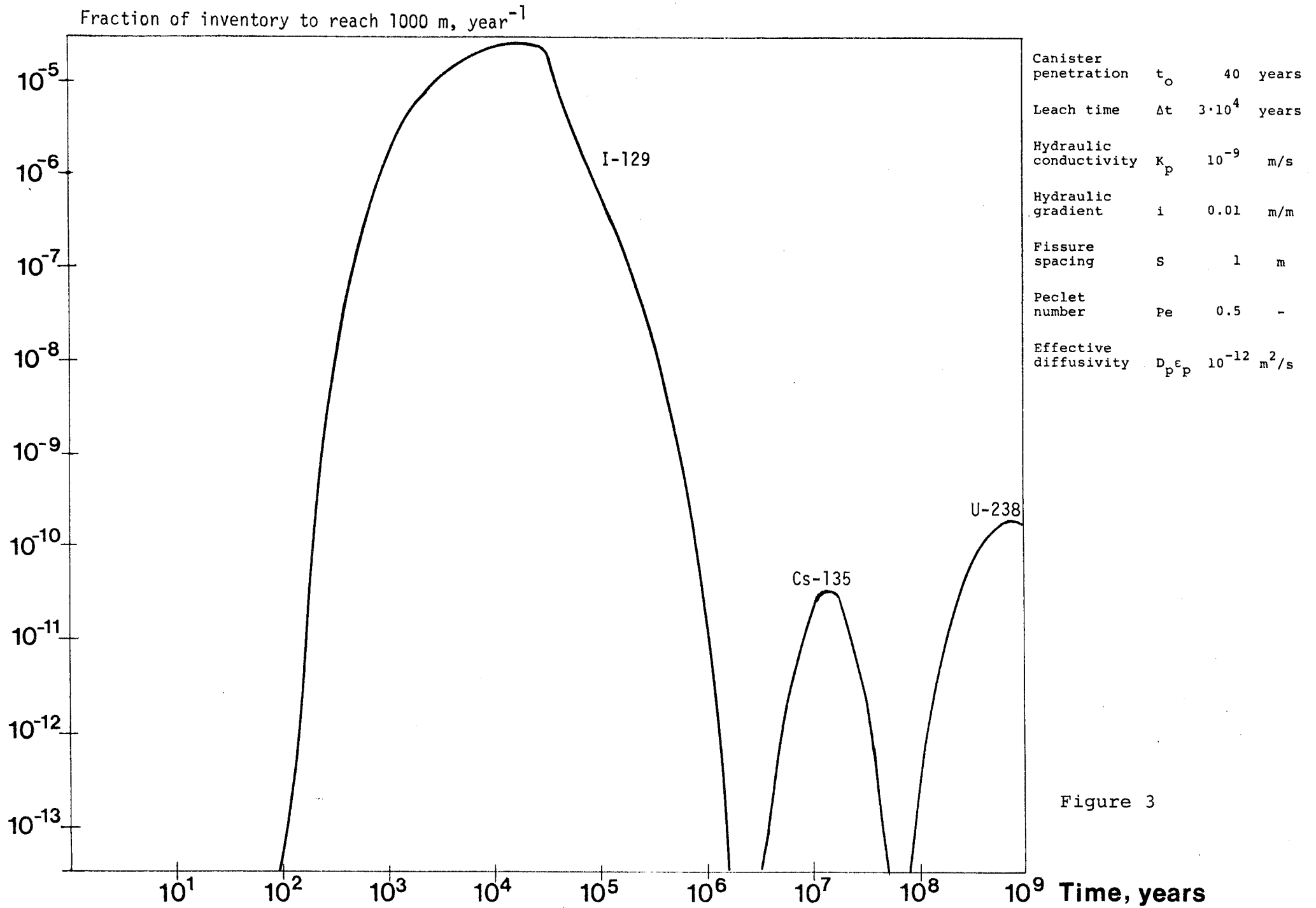


Figure 3

Fraction of inventory to reach 1000 m, year<sup>-1</sup>

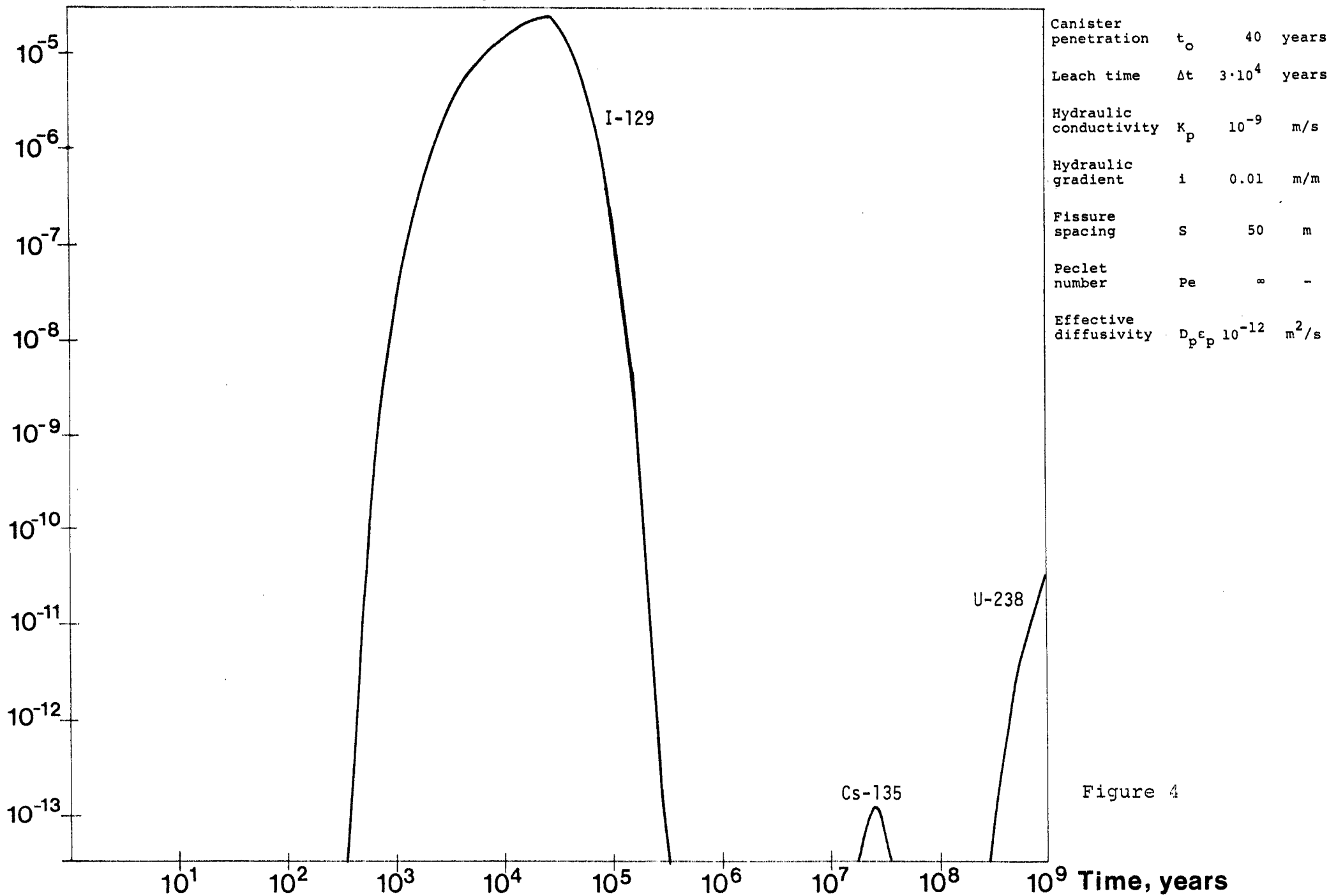
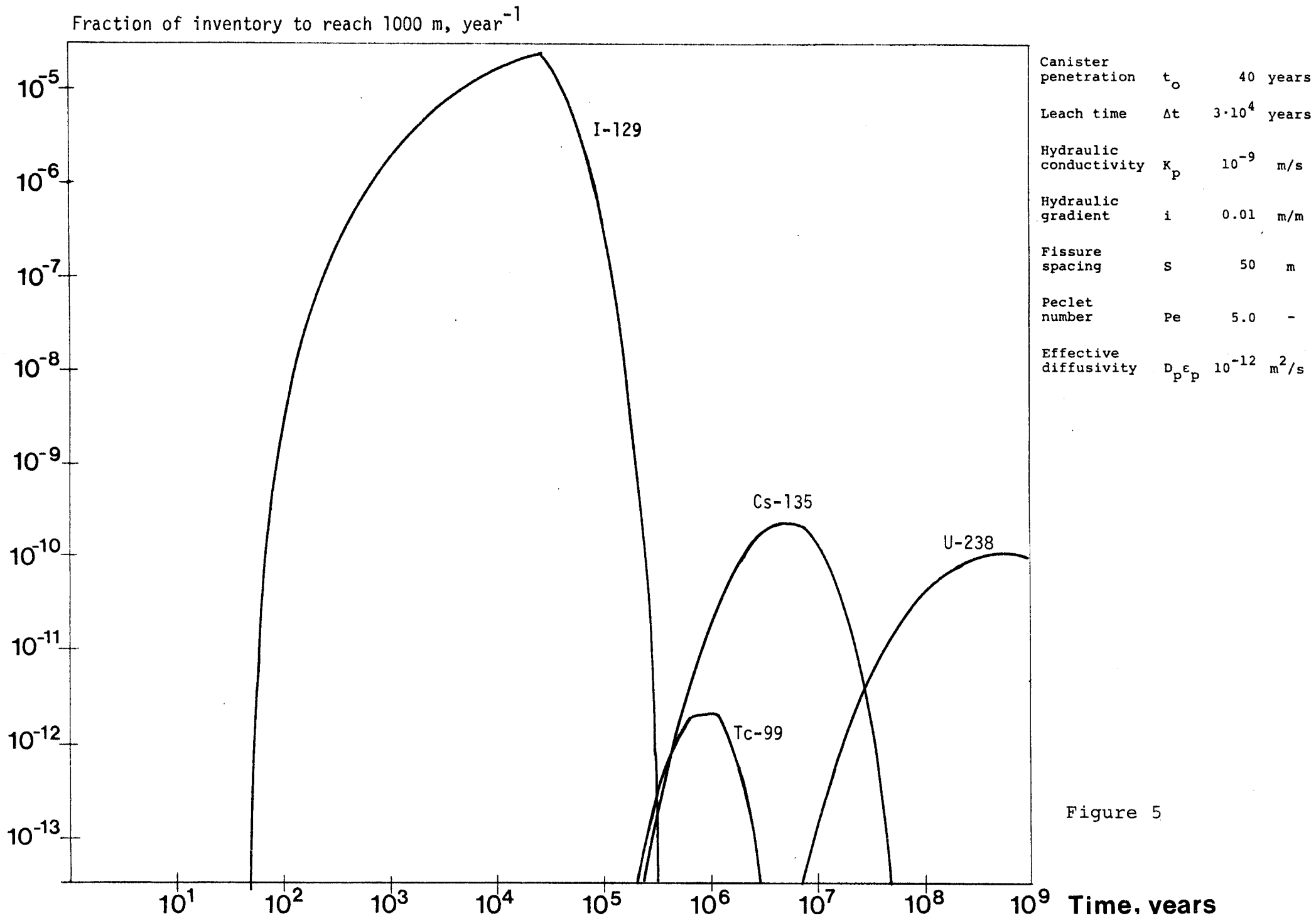


