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# DIFFUSIONAL MASS TRANSPORT PHENOMENA IN THE BUFFER MATERIAL AND DAMAGED ZONE OF A BOREHOLE WALL IN AN UNDERGROUND NUCLEAR FUEL WASTE VAULT

# PHENOMENE DE TRANSPORT DE MASSE PAR DIFFUSION DANS LE MATERIAU D'ISOLEMENT ET LA ZONE ENDOMMAGEE D'UNE PAROI DE PUITS A L'INTERIEUR D'UNE ENCEINTE SOUTERRAINE D'EVACUATION DES DECHETS DE COMBUSTIBLE NUCLEAIRE

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Etablissement de recherches
nucléaires de Whiteshell

Pinawa, Manitoba R0E 1L0
June 1983 juin

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# PHÉNOMÈNE DE TRANSPORT DE MASSE PAR DIFFUSION DANS LE MATÉRIAU D'ISOLEMENT ET LA ZONE ENDOMMAGÉE D'UNE PAROI DE PUITS À L'INTÉRIEUR D'UNE ENCEINTE SOUTERRAINE D'ÉVACUATION DES DÉCHETS DE COMBUSTIBLE NUCLÉAIRE

par

S. Page et S.C.H. Cheung

## RÉSUMÉ

On a étudié l'effet que la géométrie du forage et les caractéristiques de la paroi rocheuse endommagée du puits exercent sur le mouvement des radionucléides, à partir d'une enceinte souterraine d'évacuation de déchets de combustible nucléaire. Les données recueillies indiquent que le transport a lieu principalement par l'intermédiaire du matériau d'isolement pour atteindre la zone endommagnée de la paroi du puits. Au fur et à mesure que s'accentue le degré de fracturation de la zone endommagée, le flux des radionucléides augmente jusqu'à une limite dont on peut obtenir l'approximation grâce à un modèle de diffusion radiale unidimensionnel. Dans le cas d'une fissuration importante de la zone endommagée, le fait d'augmenter l'épaisseur du matériau d'isolement radial fait diminuer le flux total, tandis que, dans le cas de fissurations de peu d'importance, un matériau d'isolement radial plus épais peut provoquer une légère augmentation du flux total. En augmentant l'épaisseur du matériau tampon dans le plan vertical, on réduit considérablement le flux total si le degré de fissuration de la zone endommagée est peu important. Dans le sens vertical, le prolongement de la zone endommagée provoque une augmentation du flux total.

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## ABSTRACT

The effects of the geometry of the borehole and the characteristics of the damaged borehole rock wall on the movement of radionuclides from an underground nuclear waste vault have been studied. The results show that radionuclide transport will occur mainly through the buffer into the damaged zone of the borehole wall. As the degree of fracturing of the damaged zone increases, the total radionuclide flux will increase up to a limit which can be approximated by a one-dimensional radial diffusion model. For large degrees of fracturing of the damaged zone, an increase in the radial buffer material thickness will decrease the total flux, whereas, for small degrees of fracturing, an increase in the radial buffer thickness may slightly increase the total flux. Increasing the vertical buffer thickness will significantly decrease the total flux when the degree of fracturing of the damaged zone is small. An increase in the vertical extent of the damaged zone will cause an increase in total flux.

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# CONTENTS

# 1. INTRODUCTION

The Canadian research program for nuclear fuel waste management is based on the concept that the waste can be effectively isolated by deep underground disposal in stable geological formations.

At present, disposal in vaults mined into crystalline hard-rock formations, such as granite batholiths of the Precambrian shield, is considered to be the most favorable option [1]. In such a vault the only potentially significant mechanism of radionuclide release is for groundwater to penetrate to the waste, leach out the radionuclides, and carry them back to the surface. A number of protective barriers will be used to isolate the waste and minimize the probability of any significant escape. These are the waste form itself, the waste container, the buffer material surrounding the container, backfill and sealing materials that fill the remainder of the vault, and the massive geological formation itself (see Figure 1).

Two options for waste emplacement have been suggested and are being assessed [2]. These are (i) in-room and (ii) borehole emplacement, as shown in Figure 2. In this report, the near-field mass transport will be discussed only for the borehole-emplacement option by varying the geometry of the borehole and the characteristics of the damaged zone of the borehole wall.

# 2. NEAR-FIELD MASS TRANSPORT MODELS

Three models will be used to evaluate the near-field mass transport for borehole emplacement. These are shown schematically in Figures 3 and 4. Models I and II in Figure 3 will serve as bounding cases; in this study we shall focus on parameter-sensitivity analysis using Model III in Figure 4. The assumptions and boundary conditions used in these models are stated below.

## 2.1 GENERAL ASSUMPTIONS

The following assumptions are applicable to all three models:

1. Mass transport in the buffer is by diffusion.
2. The buffer is considered to be a porous medium with a constant and isotropic ionic diffusivity.
3. There are no chemical reactions to affect radionuclide migration.
4. Steady-state transport.

5. The waste container has completely failed and is uniformly permeable over its entire surface.

6. The radionuclide concentration at the container-buffer interface is constant.

## 2.2 MODEL I

In this model, as shown in Figure 3(a), the concentrations at the buffer-rock and buffer-backfill interfaces are considered to be zero, to maximize diffusive mass transport. This implies that the rock and backfill have no resistance to water flow, and water is flushing at these interfaces. This condition prevails when the rock is severely fractured and sand is used as backfill. It has been shown that, for this model, diffusional mass transport can be approximated using a one-dimensional infinite cylinder model [3]. The relevant equation is as follows:

$$F = D_b \cdot \frac{2\pi \Delta C \ell}{\ln(b/a)} \qquad (1)$$

where $F$ = total integrated radial mass flux at the buffer-rock interface,

$D_b$ = effective ionic diffusion coefficient in the buffer,

$\Delta C$ = concentration difference between the container-buffer interface and the buffer-rock interface,

$\ell$ = length of the waste container,

$b$ = radius of the borehole,

and $a$ = radius of the waste container.

## 2.3 MODEL II

In this model, as shown in Figure 3(b), the rock is considered to be intact and to have a permeability much lower than that of the buffer. Consequently, a no-diffusive-flux condition is considered to exist at the buffer-rock interface. The radionuclide concentration at the buffer-backfill interface is considered to be constant. It has been shown that the diffusional mass transport can be approximated in this case by a one-dimensional differential equation as follows [4]:

$$F = D_b \cdot A_b \cdot \frac{C_1 - C_2}{\Delta h} \qquad (2)$$

where $F$ = total integrated vertical mass flux at the buffer-backfill interface,

$D_b$ = effective ionic diffusion coefficient in the buffer,

$A_b$ = cross-sectional area of the borehole,

$C_1$ = concentration at the container-buffer interface,

$C_2$ = concentration at the buffer-backfill interface,

and $\Delta h$ = vertical buffer thickness, that is, the distance between the buffer-backfill interface and the top end surface of the waste container.

The concentration $C_2$ at the buffer-backfill interface depends on the groundwater flow rate, that is, the higher the groundwater flow rate, the smaller $C_2$ will be. The groundwater flow rate in the backfill depends on the hydraulic gradient and the permeability of the backfill. Since this information is not available, $C_2$ is considered to be zero in order to assess the effect of the geometry and the properties of the borehole rock wall on the radionuclide flux.

## 2.4 MODEL III

In this model, as shown in Figure 4, a damaged zone of borehole rock wall is considered to exist between the buffer material and the intact rock. The damaged zone is considered to be a porous medium with a constant and isotropic ionic diffusivity. Mass transport in the damaged zone of the borehole wall is by diffusion, driven only by the concentration gradient, that is, the water in the cracks of the damaged zone is assumed to be stagnant. The damaged zone may arise from excavation of the drift by blasting and from drilling of the borehole. A no-radionuclide-flux condition is considered to exist at the damaged-zone/intact-rock interface. The concentration at the buffer-backfill and damaged-zone backfill interfaces is considered to be zero, as assumed for Model II.