Figure 4



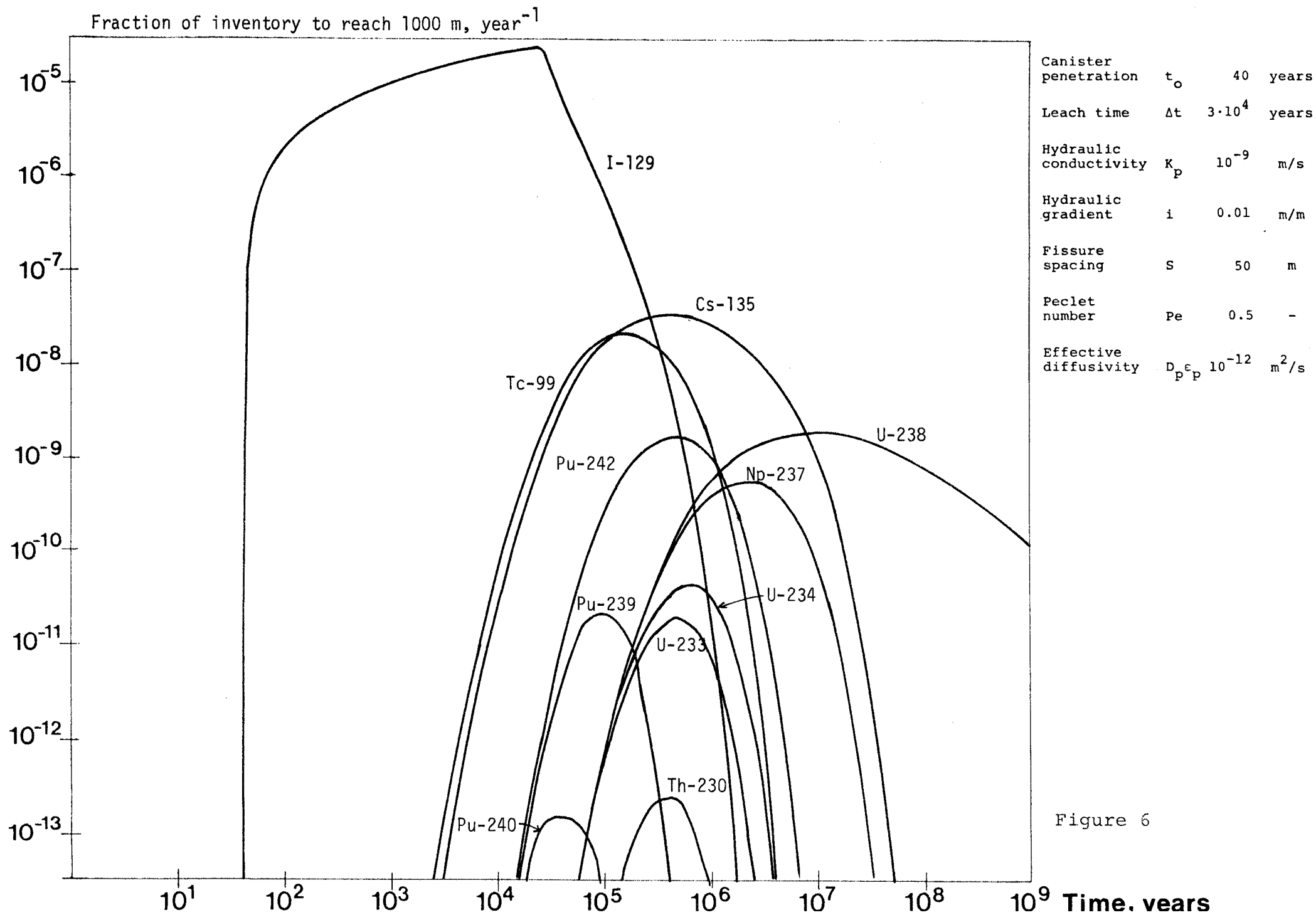


Figure 6

Fraction of inventory to reach 1000 m, year<sup>-1</sup>

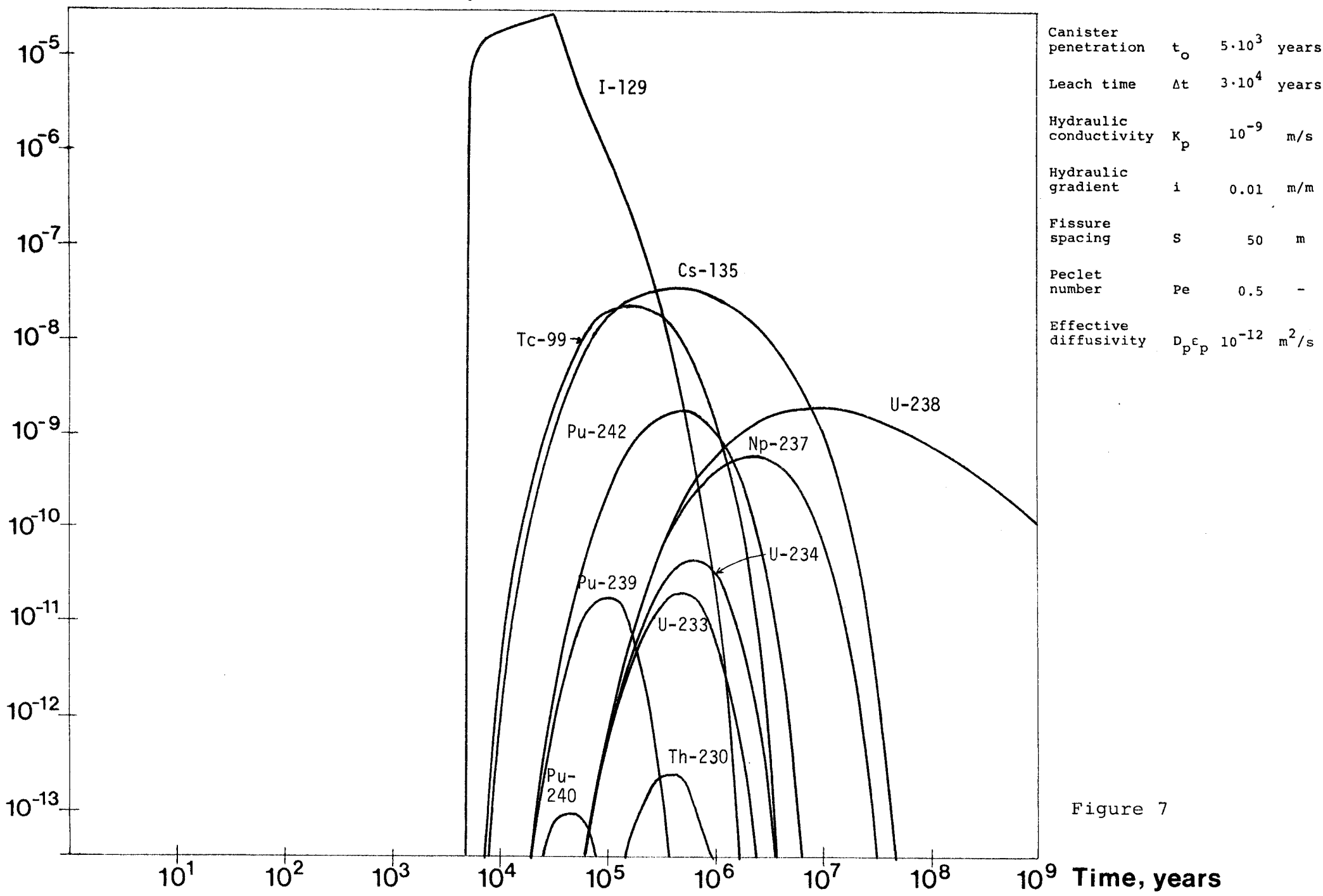


Figure 7

Time, years

Fraction of inventory to reach 1000 m, year<sup>-1</sup>

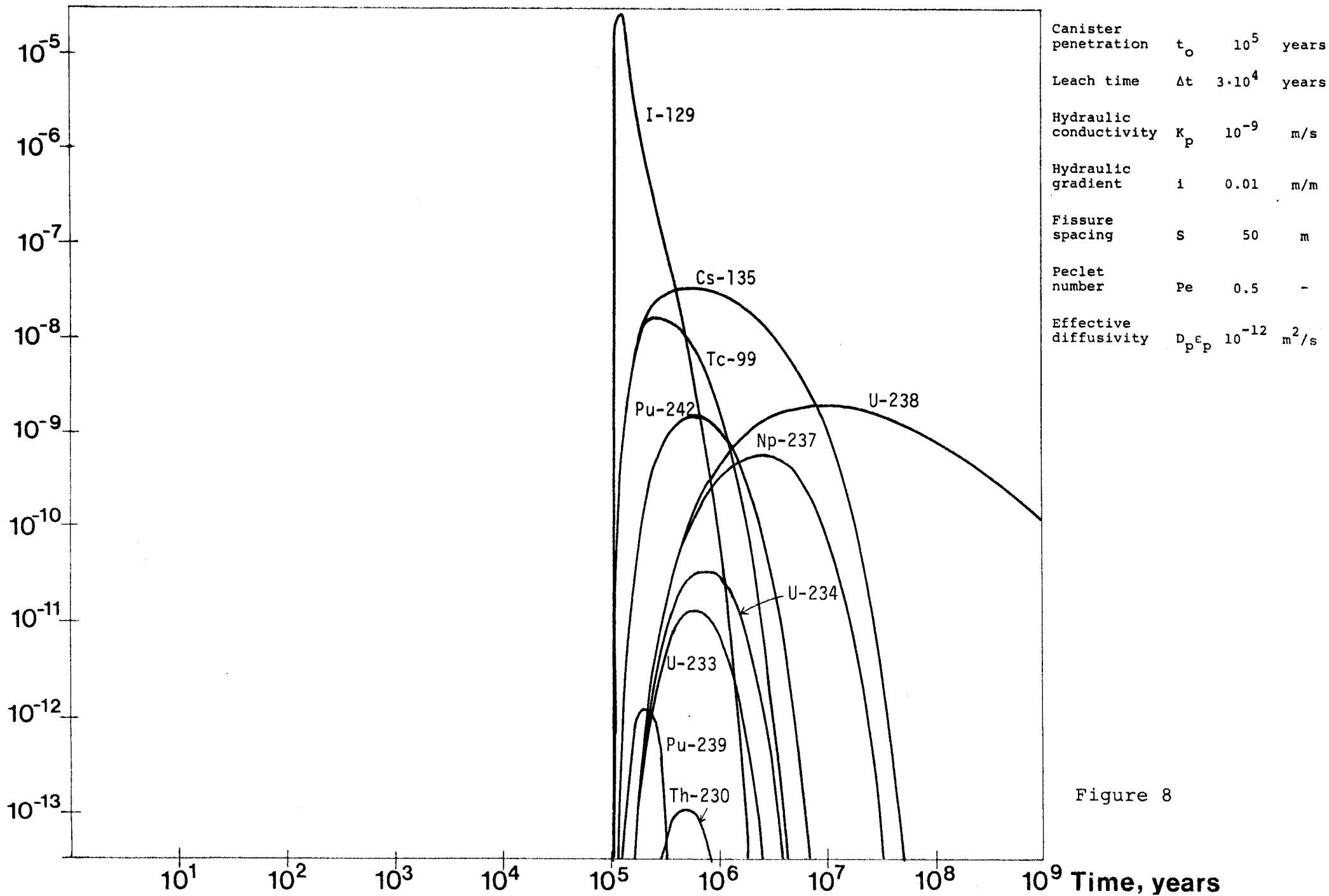


Figure 8



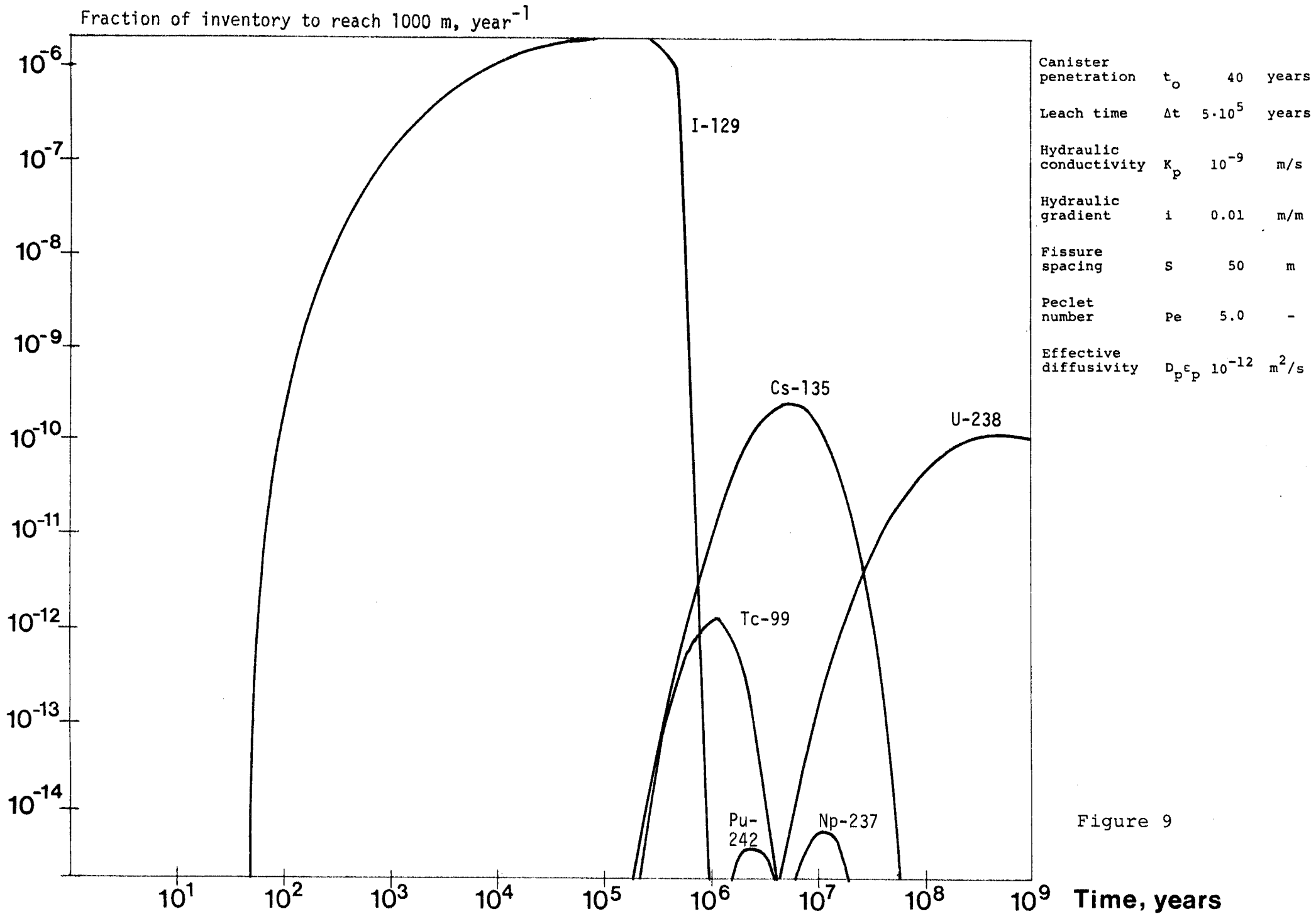


Figure 9

Fraction of inventory to reach 1000 m, year<sup>-1</sup>

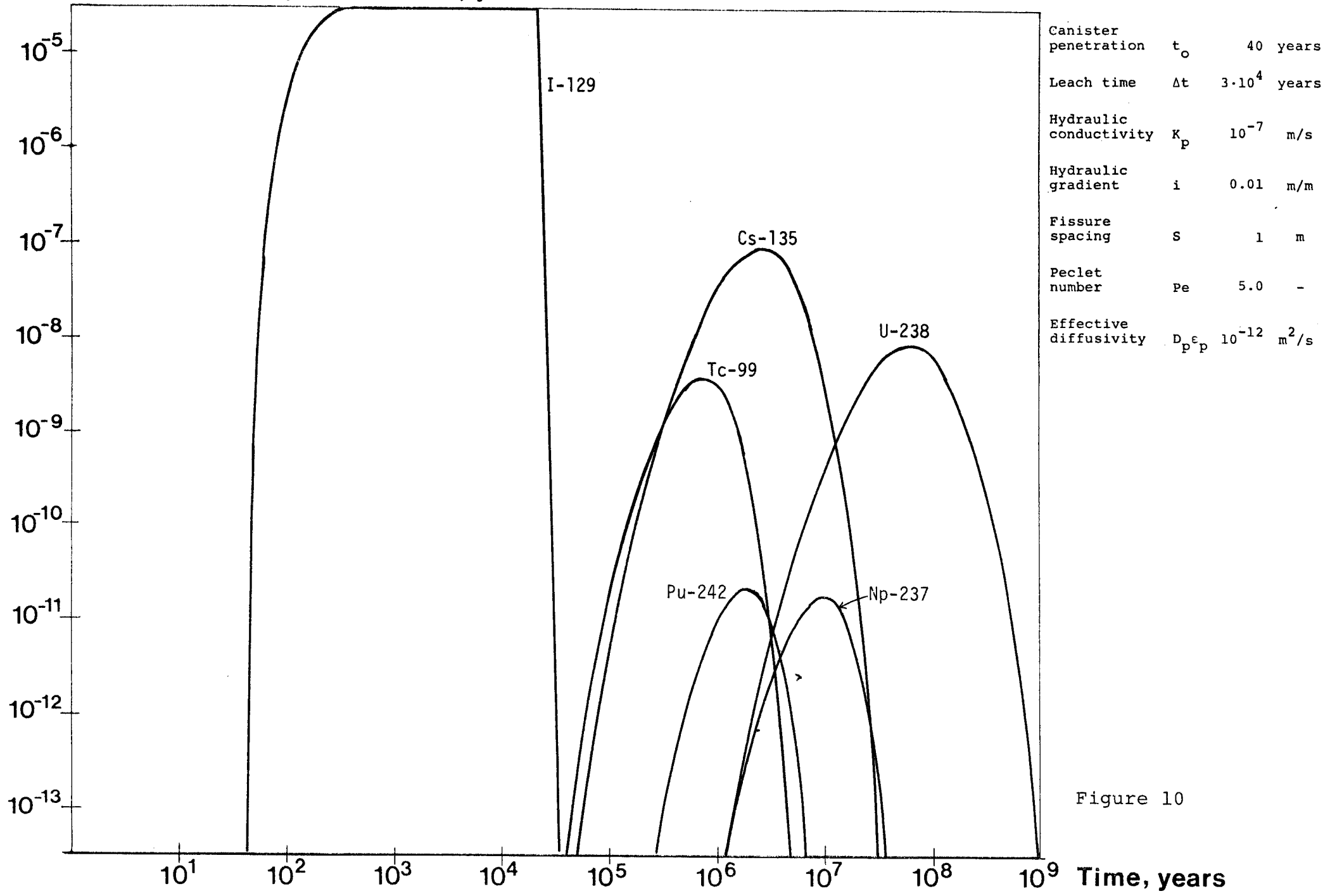
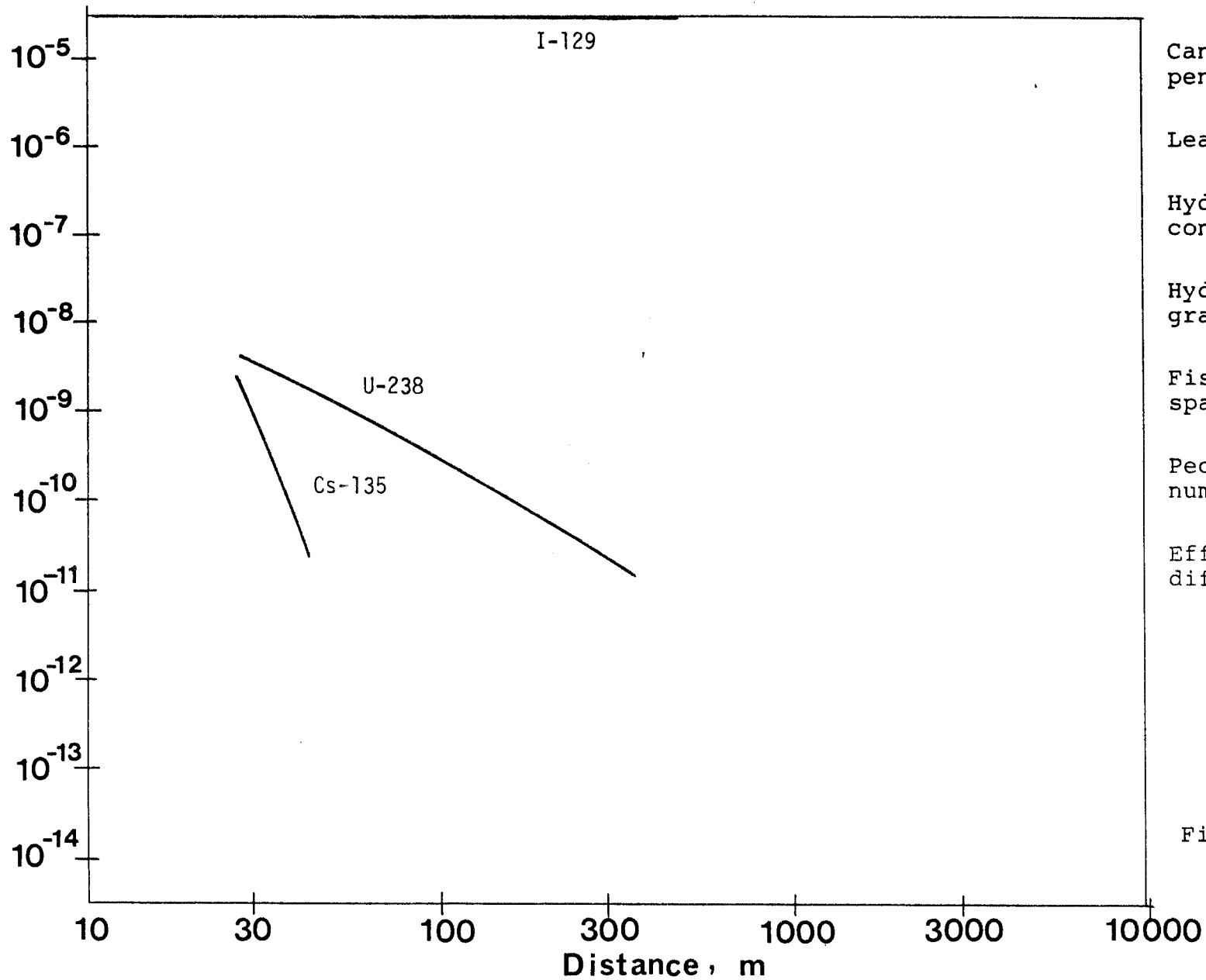


Figure 10

Time, years

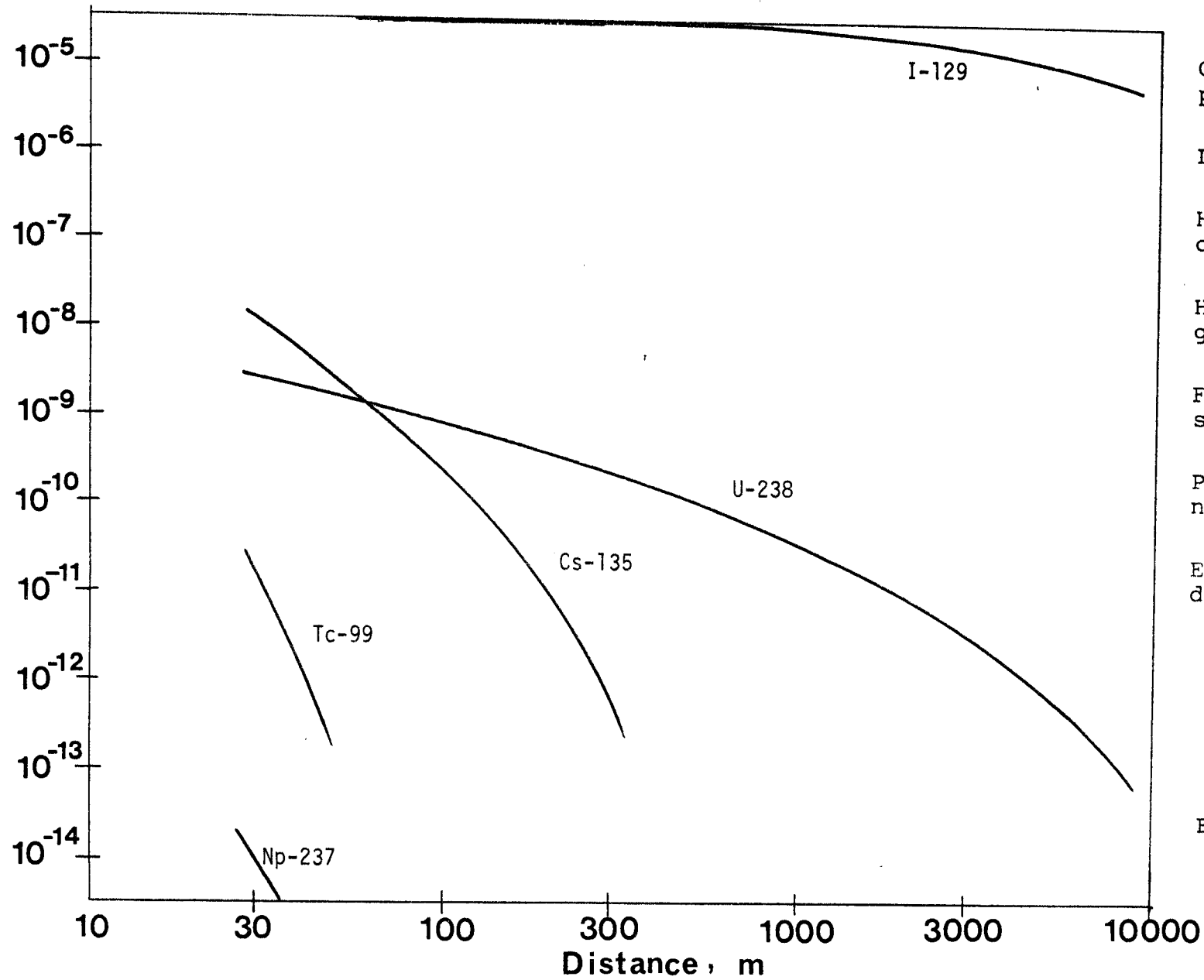
Fraction of inventory  
to reach a certain distance, year<sup>-1</sup>



Canister penetration	$t_o$	0	years
Leach time	$\Delta t$	$3 \cdot 10^4$	years
Hydraulic conductivity	$K_p$	$10^{-9}$	m/s
Hydraulic gradient	$i$	0.01	m/m
Fissure spacing	$S$	1	m
Peclet number	$Pe$	$\infty$	-
Effective diffusivity	$D_p \epsilon_p$	$10^{-12}$	m <sup>2</sup> /s

Figure 11

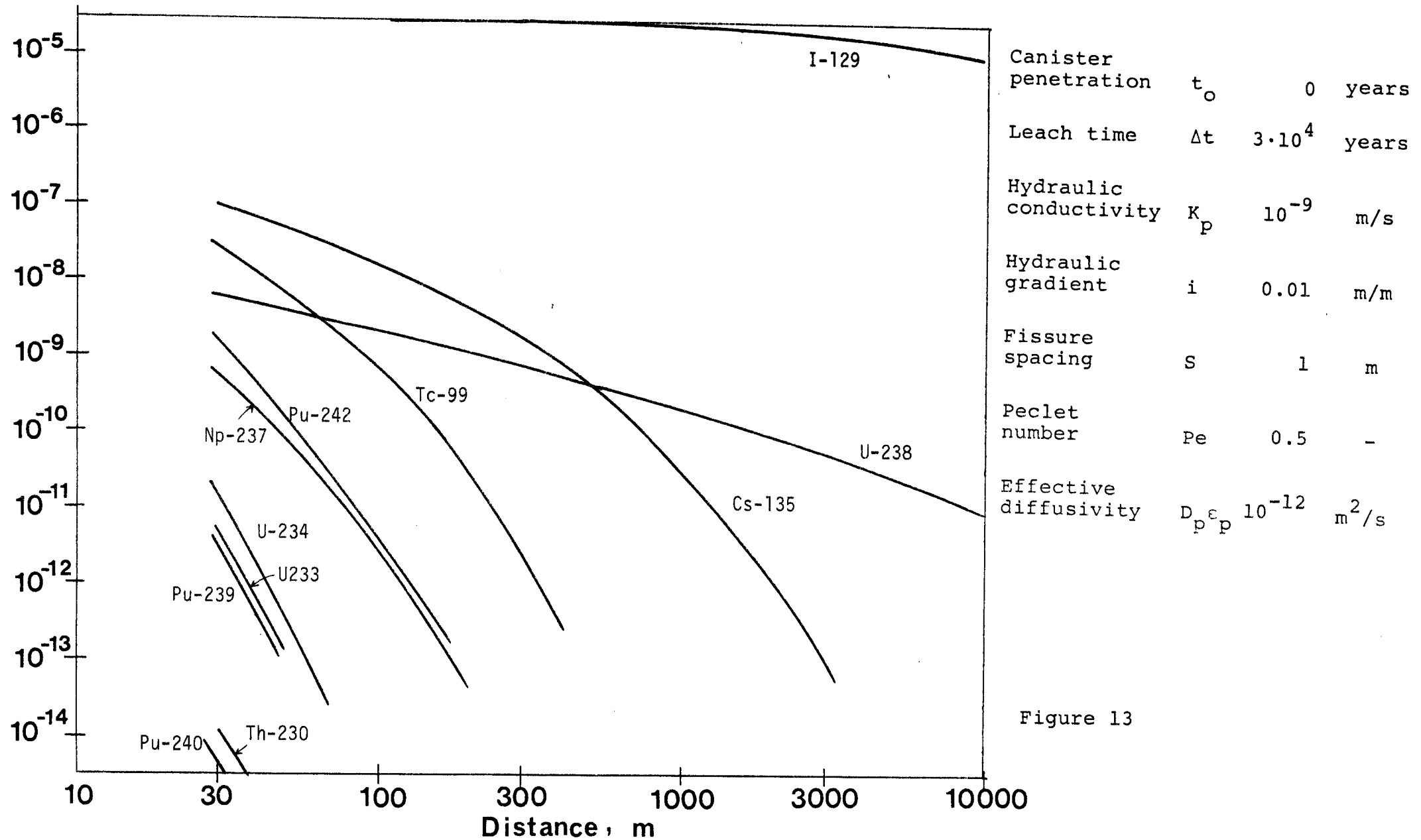
Fraction of inventory  
to reach a certain distance, year<sup>-1</sup>



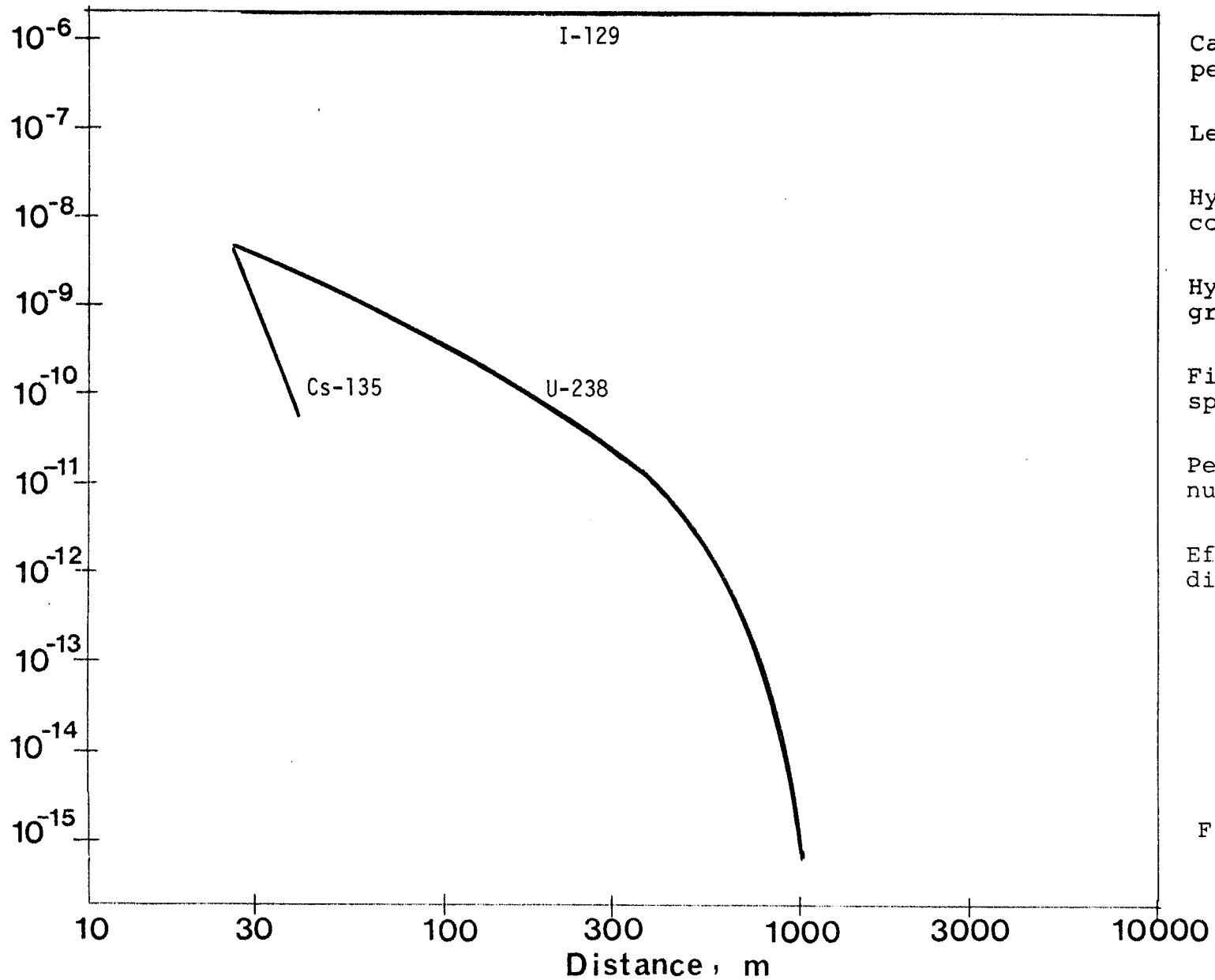
Canister penetration	$t_o$	0	years
Leach time	$\Delta t$	$3 \cdot 10^4$	years
Hydraulic conductivity	$K_p$	$10^{-9}$	m/s
Hydraulic gradient	$i$	0.01	m/m
Fissure spacing	$S$	1	m
Peclet number	$Pe$	5.0	-
Effective diffusivity	$D_p \epsilon_p$	$10^{-12}$	m <sup>2</sup> /s

Figure 12

Fraction of inventory  
to reach a certain distance, year<sup>-1</sup>



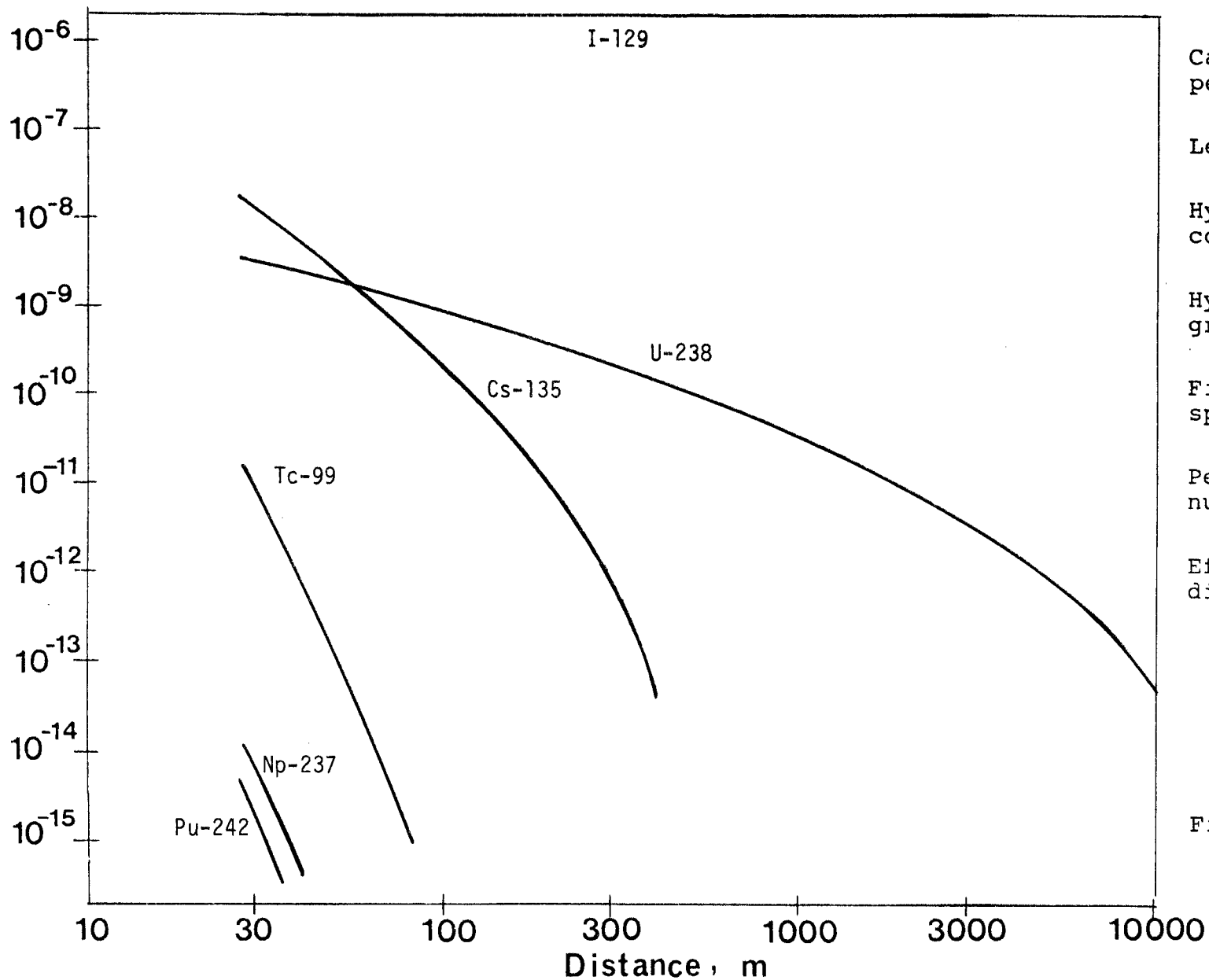
Fraction of inventory  
to reach a certain distance, year<sup>-1</sup>