In this report, the effects of borehole geometry and the characteristics of the damaged zone of the borehole rock wall on the radionuclide flux will be studied by varying five parameters in Model III: (i) vertical buffer thickness, (ii) radial buffer thickness, (iii) radial damaged-zone thickness, (iv) depth of the damaged zone, and (v) effective diffusion coefficient of the rock, indicating the degree of fracture in the damaged zone. The vertical buffer thickness is defined as the distance between the buffer-backfill interface and the top end surface of the waste container. The radial buffer thickness is defined as the distance between the buffer-container and buffer-rock interfaces. The radial damaged-zone thickness is defined as the distance between the damaged-zone/buffer and the damaged-zone/intact-rock interfaces. The depth of the damaged zone is defined as the vertical distance between the damaged-zone/backfill and damaged-zone/intact-rock interfaces. These are indicated in Figure 4. The effective diffusion coefficient is defined as follows [5]:

$$D_R = \frac{D \cdot \varepsilon}{\tau^2} \qquad (3)$$

where $D_R$ = effective diffusion coefficient in damaged rock,

$D$ = ionic diffusivity in bulk water,

$\varepsilon$ = porosity,

and $\tau$ = tortuosity.

To calculate the radionuclide flux, a computer code known as the DOT program was used [6]. This program simulates heat conduction using the finite-element method. The thermal solution given by the DOT program has been validated against temperature data from an underground heating experiment in granitic rock [7]. Since concentration diffusion is governed by the same partial differential equation as heat conduction, the DOT program is also applicable to the diffusion problem. The results obtained from the DOT program agree very well with those predicted by the analytical solutions [6].

## 3. RESULTS AND DISCUSSION

Figure 5 shows several radionuclide concentration profiles for a half longitudinal section of the borehole, as produced by the DOT program. The waste container considered is 0.35 m in diameter and 3 m long. In the first profile, $D_b$ represents the effective diffusion coefficient in the buffer. The effective diffusion coefficient in the damaged zone is expressed relative to the diffusion coefficient of the buffer. For example, when the relative diffusion coefficient of the damaged zone is two, the effective diffusion coefficient of the damaged zone is twice that of the buffer. The concentration is expressed as a percentage of the concentration at the container-buffer interface. As shown in profile 1, when the relative diffusion coefficient of the damaged zone is small, diffusion occurs mainly in the vertical direction, since the concentration contours are mainly horizontal. As the relative diffusion coefficient increases, the radionuclide flux occurs more in the radial direction because the concentration contours become more vertical. In this case, the radionuclides would migrate mainly into the damaged zone through the buffer, and then travel vertically into the drift.

Figure 6 shows the same trend of concentration profiles when the radial damaged-zone thickness is reduced to 0.1 m.

In Figures 7 - 12, the total flux is defined as the total integrated mass flux through the cross-sectional area of the buffer and/or the damaged zone at the backfill-buffer or backfill-rock interface, available for diffusion into the drift. The total flux has been normalized and has no units. The normalization of flux is obtained by using unit diffusion coefficient of buffer and unit concentration at the buffer-container interface.

In Figure 7, six curves are shown for six relative diffusion coefficients (RDC) of the damaged zone for a radial buffer thickness (RBT) of 0.275 m and a vertical buffer thickness (VBT) of 1.0 m. All curves begin at the same point when the damaged-zone thickness is zero. This value corresponds to the total vertical radionuclide flux predicted by Equation (2) from Model II. As the radial thickness of the damaged zone increases, the total flux increases. This is due to the dominant increase in the cross-sectional area for diffusion into the drift as compared to the decrease in concentration gradient shown in Figures 5 and 6. As expected, when the relative diffusion coefficient in the damaged zone is higher, there is a sharper increase in the total flux. As the radial damaged-zone thickness becomes very large, the curves begin to level off. This levelling off is most apparent at a relative diffusion coefficient of 100, where the curve seems to approach a total flux limit, which corresponds closely to that predicted by Equation (1) of Model I. In Figure 8, four curves representing different radial thicknesses of the damaged zone (RDZT) are shown. These curves are very similar to those shown in Figure 7 because all curves start at the same point and increase towards the same flux limit as observed for increases in the relative diffusion coefficient.

Figure 9 shows the effect of the radial buffer thickness on the total flux for a given radial damaged-zone thickness of 0.25 m, and a given vertical buffer thickness of 1.0 m. Curves are shown for six relative diffusion coefficients of the damaged zone. The curves indicate that, for small relative diffusion coefficients, an increase in the radial buffer thickness will slightly increase the total flux. This increase is due to an increase in the cross-sectional area for diffusion into the drift. For large relative diffusion coefficients of 50 or more, an increase in the radial buffer thickness will decrease the total flux into the drift.

Figure 10 shows the effect of radial buffer thickness on the total flux for a relative diffusion coefficient of 10 and a vertical buffer thickness 1.0 m. Curves are shown for four radial damaged-zone thicknesses. For radial damaged-zone thicknesses above 0.5 m, increasing the radial buffer thickness decreases the total flux slightly, whereas below 0.5 m, increasing the radial buffer thickness increases the total flux slightly.

Figures 11 and 12 show the effect of vertical buffer thickness on the total flux for a radial buffer thickness of 0.275 m, and a radial damaged-zone thickness or relative diffusion coefficient as indicated on each figure. All curves indicate that an increase in the vertical buffer thickness will decrease the total flux. However, the fractional decrease in total flux is greater when the relative diffusion coefficient is lower (Figure 11), or the radial damaged-zone thickness is smaller (Figure 12).

Figure 13 shows the effect of the depth of the damaged zone on the total flux for a radial buffer thickness of 0.1375 m, a vertical buffer thickness of 0.5 m, a radial damaged-zone thickness of 0.425 m, and a relative diffusion coefficient of 100. The total flux in this case is expressed as a percent of the total flux at a damaged-zone depth of 4.0 m. As can be seen, an increase in the depth of the damaged zone results in an increase in total flux. The greatest rate of increase occurs between 0.5 m and 2.0 m, where the total flux increases from 14% to 75%. This implies that, if the damaged zone is 4 m deep, then lowering the container 2 to 4 m would significantly reduce the total flux.

## 4. SUMMARY AND CONCLUSIONS

The effects of borehole geometry and the characteristics of the damaged zone on the total radionuclide flux into the drift have been studied using Model III. Their results are summarized below:

1) For large relative diffusion coefficients or radial damaged-zone thicknesses, diffusion will occur mainly from the container, through the buffer and into the damaged zone.

2) An increase in the degree of fracturing or the radial thickness of the damaged zone will increase the total flux. However, the total flux will approach a limit which can be approximated by a one-dimensional radial diffusion model for an infinite cylinder.

3) For large relative diffusion coefficients or radial damaged-zone thicknesses, an increase in the radial buffer thickness will slightly decrease the total flux, whereas, for small relative diffusion coefficients or radial damaged-zone thicknesses, an increase in buffer thickness will increase total flux.

4) An increase in the vertical buffer thickness will decrease the total flux significantly when the relative diffusion coefficient or the radial damaged-zone thickness is small.

5) Increasing the depth of the damaged zone will increase the total flux into the drift.

In conclusion, this approach can be used to assess the geometry of the borehole required to optimize the total radionuclide flux, when the hydraulic properties of the buffer, the backfill, and the damaged zone of the borehole rock wall are known

## ACKNOWLEDGEMENTS

Reviews by T. Chan, V. Guvanasen and T. Melnyk substantially improved this manuscript.

The DOT program used in the present study is a modified version provided by T. Chan and O. Wan, formerly of the Lawrence Berkeley Laboratory.

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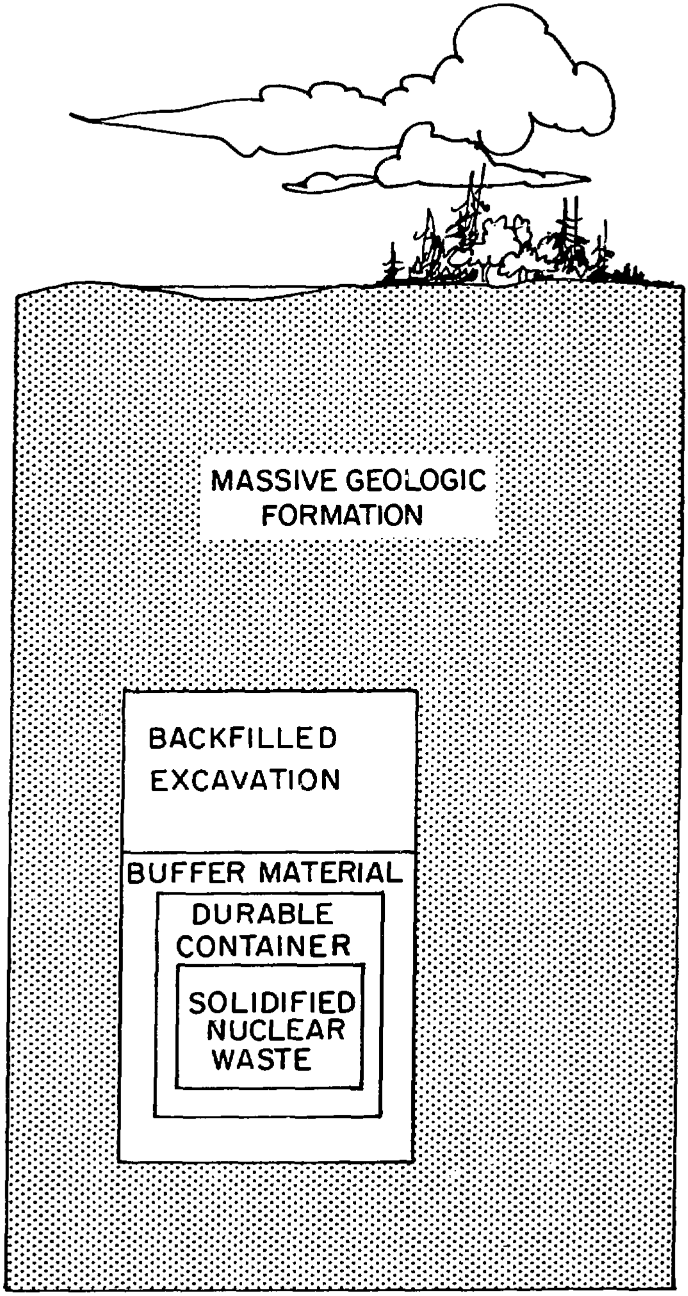
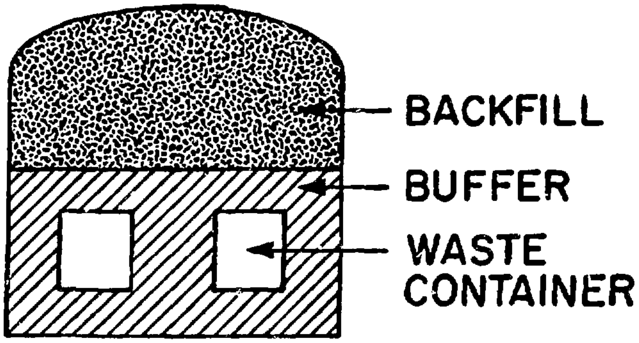
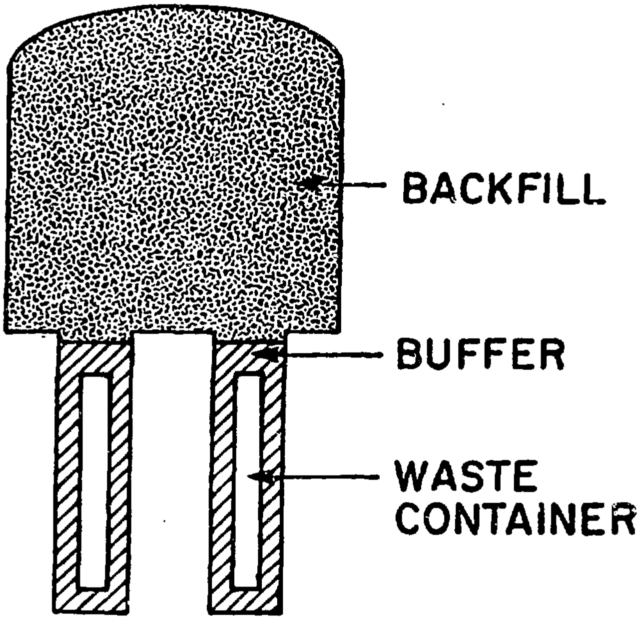


FIGURE 1: Schematic Illustration of the Sequence of Barriers to Prevent the Release of Radionuclides to Man and the Biosphere



(a)
IN-ROOM
EMPLACEMENT



(b)
BOREHOLE
EMPLACEMENT

FIGURE 2: Schematic Illustration of the Two Disposal Concepts (not to scale)