Canister penetration	$t_o$	0	years
Leach time	$\Delta t$	$5 \cdot 10^5$	years
Hydraulic conductivity	$K_p$	$10^{-9}$	m/s
Hydraulic gradient	$i$	0.01	m/m
Fissure spacing	$S$	1	m
Peclet number	$Pe$	$\infty$	-
Effective diffusivity	$D_p \epsilon_p$	$10^{-12}$	m <sup>2</sup> /s

Figure 14

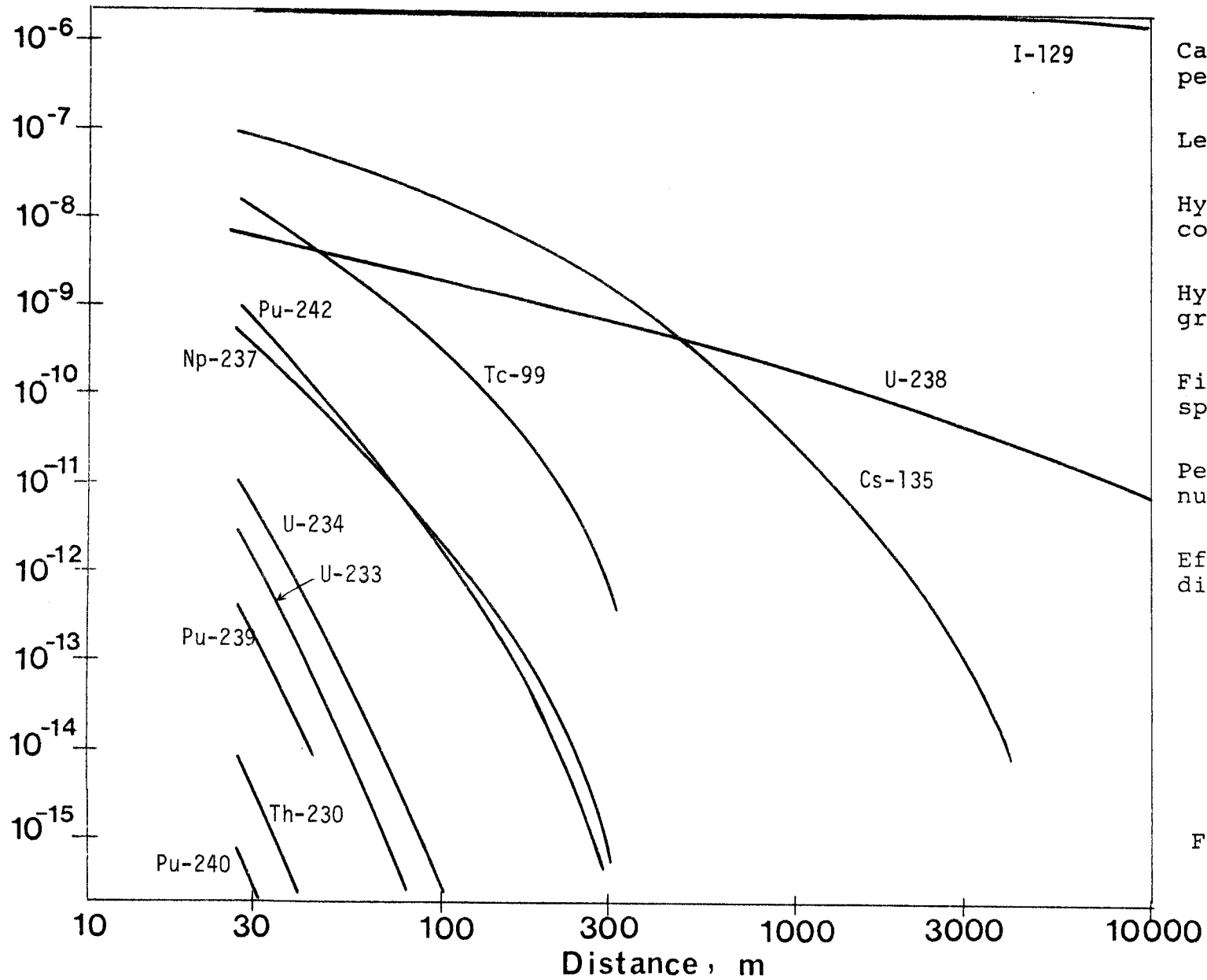
Fraction of inventory  
to reach a certain distance, year<sup>-1</sup>



Canister penetration	$t_o$	0	years
Leach time	$\Delta t$	$5 \cdot 10^5$	years
Hydraulic conductivity	$K_p$	$10^{-9}$	m/s
Hydraulic gradient	$i$	0.01	m/m
Fissure spacing	$S$	1	m
Peclet number	$Pe$	5.0	-
Effective diffusivity	$D_p \epsilon_p$	$10^{-12}$	m <sup>2</sup> /s

Figure 15

Fraction of inventory  
to reach a certain distance, year<sup>-1</sup>

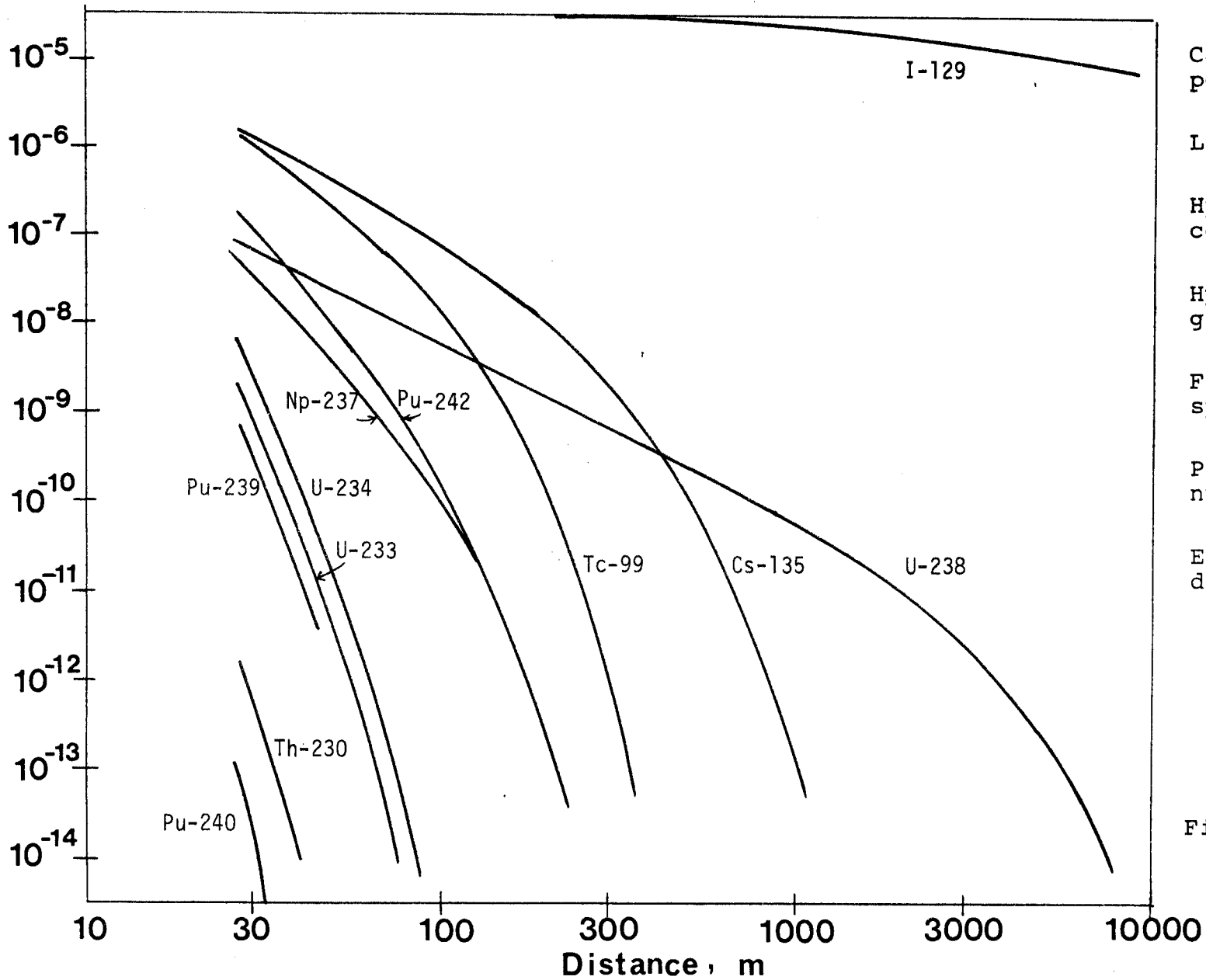


Canister penetration	$t_o$	0	years
Leach time	$\Delta t$	$5 \cdot 10^5$	years
Hydraulic conductivity	$K_p$	$10^{-9}$	m/s
Hydraulic gradient	$i$	0.01	m/m
Fissure spacing	$S$	1	m
Peclet number	$Pe$	0.5	-
Effective diffusivity	$D_p \epsilon_p$	$10^{-12}$	m <sup>2</sup> /s

Figure 16



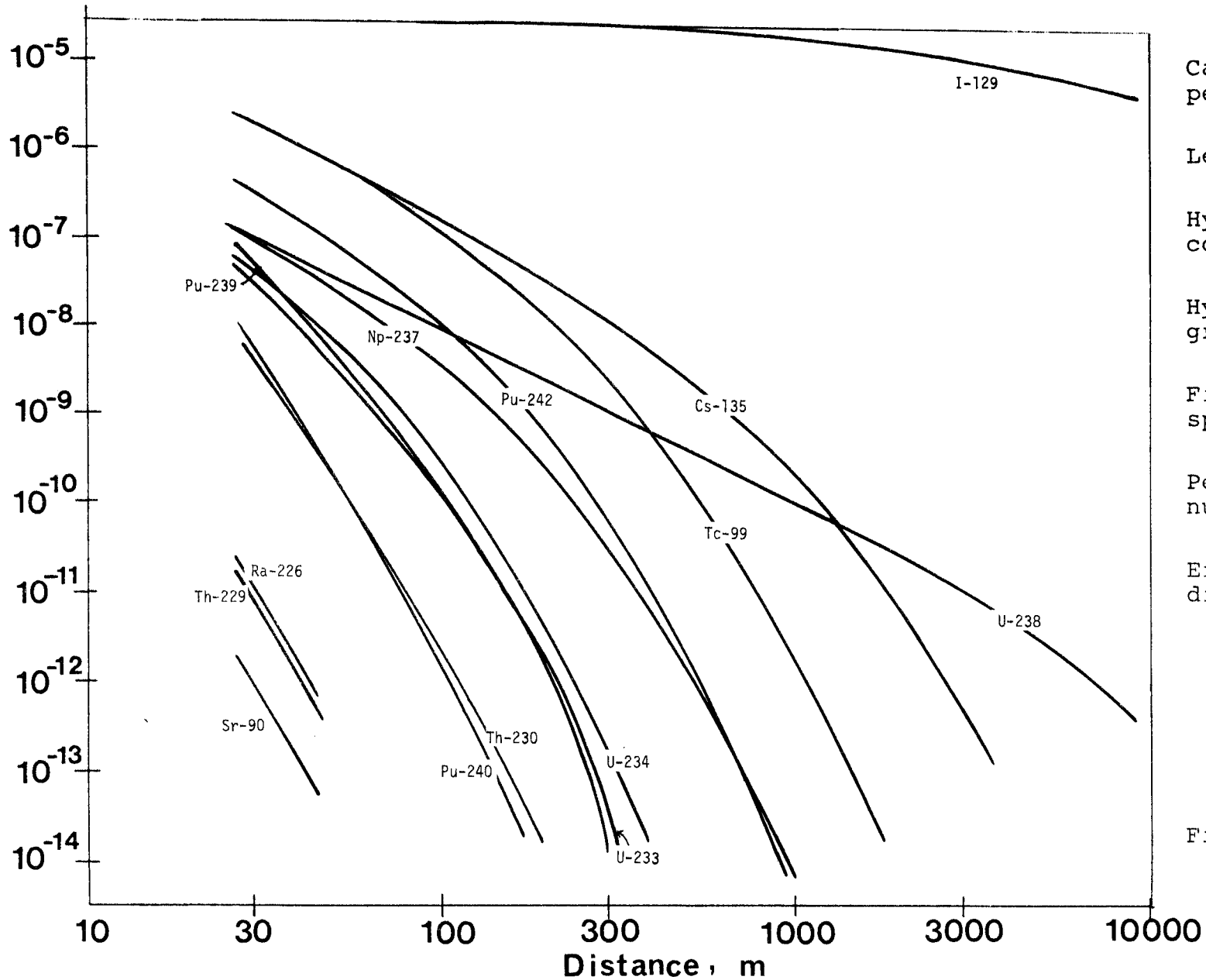
Fraction of inventory  
to reach a certain distance, year<sup>-1</sup>



Canister penetration	$t_0$	0	year
Leach time	$\Delta t$	$3 \cdot 10^4$	year
Hydraulic conductivity	$K_p$	$10^{-9}$	m/s
Hydraulic gradient	$i$	0.01	m/m
Fissure spacing	$S$	50	m
Peclet number	$Pe$	$\infty$	-
Effective diffusivity	$D_p \epsilon_p$	$10^{-12}$	$m^2/s$

Figure 17

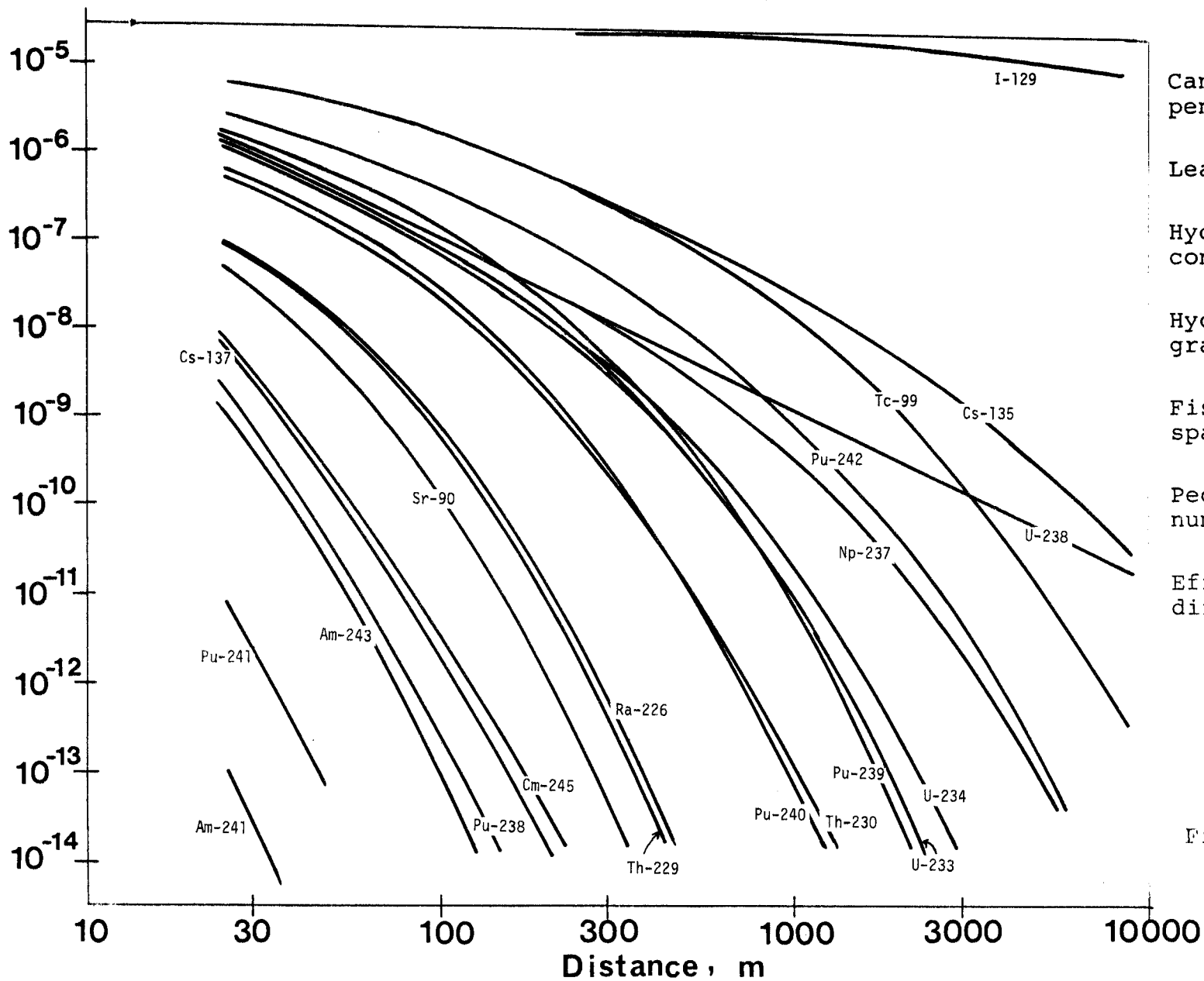
Fraction of inventory  
to reach a certain distance, year<sup>-1</sup>