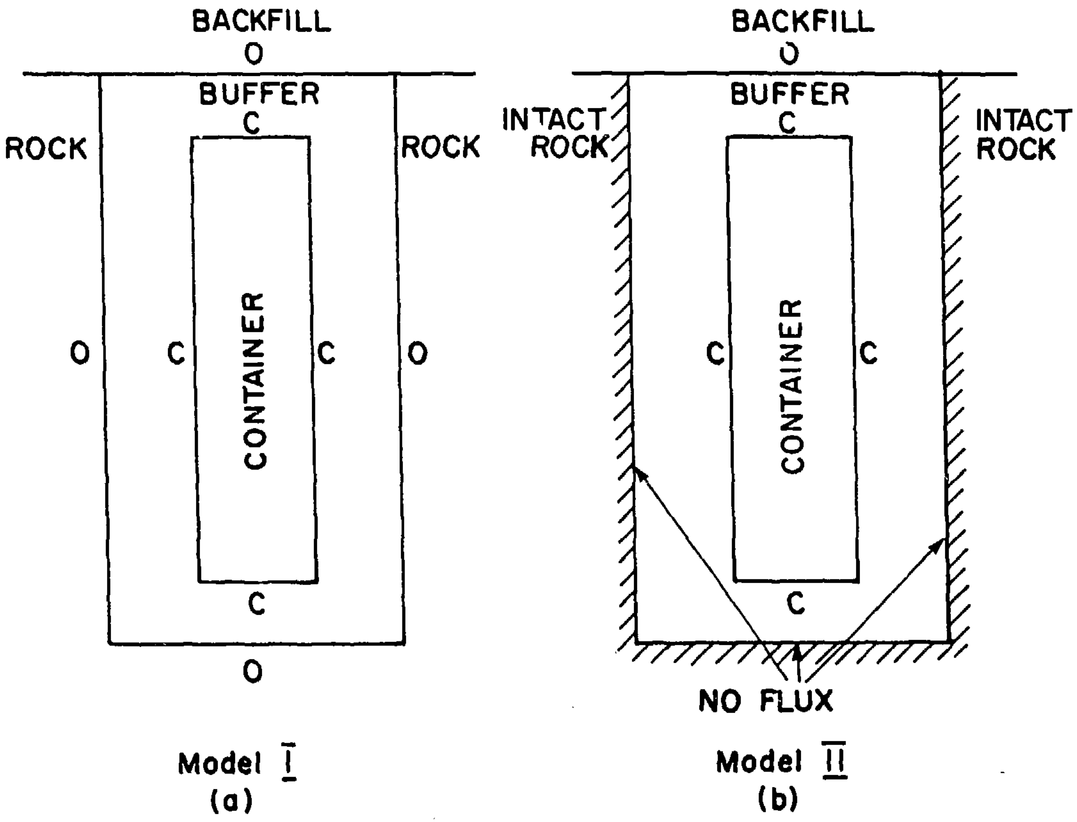


FIGURE 3: Schematic Illustration of Models I and II for Borehole Emplacement

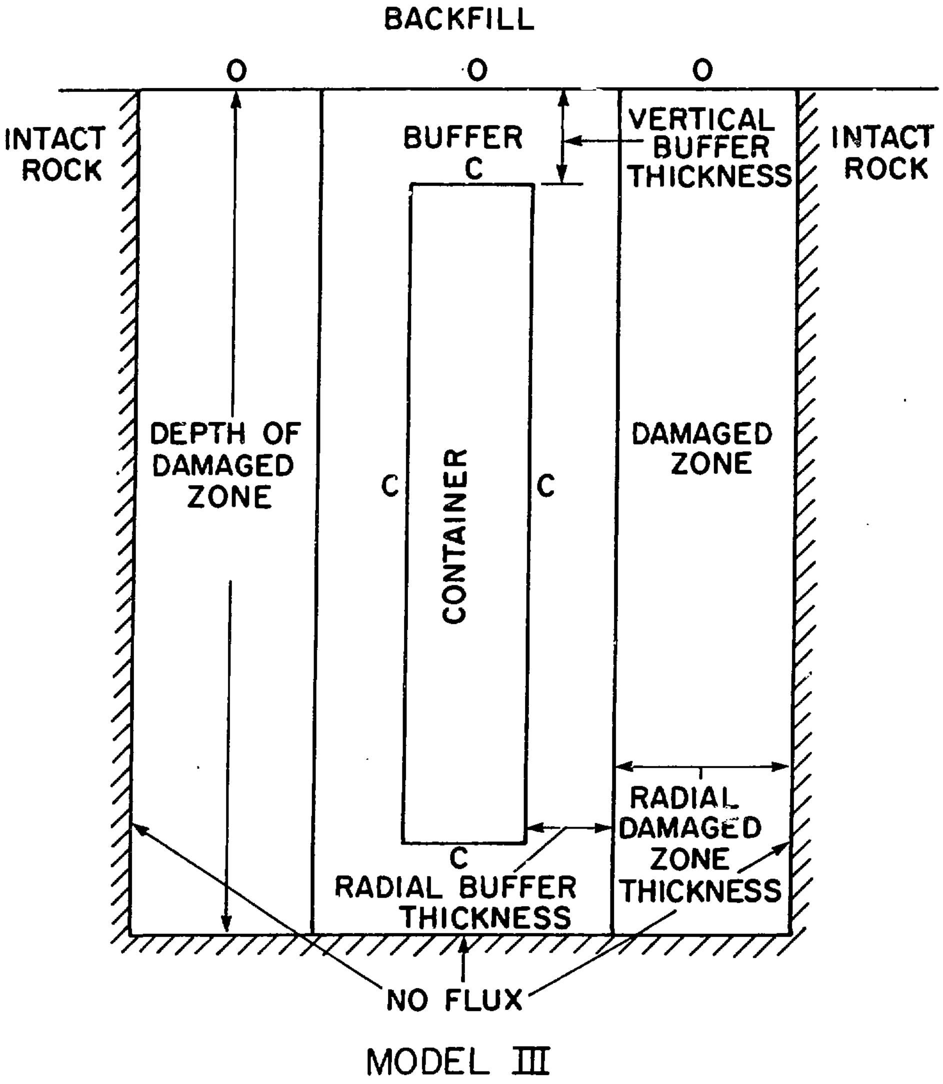


FIGURE 4: Schematic Illustration of Model III for Borehole Emplacement

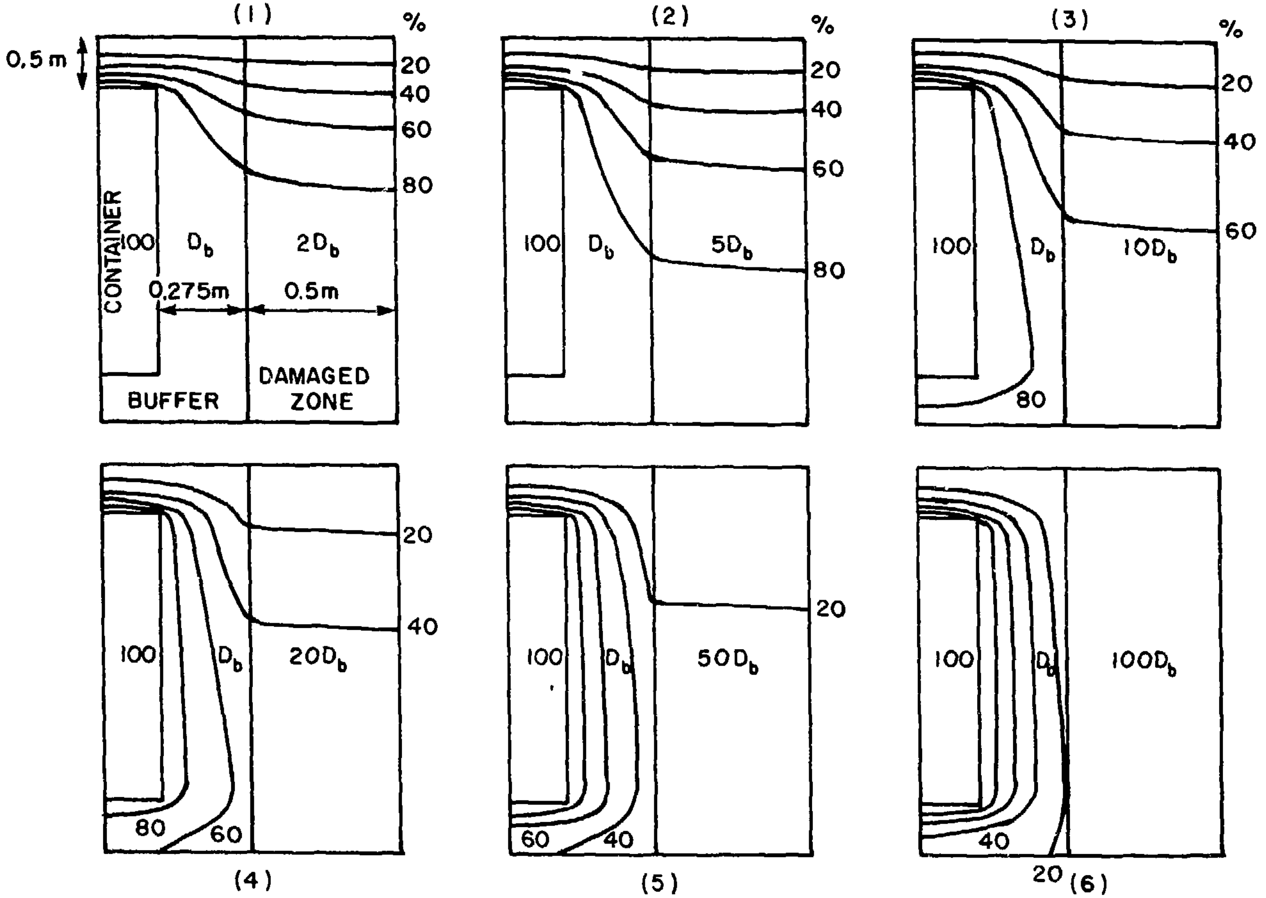


FIGURE 5: Concentration Profiles for a Half Longitudinal Section of the Borehole for a Damaged-Zone Thickness of 0.5 m

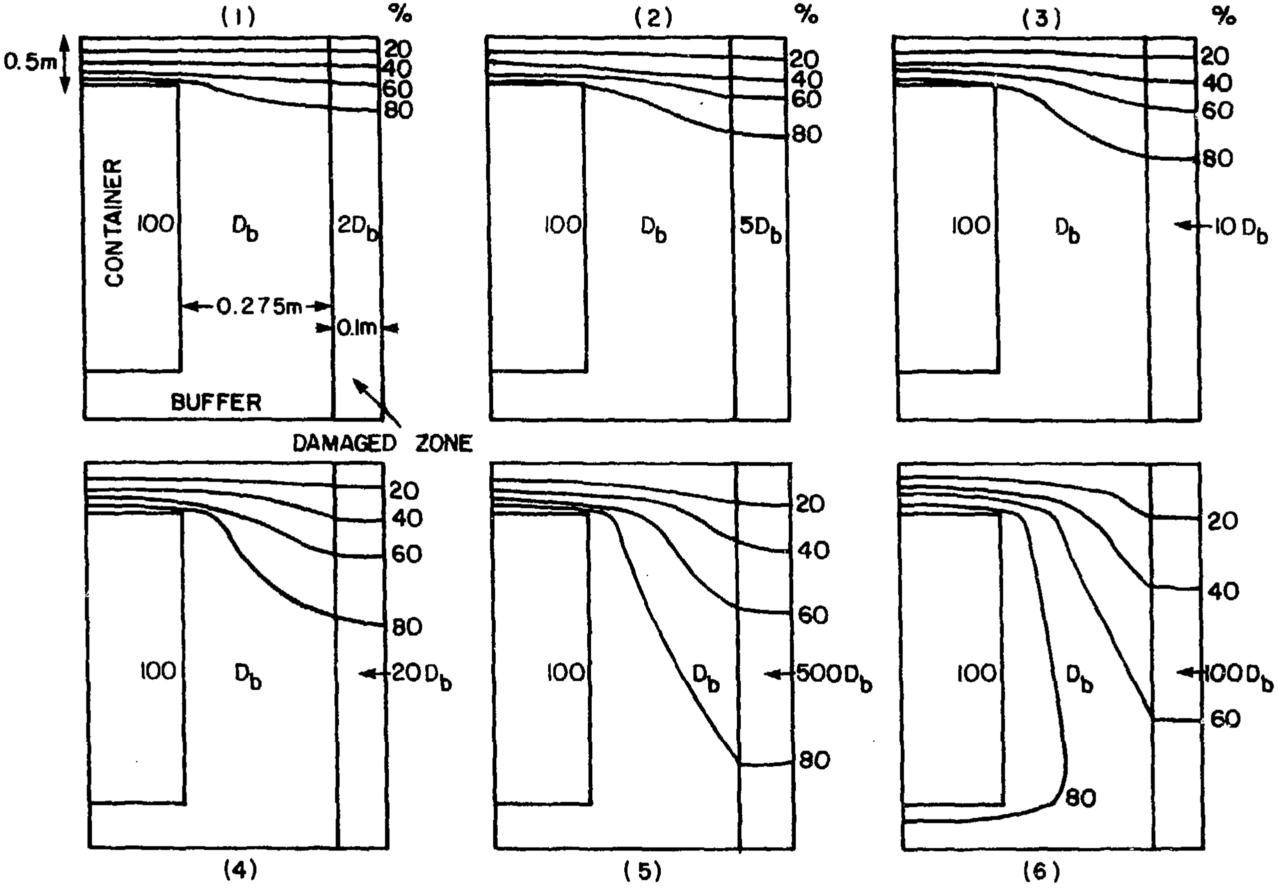


FIGURE 6: Concentration Profiles for a Half Longitudinal Section of the Borehole for a Damaged-Zone Thickness of 0.1 m

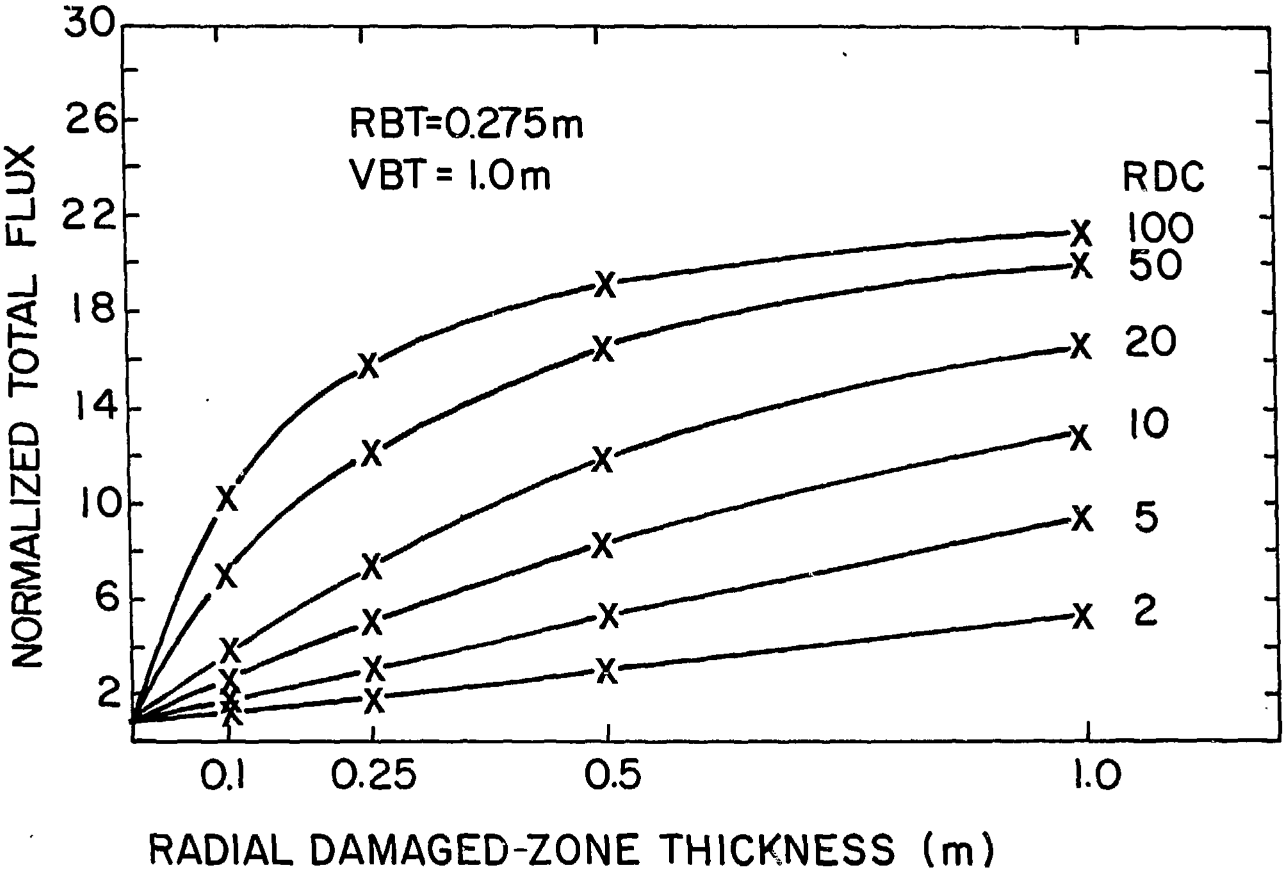


FIGURE 7: The Effect of Radial Damaged-Zone Thickness on the Total Flux for Various Damaged-Zone Relative Diffusion Coefficients