Canister penetration	$t_0$	0	years
Leach time	$\Delta t$	$3 \cdot 10^4$	years
Hydraulic conductivity	$K_p$	$10^{-9}$	m/s
Hydraulic gradient	$i$	0.01	m/m
Fissure spacing	$S$	50	m
Peclet number	$Pe$	5.0	-
Effective diffusivity	$D_p \epsilon_p$	$10^{-12}$	$m^2/s$

Figure 18

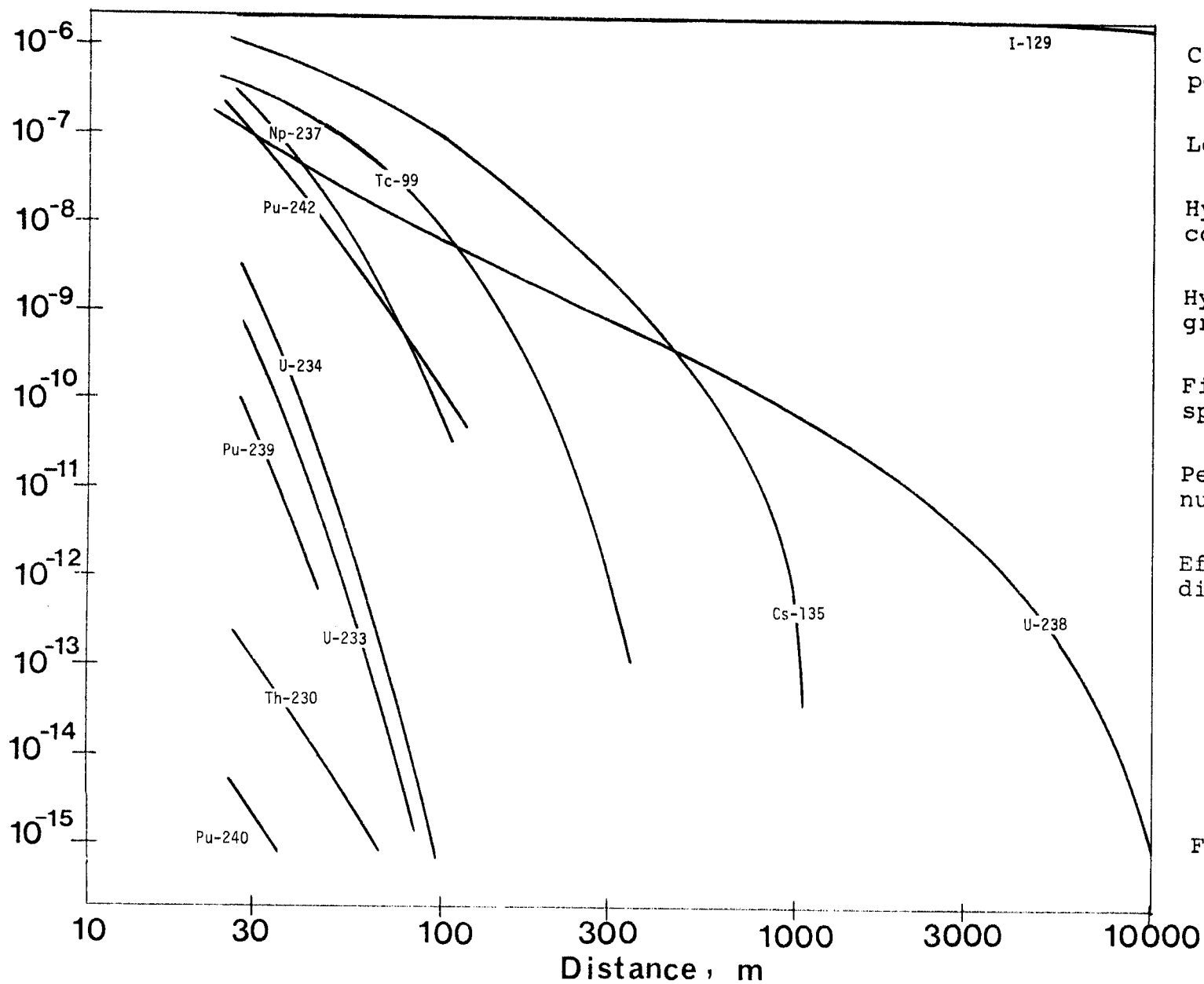
Fraction of inventory  
to reach a certain distance, year<sup>-1</sup>



Canister penetration	$t_0$	0	years
Leach time	$\Delta t$	$3 \cdot 10^4$	years
Hydraulic conductivity	$K_p$	$10^{-9}$	m/s
Hydraulic gradient	$i$	0.01	m/m
Fissure spacing	$S$	50	m
Peclet number	$Pe$	0.5	-
Effective diffusivity	$D_p \epsilon_p$	$10^{-12}$	$m^2/s$

Figure 19

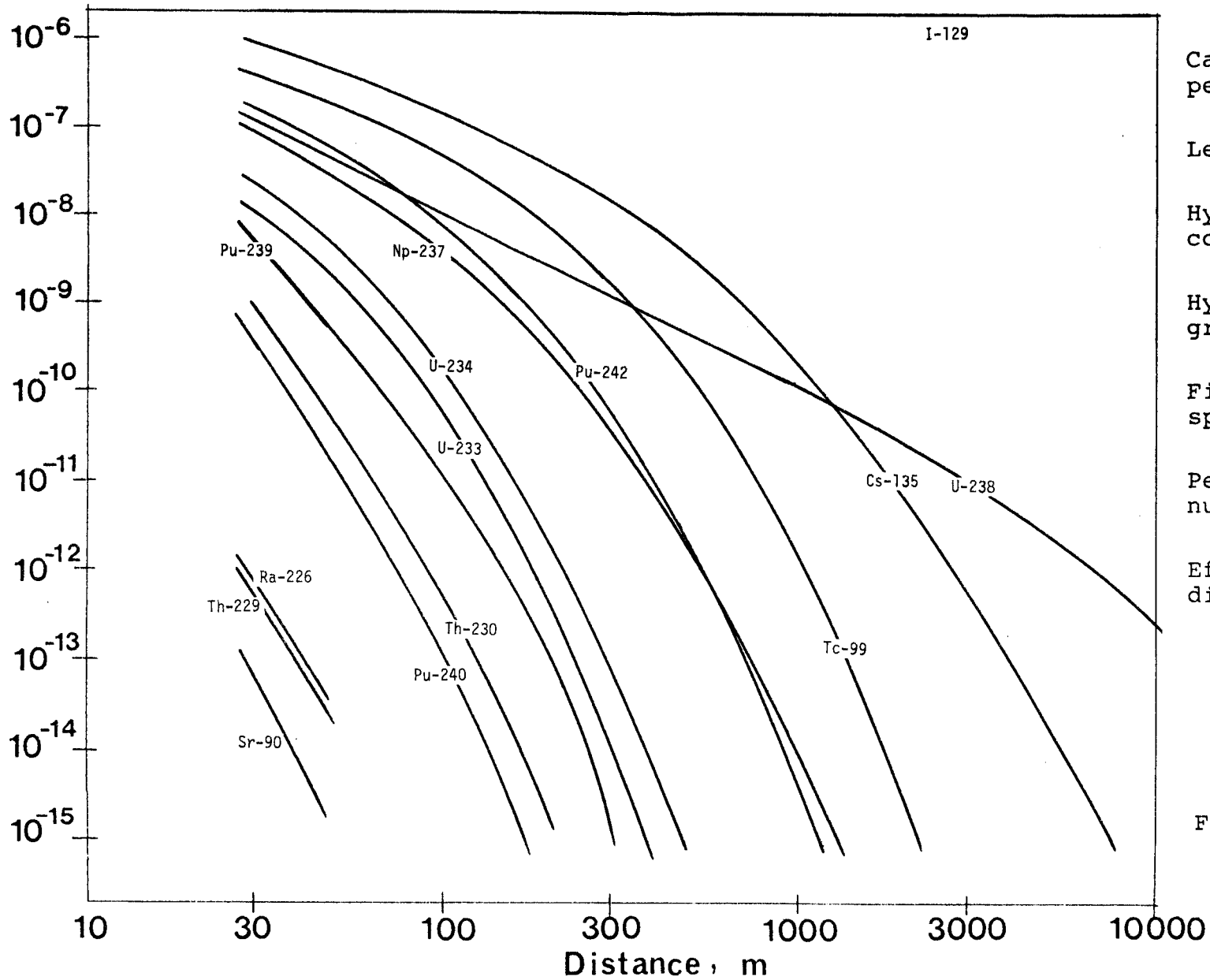
Fraction of inventory  
to reach a certain distance, year<sup>-1</sup>



Canister penetration	$t_o$	0	years
Leach time	$\Delta t$	$5 \cdot 10^5$	years
Hydraulic conductivity	$K_p$	$10^{-9}$	m/s
Hydraulic gradient	$i$	0.01	m/m
Fissure spacing	$S$	50	m
Peclet number	$Pe$	$\infty$	-
Effective diffusivity	$D_p \epsilon_p$	$10^{-12}$	m <sup>2</sup> /s

Figure 20

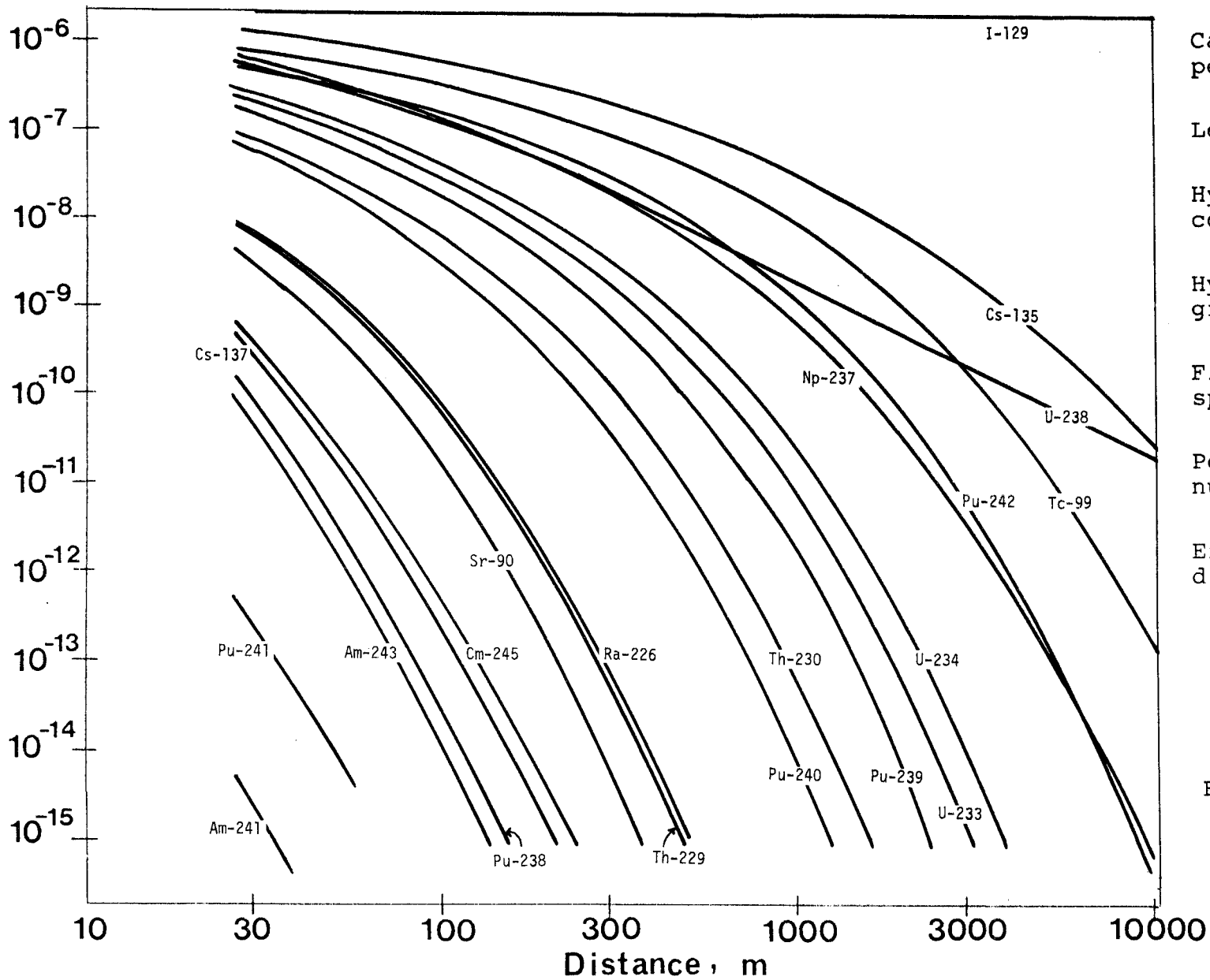
Fraction of inventory  
to reach a certain distance, year<sup>-1</sup>



Canister penetration	$t_o$	0 years
Leach time	$\Delta t$	$5 \cdot 10^5$ years
Hydraulic conductivity	$K_p$	$10^{-9}$ m/s
Hydraulic gradient	$i$	0.01 m/m
Fissure spacing	$S$	50 m
Peclet number	$Pe$	5.0 -
Effective diffusivity	$D_p \epsilon_p$	$10^{-12}$ m <sup>2</sup> /s