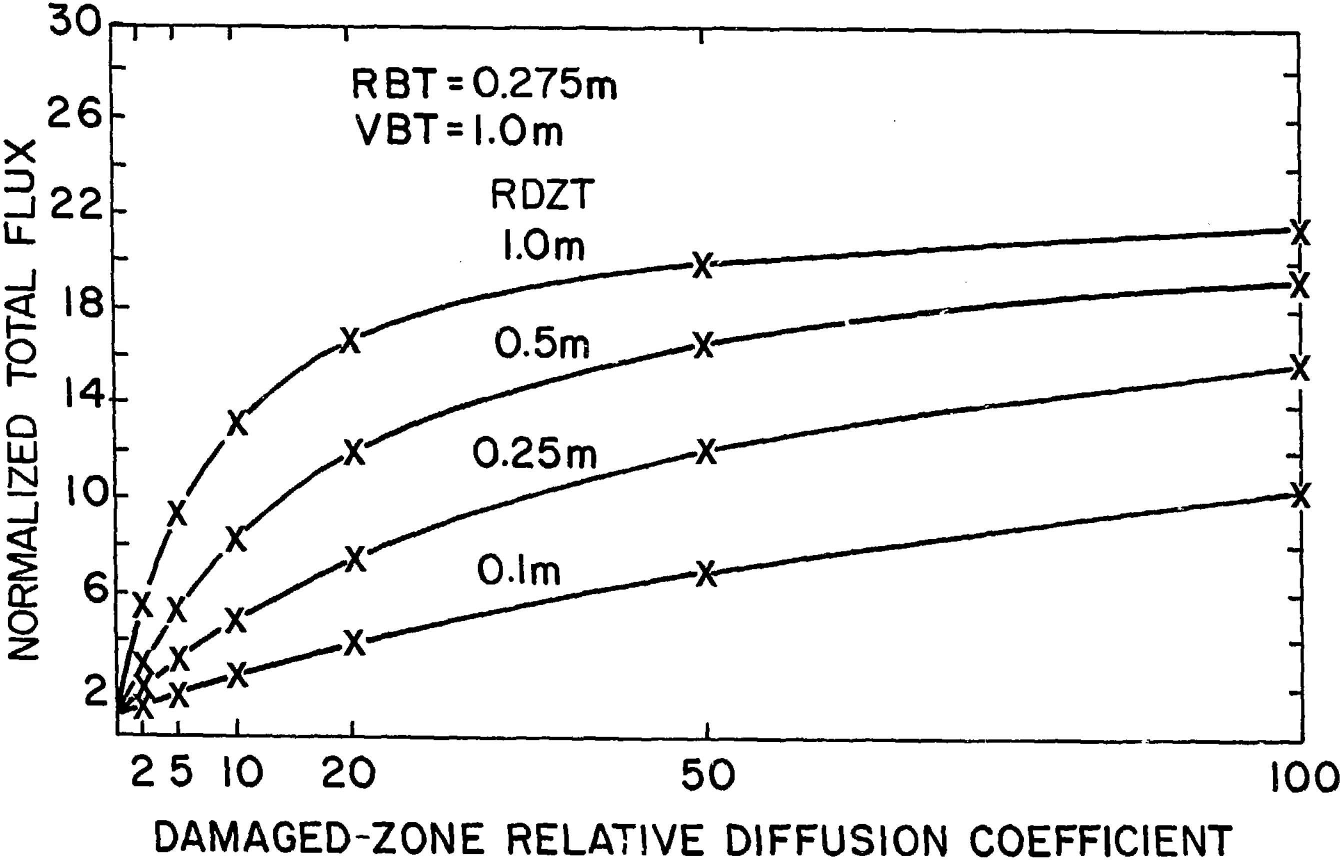


FIGURE 8: The Effect of Damaged-Zone Relative Diffusion Coefficient on the Total Flux for Various Radial Damaged-Zone Thicknesses

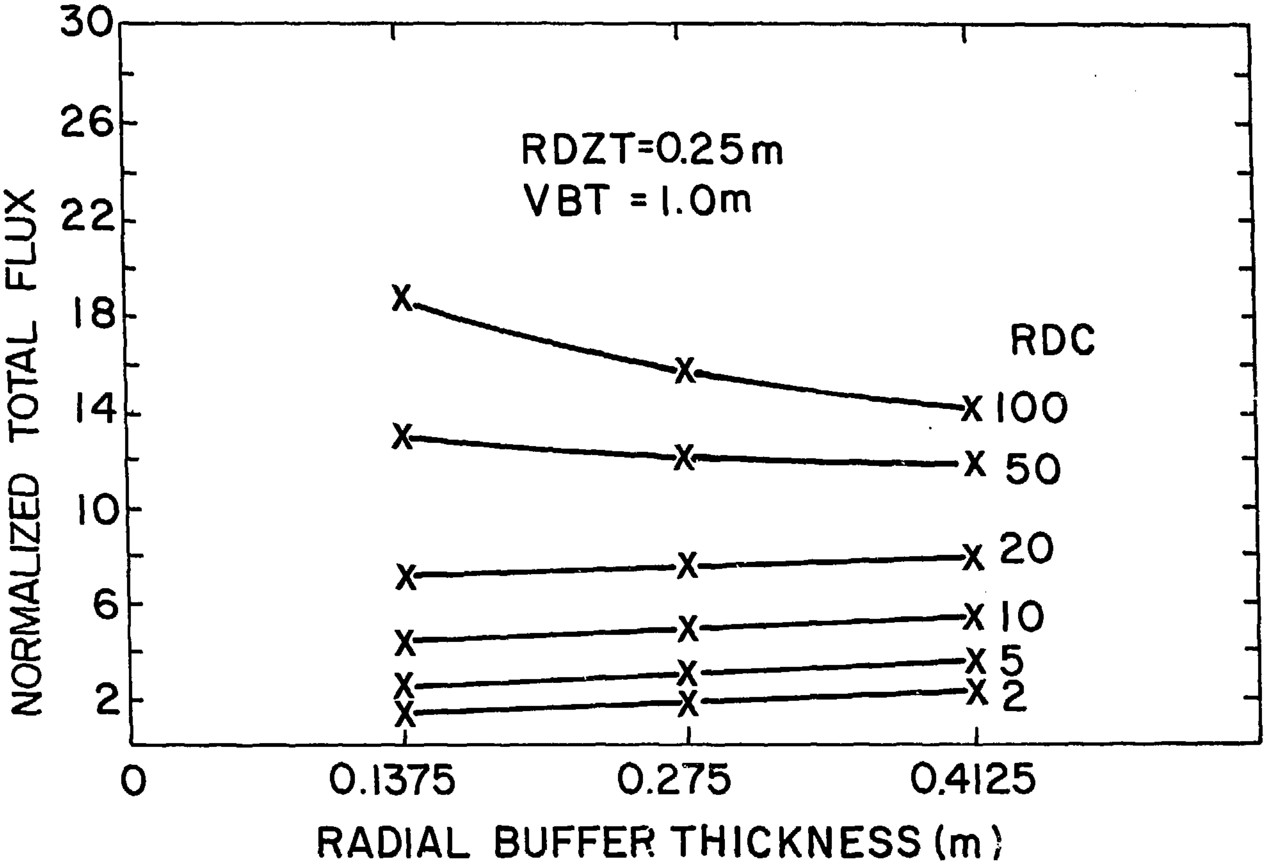


FIGURE 9: The Effect of Radial Buffer Thickness on the Total Flux for Various Damaged-Zone Relative Diffusion Coefficients