Figure 21

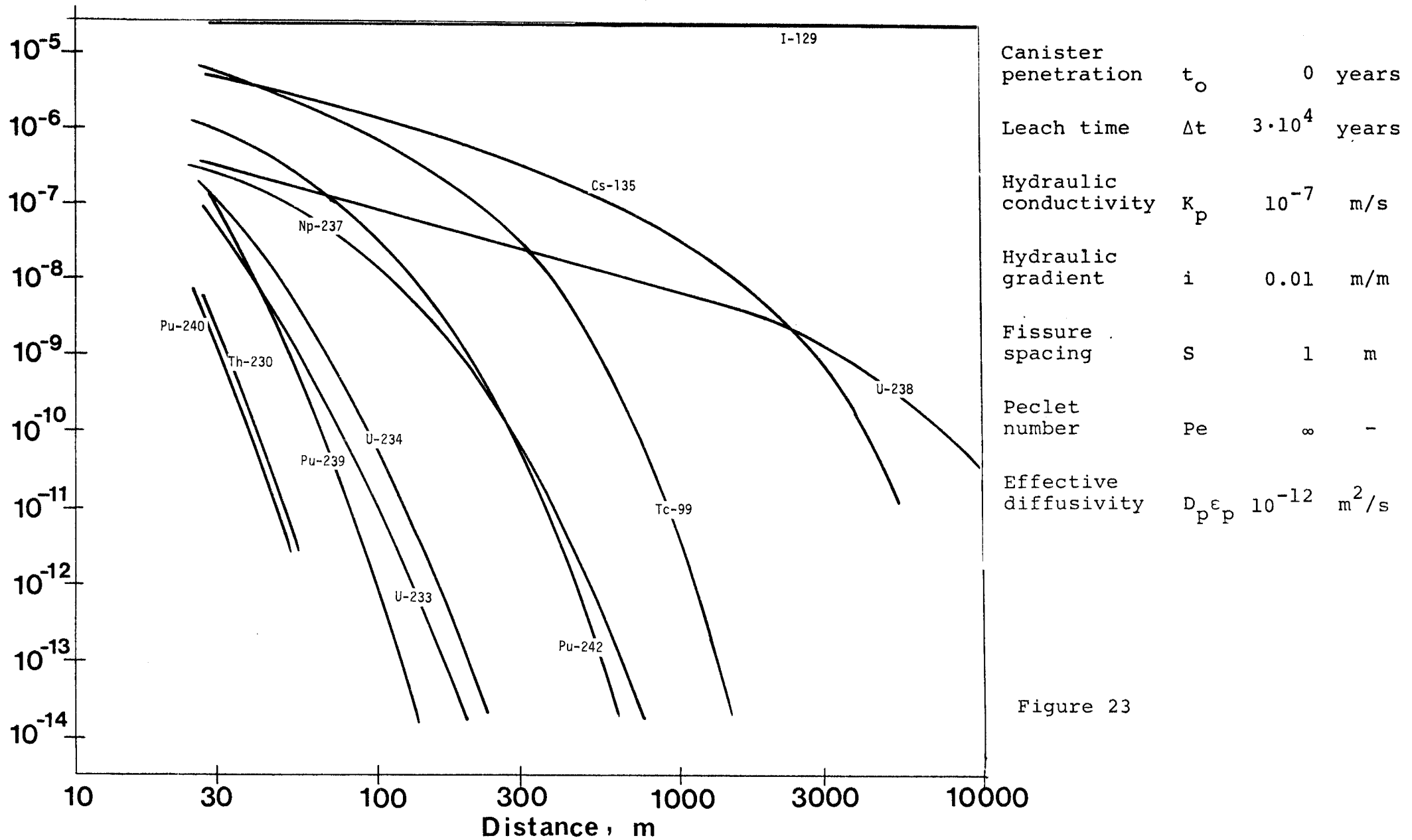
Fraction of inventory  
to reach a certain distance, year<sup>-1</sup>



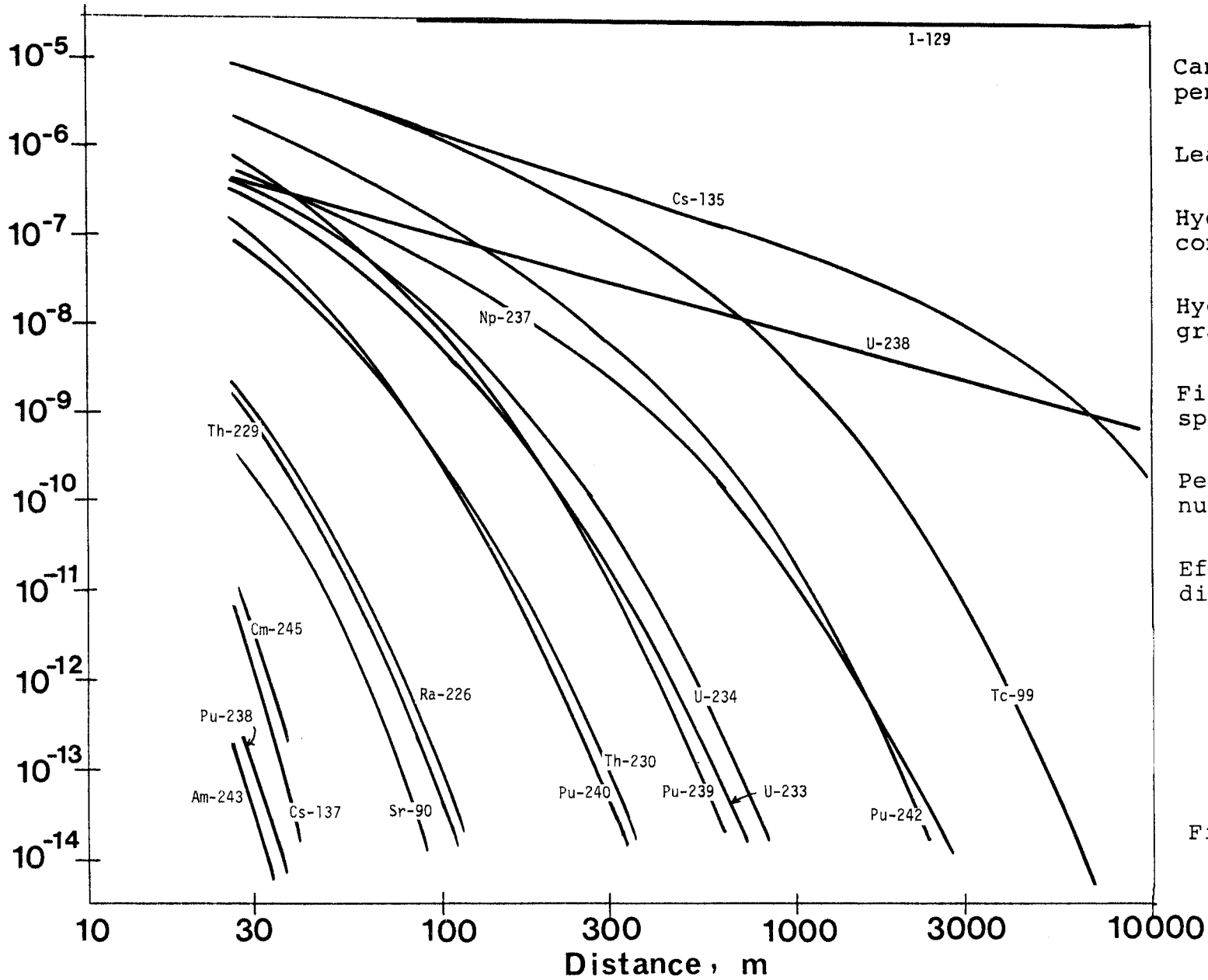
Canister penetration	$t_0$	0	years
Leach time	$\Delta t$	$5 \cdot 10^5$	years
Hydraulic conductivity	$K_p$	$10^{-9}$	m/s
Hydraulic gradient	$i$	0.01	m/m
Fissure spacing	$S$	50	m
Peclet number	$Pe$	0.5	-
Effective diffusivity	$D_p \epsilon_p$	$10^{-12}$	$m^2/s$

Figure 22

Fraction of inventory  
to reach a certain distance, year<sup>-1</sup>



Fraction of inventory  
to reach a certain distance, year<sup>-1</sup>

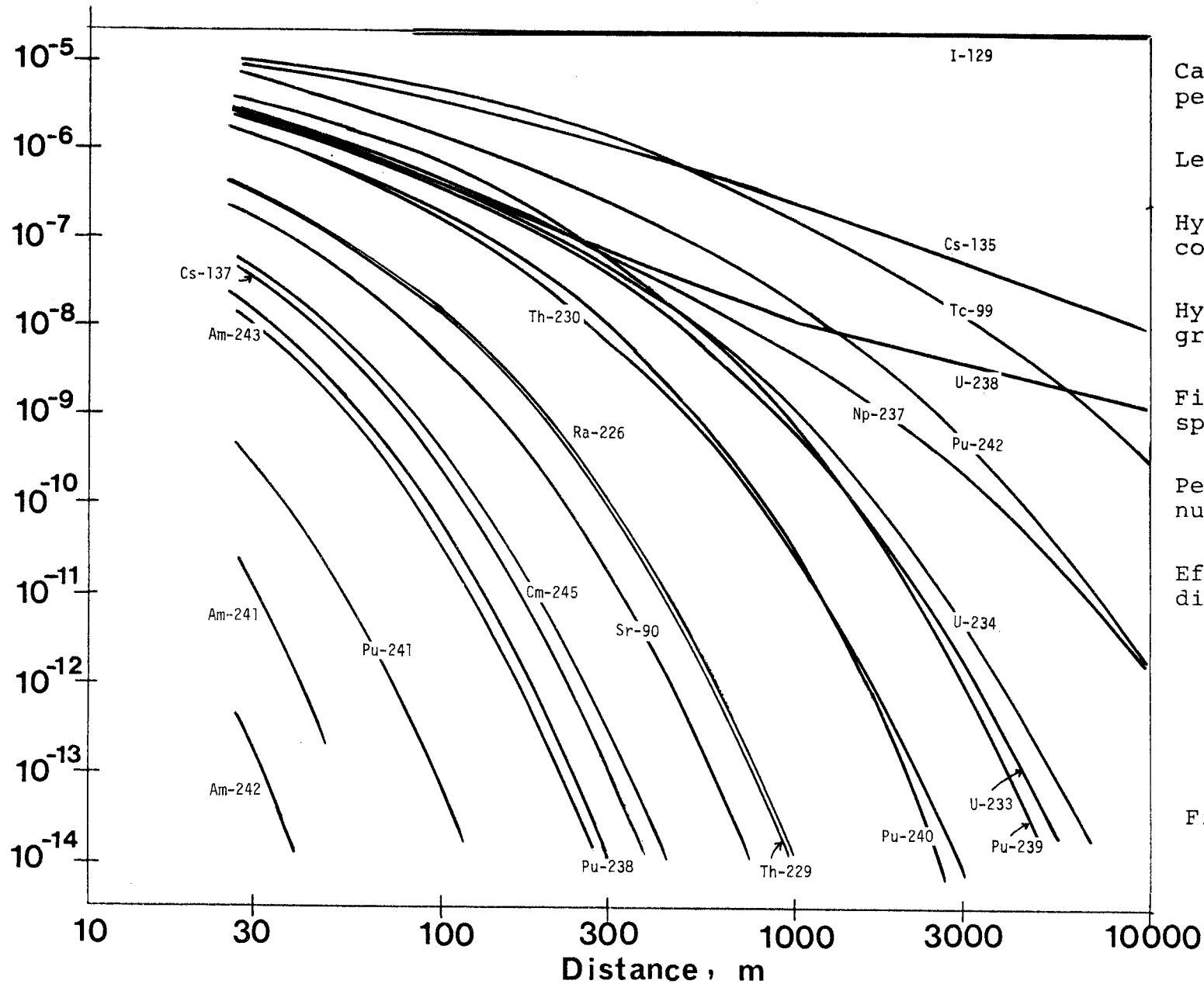


Canister penetration	$t_0$	0	years
Leach time	$\Delta t$	$3 \cdot 10^4$	years
Hydraulic conductivity	$K_p$	$10^{-7}$	m/s
Hydraulic gradient	$i$	0.01	m/m
Fissure spacing	$S$	1	m
Peclet number	$Pe$	5.0	-
Effective diffusivity	$D_p \epsilon_p$	$10^{-12}$	$m^2/s$

Figure 24



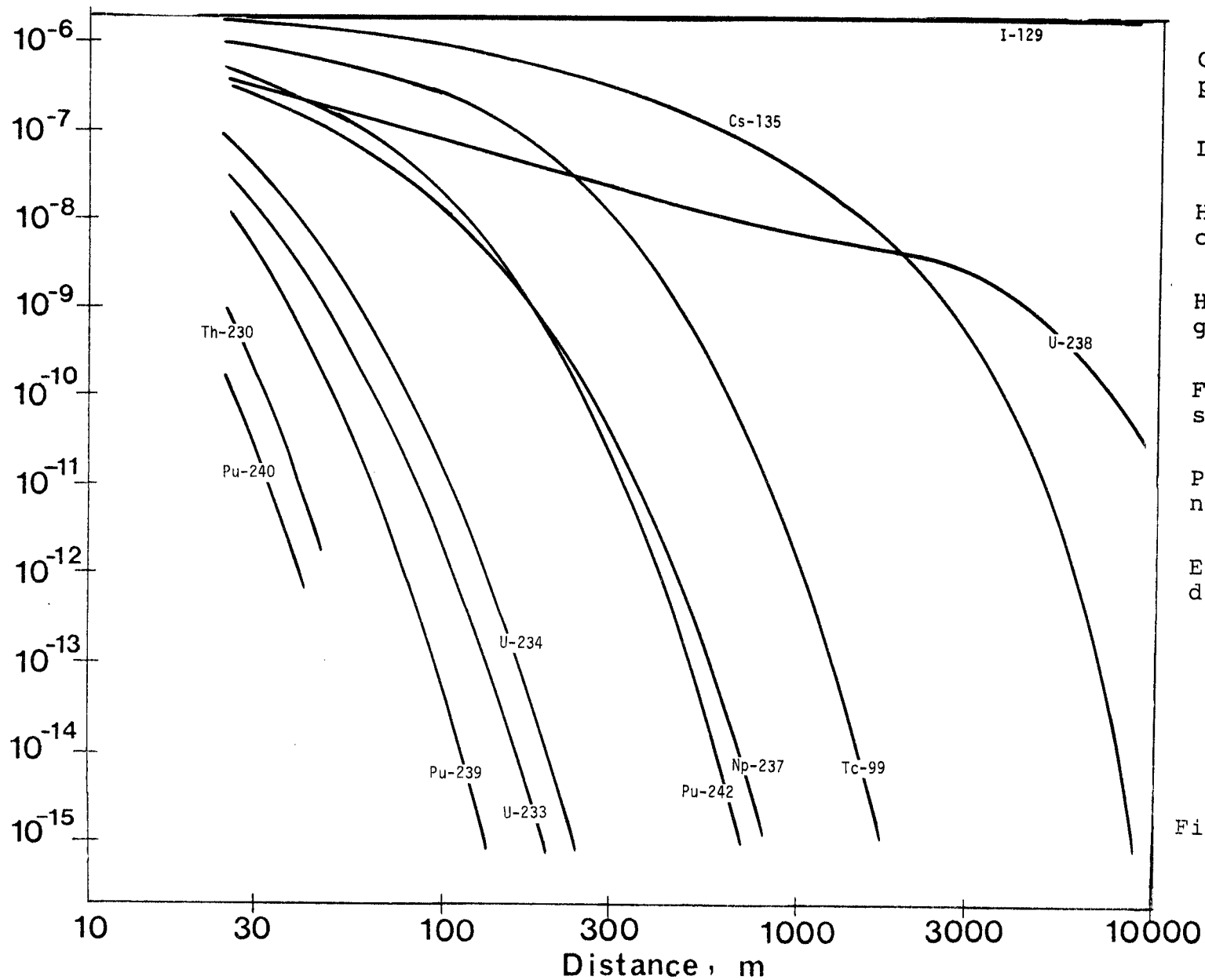
Fraction of inventory  
to reach a certain distance, year<sup>-1</sup>



Canister penetration	$t_0$	0	years
Leach time	$\Delta t$	$3 \cdot 10^4$	years
Hydraulic conductivity	$K_p$	$10^{-7}$	m/s
Hydraulic gradient	$i$	0.01	m/m
Fissure spacing	$S$	1	m
Peclet number	$Pe$	0.5	-
Effective diffusivity	$D_p \epsilon_p$	$10^{-12}$	$m^2/s$