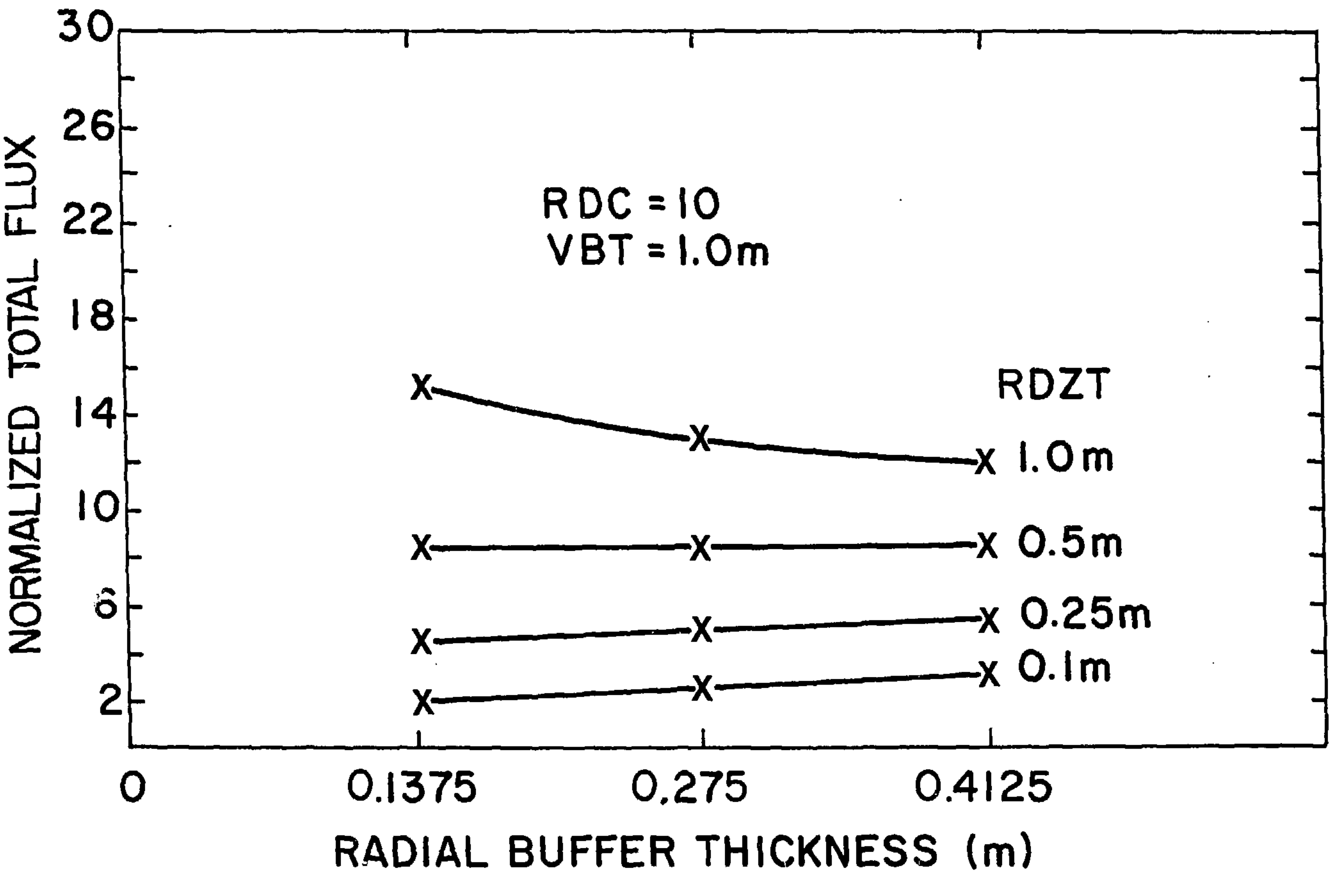


FIGURE 10: The Effect of Radial Buffer Thickness on the Total Flux for Various Radial Damaged-Zone Thicknesses

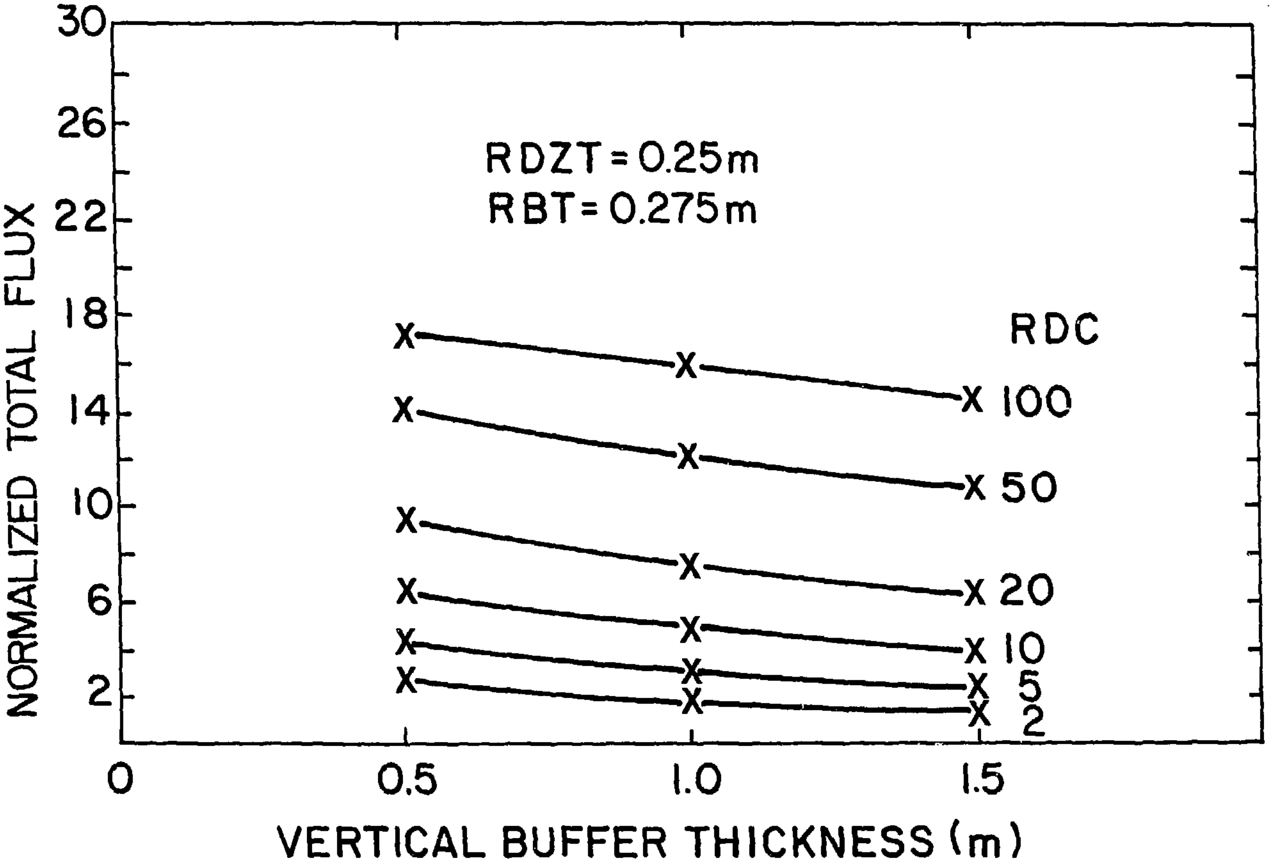


FIGURE 11: The Effect of Vertical Buffer Thickness on the Total Flux for Various Damaged-Zone Relative Diffusion Coefficients