Figure 25

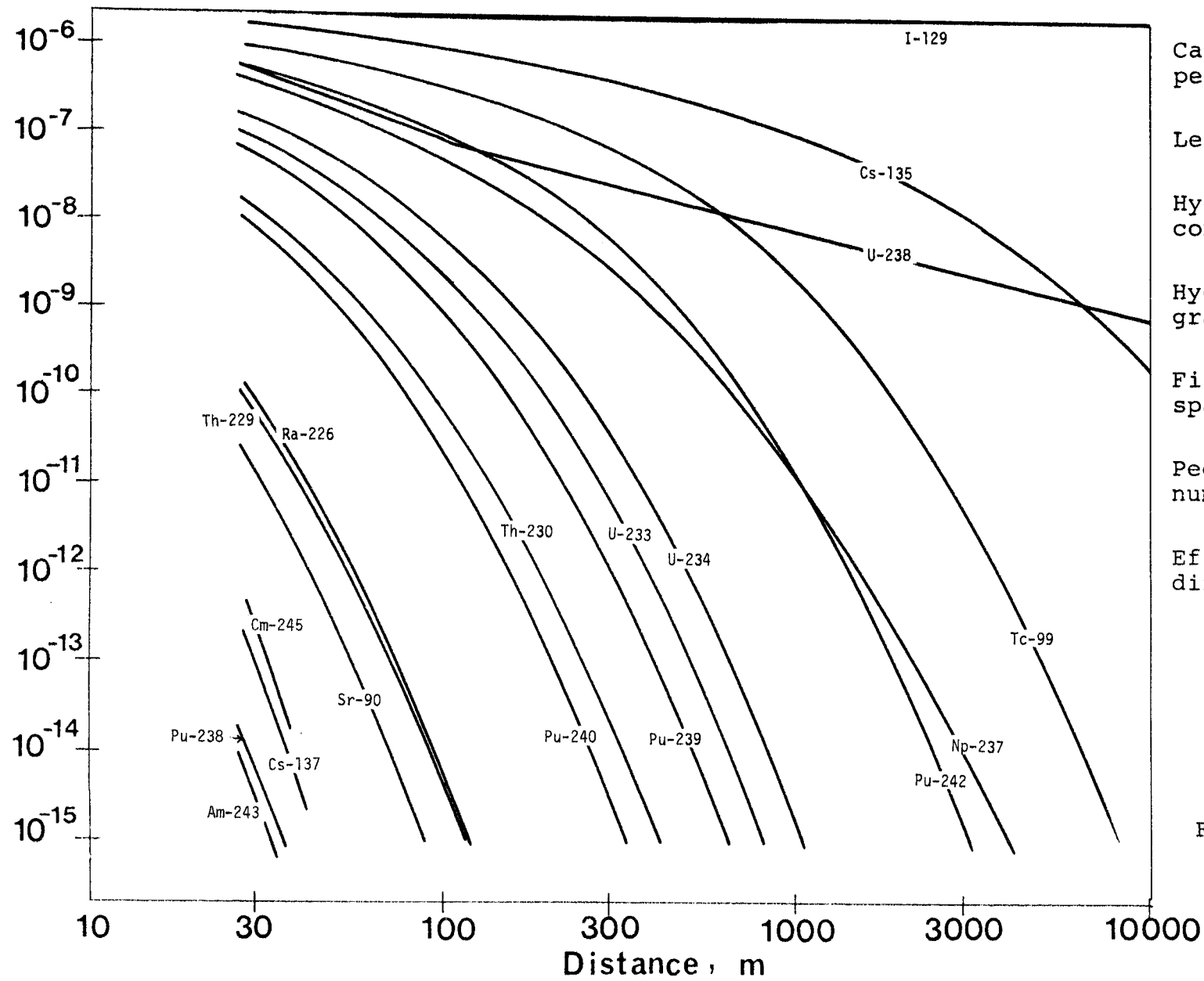
Fraction of inventory  
to reach a certain distance, year<sup>-1</sup>



Canister penetration	$t_o$	0	years
Leach time	$\Delta t$	$5 \cdot 10^5$	years
Hydraulic conductivity	$K_p$	$10^{-7}$	m/s
Hydraulic gradient	$i$	0.01	m/m
Fissure spacing	$S$	1	m
Peclet number	$Pe$	$\infty$	-
Effective diffusivity	$D_p \epsilon_p$	$10^{-12}$	$m^2/s$

Figure 26

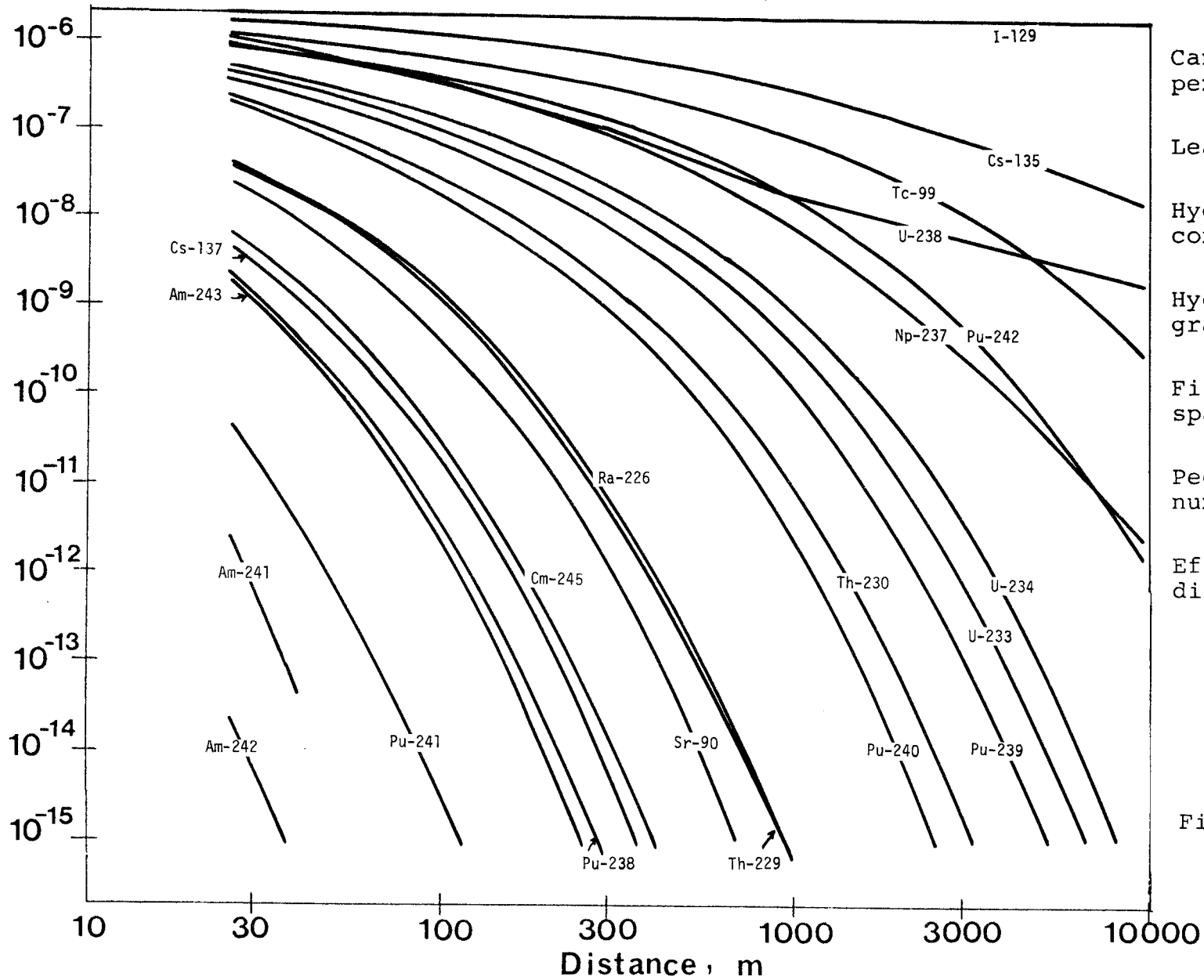
Fraction of inventory  
to reach a certain distance, year<sup>-1</sup>



Canister penetration	$t_o$	0	years
Leach time	$\Delta t$	$5 \cdot 10^5$	years
Hydraulic conductivity	$K_p$	$10^{-7}$	m/s
Hydraulic gradient	$i$	0.01	m/m
Fissure spacing	$S$	1	m
Peclet number	$Pe$	5.0	-
Effective diffusivity	$D_p \epsilon_p$	$10^{-12}$	$m^2/s$

Figure 27

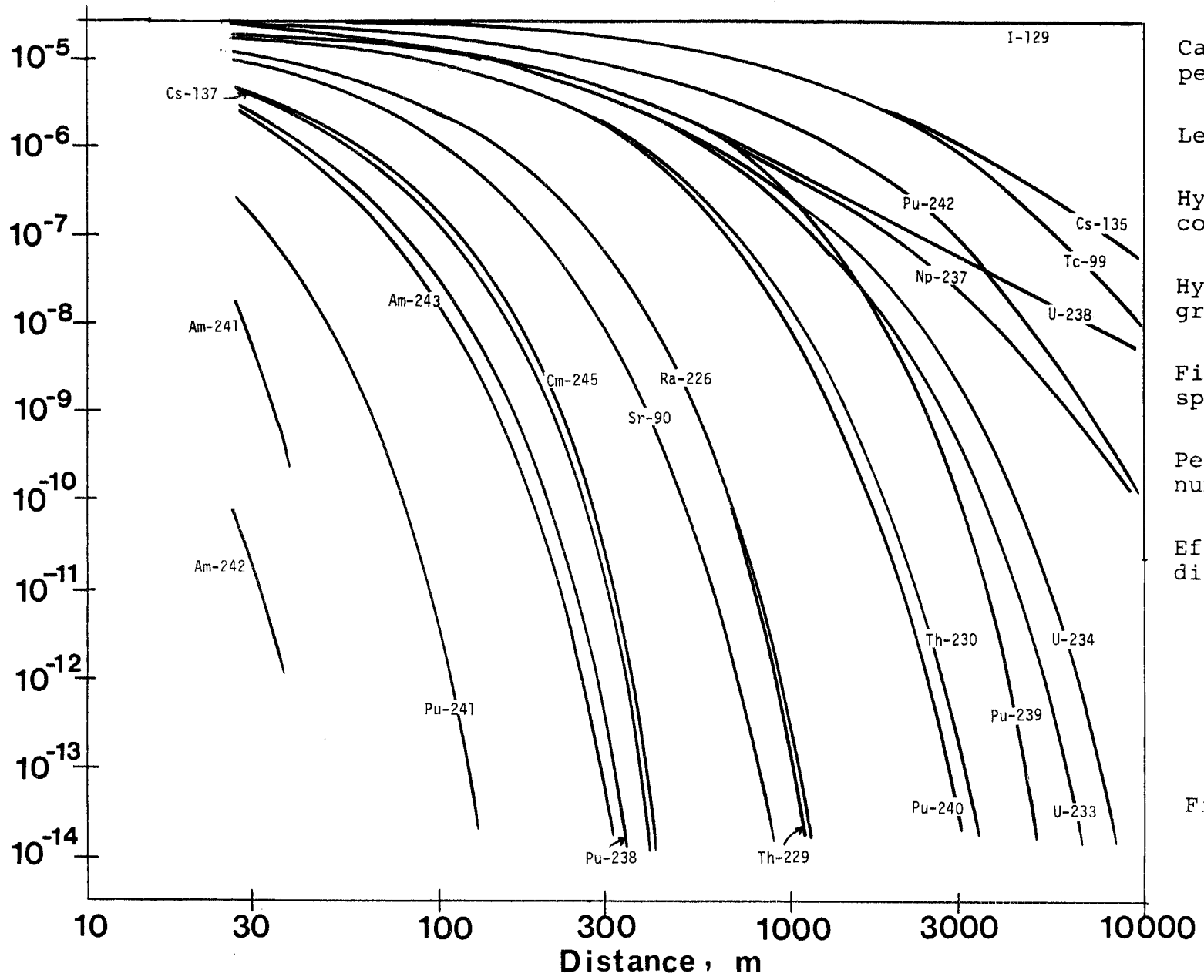
Fraction of inventory  
to reach a certain distance, year<sup>-1</sup>



Canister penetration	$t_0$	0	years
Leach time	$\Delta t$	$5 \cdot 10^5$	years
Hydraulic conductivity	$K_p$	$10^{-7}$	m/s
Hydraulic gradient	$i$	0.01	m/m
Fissure spacing	$S$	1	m
Peclet number	$Pe$	0.5	-
Effective diffusivity	$D_p \epsilon_p$	$10^{-12}$	$m^2/s$

Figure 28

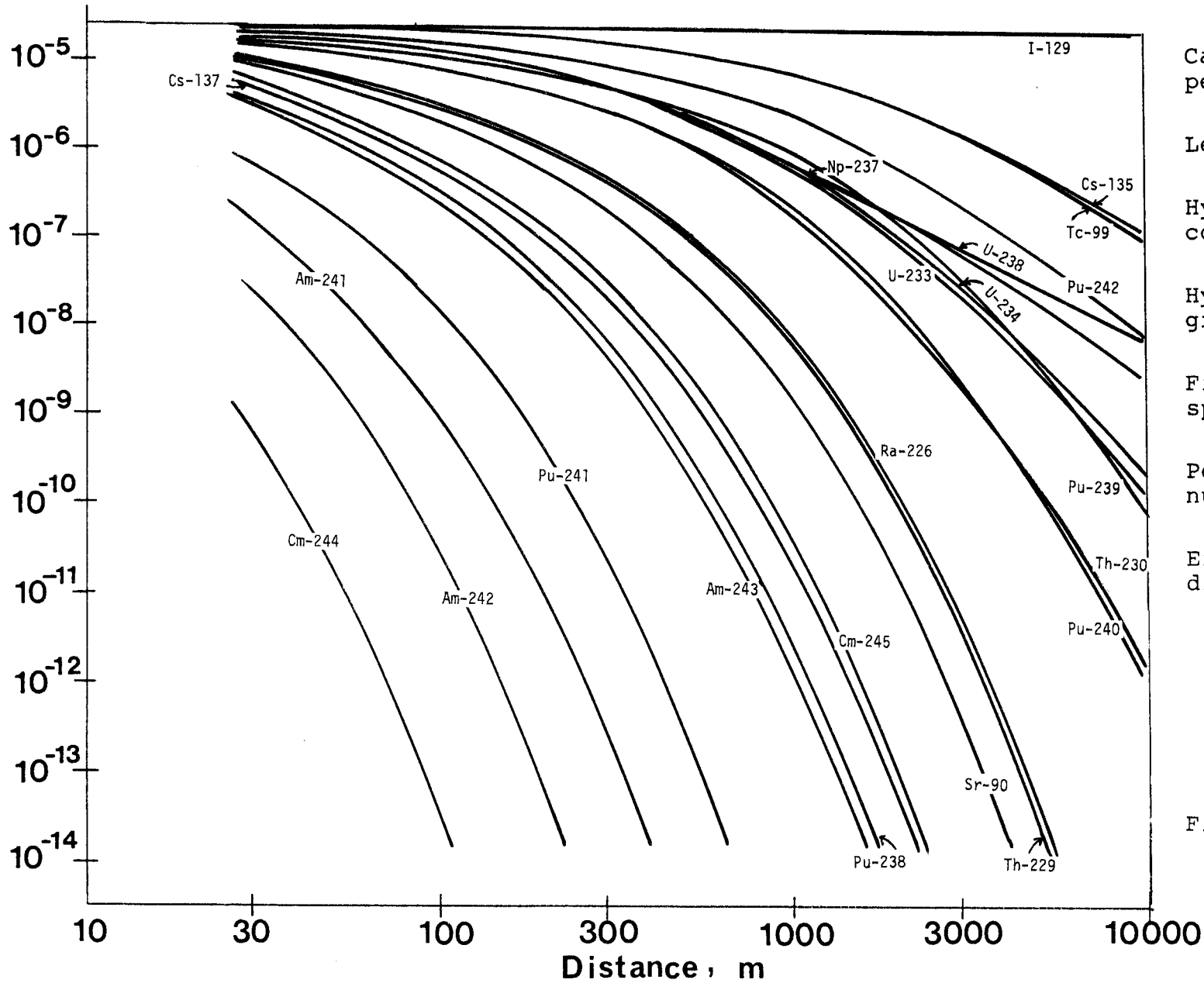
Fraction of inventory  
to reach a certain distance, year<sup>-1</sup>



Canister penetration	$t_0$	0	years
Leach time	$\Delta t$	$3 \cdot 10^4$	years
Hydraulic conductivity	$K_p$	$10^{-7}$	m/s
Hydraulic gradient	$i$	0.01	m/m
Fissure spacing	$S$	50	m
Peclet number	$Pe$	$\infty$	-
Effective diffusivity	$D_p \epsilon_p$	$10^{-12}$	m <sup>2</sup> /s

Figure 29

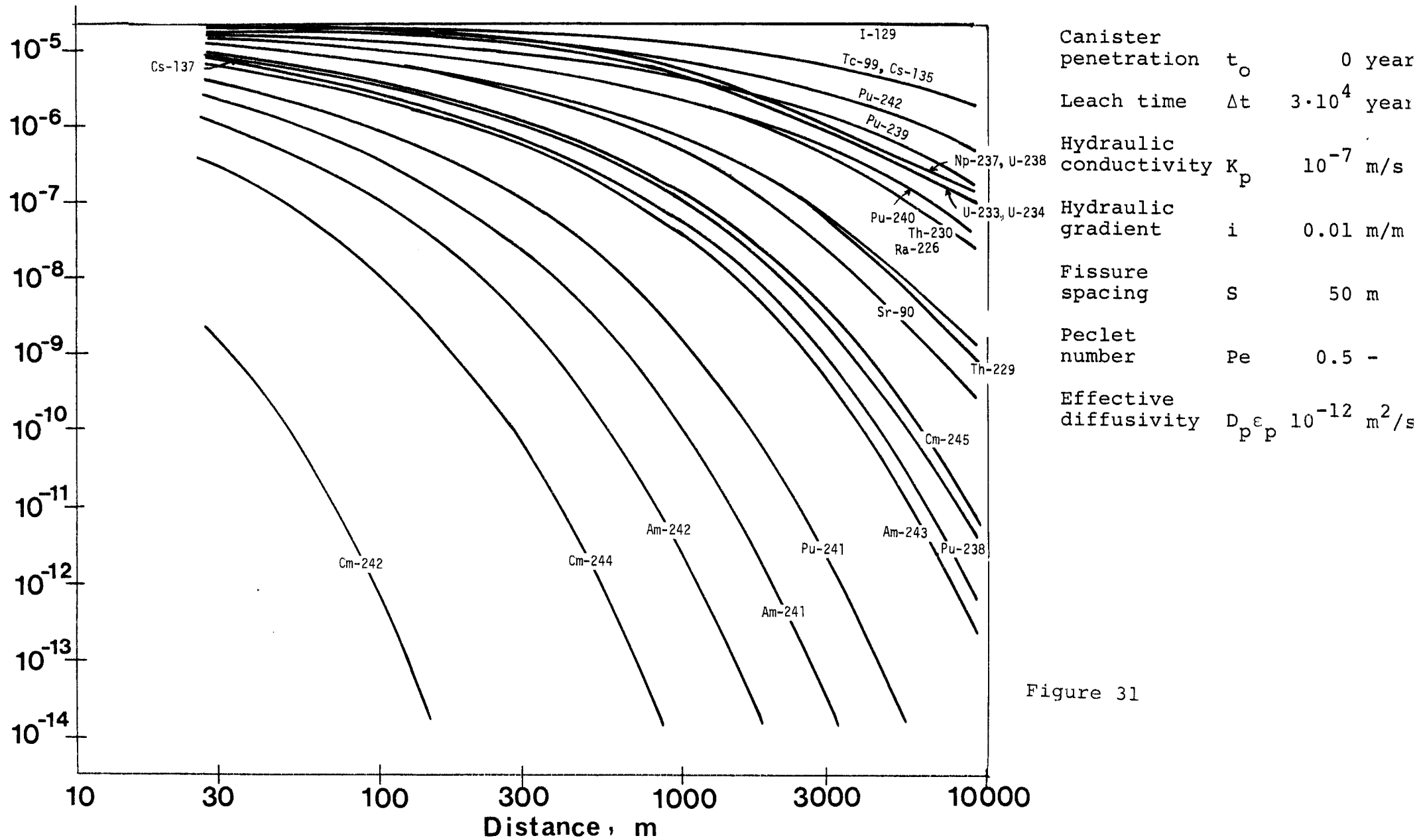
Fraction of inventory  
to reach a certain distance, year<sup>-1</sup>



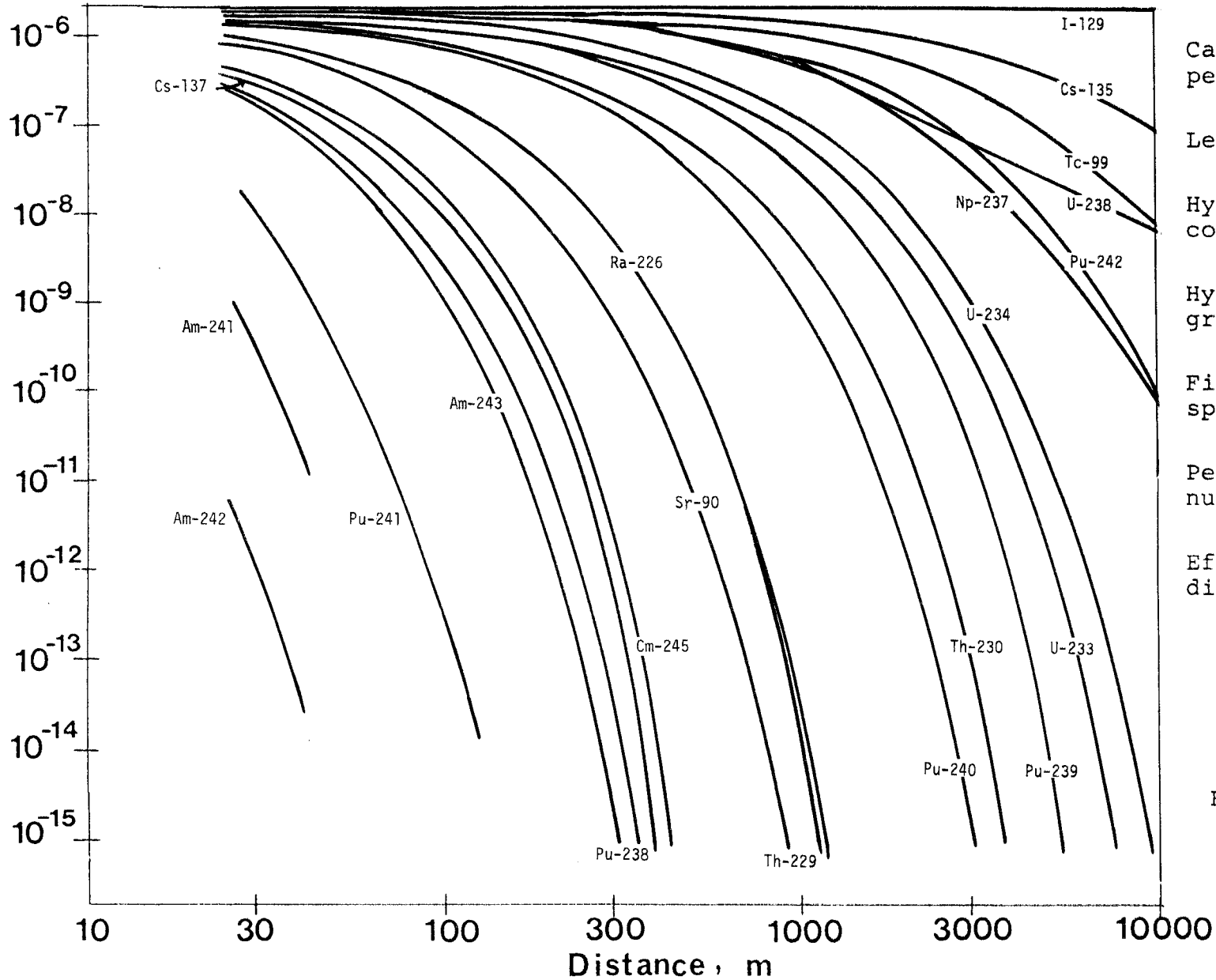
Canister penetration	$t_0$	0	years
Leach time	$\Delta t$	$3 \cdot 10^4$	years
Hydraulic conductivity	$K_p$	$10^{-7}$	m/s
Hydraulic gradient	$i$	0.01	m/m
Fissure spacing	$S$	50	m
Peclet number	$Pe$	5.0	-
Effective diffusivity	$D_p \epsilon_p$	$10^{-12}$	$m^2/s$

Figure 30

Fraction of inventory  
to reach a certain distance, year<sup>-1</sup>



Fraction of inventory  
to reach a certain distance, year<sup>-1</sup>

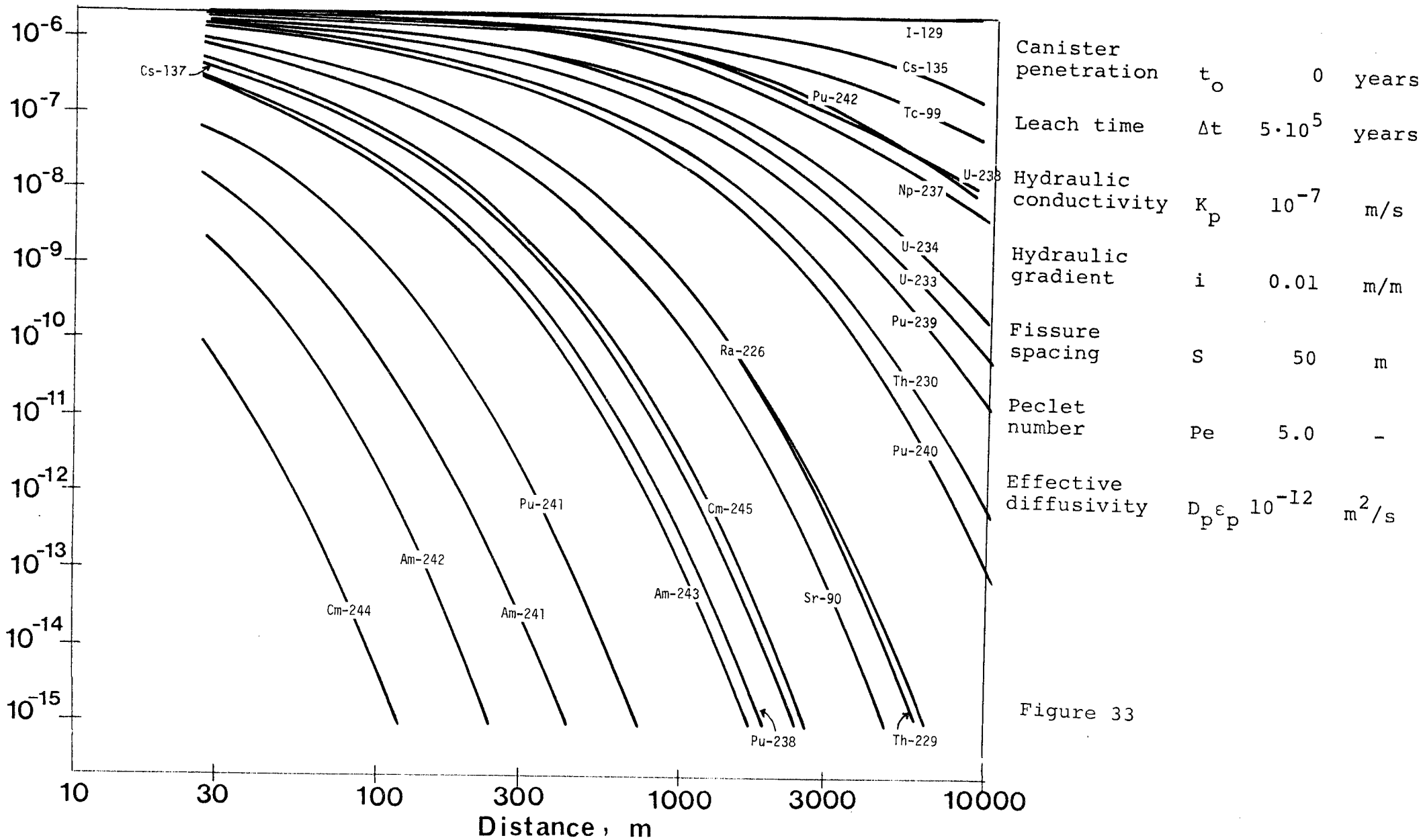


Canister penetration	$t_o$	0	years
Leach time	$\Delta t$	$5 \cdot 10^5$	years
Hydraulic conductivity	$K_p$	$10^{-7}$	m/s
Hydraulic gradient	$i$	0.01	m/m
Fissure spacing	$S$	50	m
Peclet number	$Pe$	$\infty$	-
Effective diffusivity	$D_p \epsilon_p$	$10^{-12}$	$m^2/s$

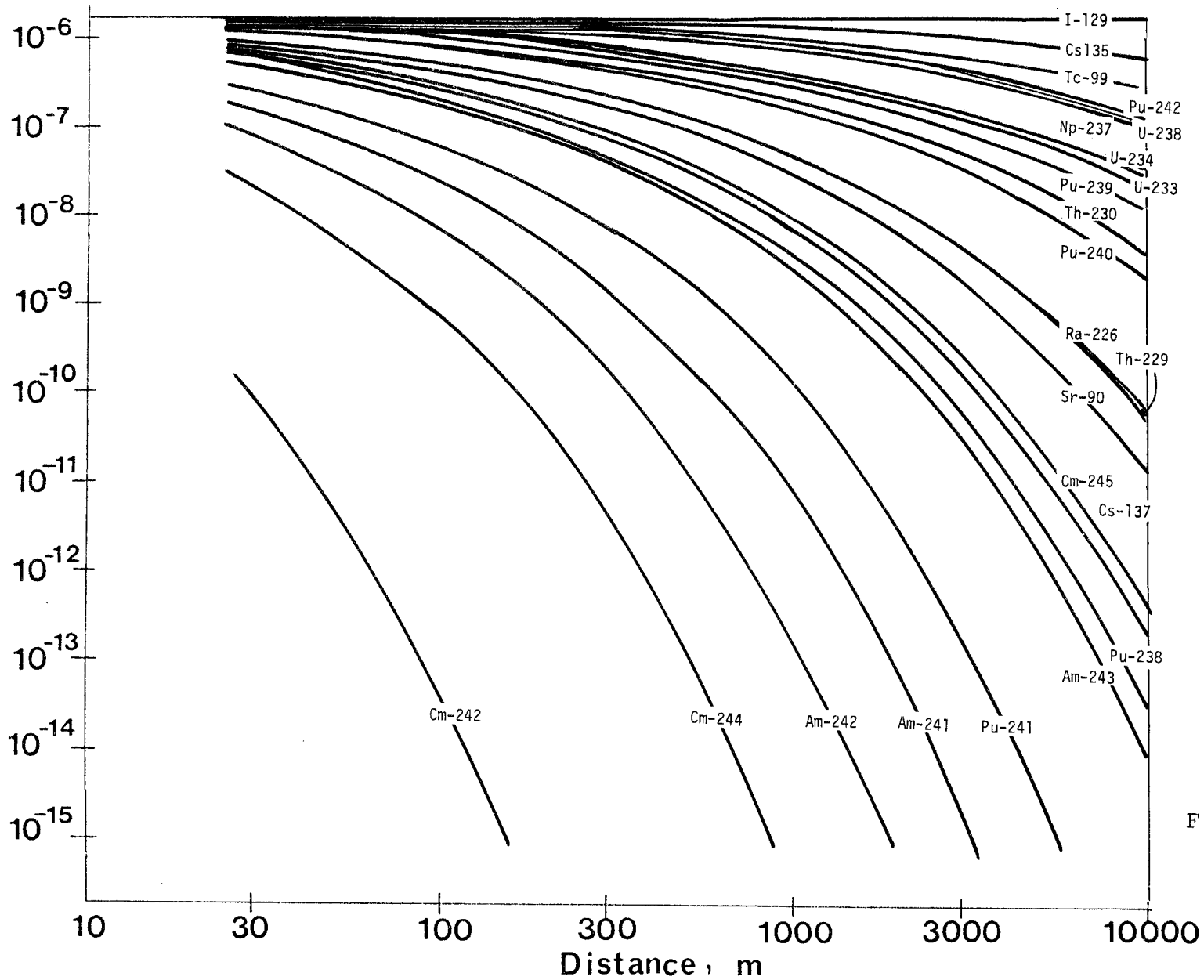
Figure 32



Fraction of inventory  
to reach a certain distance, year<sup>-1</sup>



Fraction of inventory  
to reach a certain distance, year<sup>-1</sup>



Canister penetration	$t_0$	0	year
Leach time	$\Delta t$	$5 \cdot 10^5$	year
Hydraulic conductivity	$K_p$	$10^{-7}$	m/day
Hydraulic gradient	$i$	0.01	m/m
Fissure spacing	$S$	50	m
Peclet number	$Pe$	0.5	-
Effective diffusivity	$D_p \epsilon_p$	$10^{-12}$	m <sup>2</sup> /year

Figure 34

FÖRTECKNING ÖVER KBS TEKNISKA RAPPORTER

1977-78

TR 121 KBS Technical Reports 1 - 120.  
Summaries. Stockholm, May 1979.

1979

TR 79-28 The KBS Annual Report 1979.  
KBS Technical Reports 79-01--79-27.  
Summaries. Stockholm, March 1980.

1980

TR 80-26 The KBS Annual Report 1980.  
KBS Technical Reports 80-01--80-25.  
Summaries. Stockholm, March 1981.

1981

TR 81-17 The KBS Annual Report 1981.  
KBS Technical Reports 81-01--81-16  
Summaries. Stockholm, April 1982.

1982

TR 82-01 Hydrothermal conditions around a radioactive waste  
repository  
Part 3 - Numerical solutions for anisotropy  
Roger Thunvik  
Royal Institute of Technology, Stockholm, Sweden  
Carol Braester  
Institute of Technology, Haifa, Israel  
December 1981

TR 82-02 Radiolysis of groundwater from HLW stored in copper  
canisters  
Hilbert Christensen  
Erling Bjergbakke  
Studsvik Energiteknik AB, 1982-06-29

- TR 82-03 Migration of radionuclides in fissured rock:  
Some calculated results obtained from a model based  
on the concept of stratified flow and matrix  
diffusion  
Ivars Neretnieks  
Royal Institute of Technology  
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The influence of matrix diffusion  
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