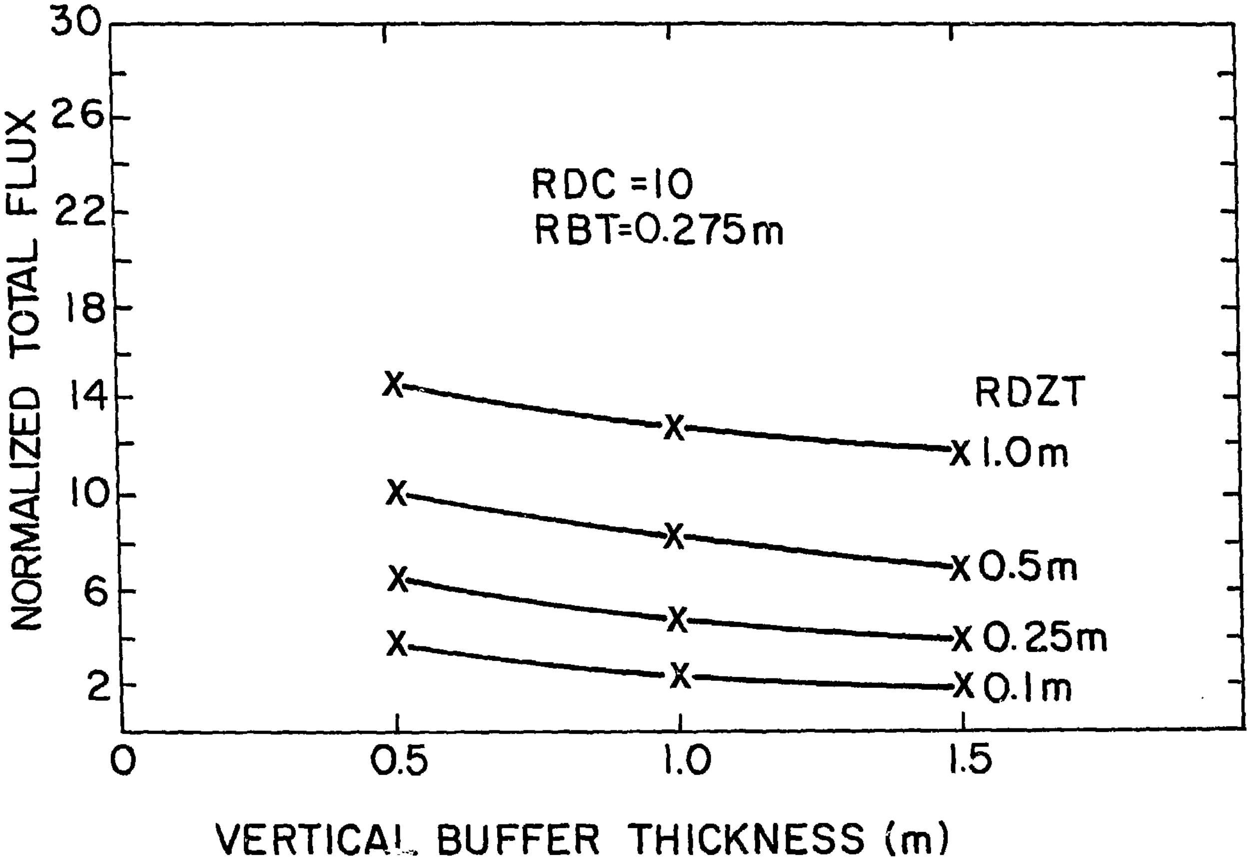


FIGURE 12: The Effect of Vertical Buffer Thickness on the Total Flux for Various Radial Damaged-Zone Thicknesses

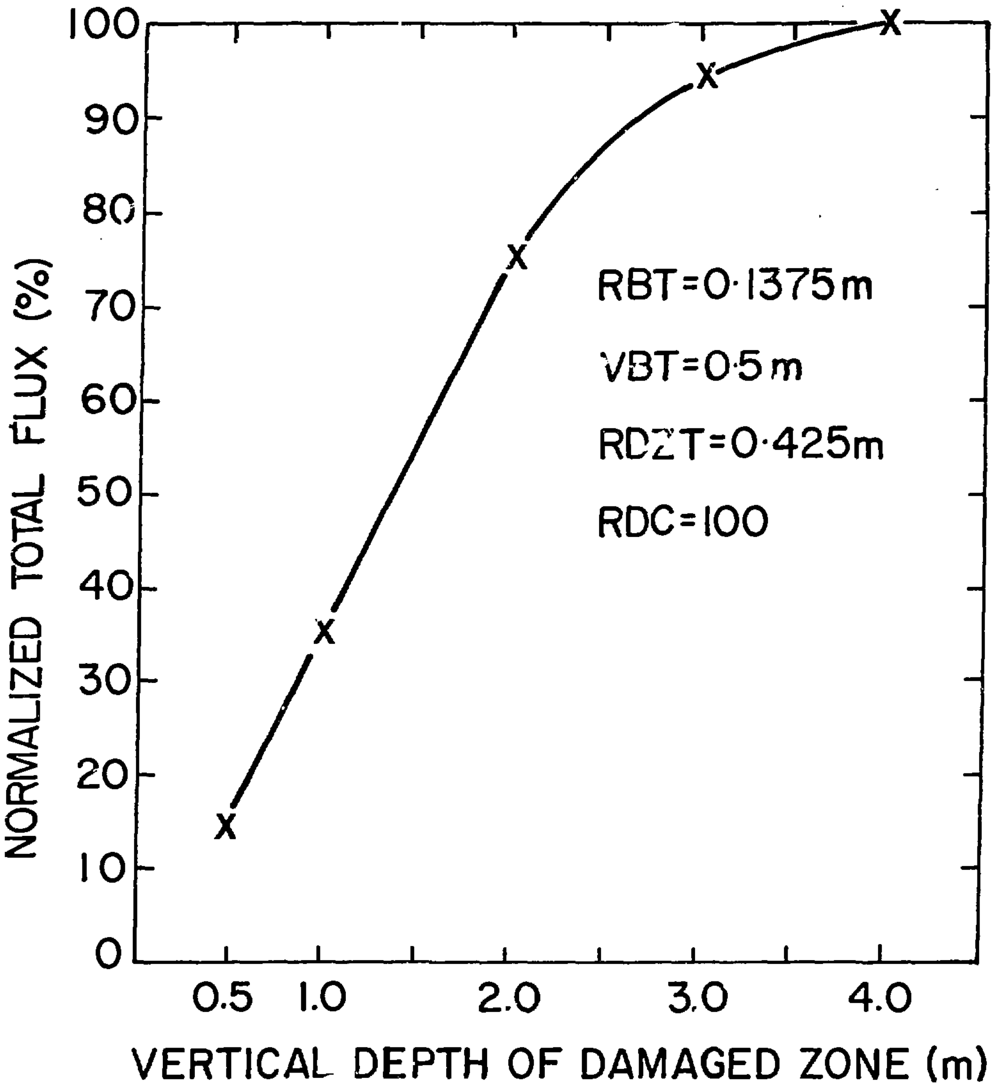


FIGURE 13: The Effect of Vertical Depth of the Damaged Zone on the Total Flux

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