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Discretization in COMP23 for SR97

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SUMMARY

The discretization of the near field compartment model COM23 used in e.g. the SR95 study is rather coarse, which results in a poor description of the first instationary phase of radionuclide release. For some nuclides the maximum release rates are somewhat overestimated.

In this study, the discretization has been investigated in a systematic manner. The division of the systems into blocks is shown in Figure 1.

First block 3 representing the bentonite outside the hole in the canister is divided into an increasing number of compartments. This block has in earlier calculations showed to be of major importance. In the SR95 study it was divided into three compartments and here it was increased to 6, 9, 12, and 15 compartments. The differences between the release rates are smaller for each increase, but also between 12 and 15 compartments there was some difference. The release rate decreases with increased number of compartments. It was decided to use six compartments, to achieve reasonable total number of compartments and thereby reasonable calculation times.

The whole system was then studied in a corresponding way. The original discretization was found to be sufficient for all other blocks if only the total release is of interest. The final discretization was however proposed to include three compartments in block 5 and changed proportions between the size of the two compartments in block 4. The resulting discretization resulted in 19 compartments compared to the 14 compartments used in the SR95 study.

The calculation time was recorded for all the studied cases. It was found that the calculation time increases in proportion to the square of the number of compartments. The calculation time increases about 20 % with the proposed discretization compared to the one earlier used.

SAMMANFATTNING

Diskretiseringen av närzonen i boxmodellen COMP23 som användes i tex SR95-studien är relativt grov, vilket resulterar i en dålig beskrivning av den första instationära fasen av radionuklidutsläppet. För en del nuklider är maxutsläppet överskattat.

I den här studien har diskretiseringen undersökts systematiskt. Indelningen av systemet i block visas i Figur 1.

Först delades blocket som representerar bentoniten utanför hålet i kapseln in i ett ökande antal boxar. Detta block har i tidigare beräkningar visat sig vara av stor betydelse. I SR-95-studien var det indelat i 3 boxar och här ökades det till 6, 9, 12 och 15 boxar. Skillnaderna mellan utsläppshastigheterna är mindre för varje ökningen, men även mellan 12 och 15 boxar är det en skillnad. Utsläppshastigheten minskar med ökande antal boxar. Det beslutades att använda 6 boxar, för att erhålla ett rimligt totalt antal boxar och därmed rimliga beräkningstider.

Hela systemet studerades sedan på motsvarande sätt. Den ursprungliga diskretiseringen visade sig vara tillräcklig för alla andra block om bara totala utsläppet är av intresse. Den slutgiltiga diskretiseringen föreslås dock innehålla 3 boxar i block 5 och förändrade proportioner mellan de två boxarna i block 4. Den slutgiltiga diskretiseringen innehåller 19 boxar jämfört med de 14 boxar som användes i SR95-studien.

Beräkningstiden för varje fall noterades. Det visade sig att beräkningstiden ökar proportionellt till kvadraten på antalet boxar. Beräkningstiden ökar med ungefär 20 % med den föreslagna diskretiseringen jämfört med den som använts tidigare.

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1 INTRODUCTION

The discretization of the near field compartment model COM23 used in e.g. the SR95 study is rather coarse, which results in a poor description of the first instationary phase of radionuclide release. For some nuclides the maximum release rates are somewhat overestimated.

In this study, the discretization has been investigated in a systematic manner. In Figure 1 the division of the system into blocks is shown. In the SR95 calculations, block 3 was divided into three compartments, block 4 into two compartments and block 7 into three compartments. In this study one block at a time was divided into an increasing number of compartments to investigate the differences in the release rates. The dominating release is through Q1 and Q2 and hence the blocks passed on the way out to these points are more closely investigated, i.e. block 3, 5 and 6. Block 8 and 9 was not studied. An important parameter in the choice of number of compartments is the calculation time and hence this is also shown for each calculation.

The following nuclides are studied: U-238 and U-234 in chain, Am-243, I-129, Sr-90, Ni-59, Cs-137 and Cs-135. The transport is modelled with diffusion through the barriers and with boundary conditions described by Q_{eq}-values. The parameters for bentonite were taken from *[Yu and Neretnieks, 1997]* and the parameters for rock from *[Carbol and Engkvist, 1997]*. For sand-bentonite the same parameter values as in *[Widén and Hedin, 1998]* were used.

The behaviour of the different nuclides is easier to understand if the penetration depth in bentonite after one half-life is known. In Table 1 the penetration depth in bentonite for the studied nuclides after one half-life is given. The penetration depth is calculated as:

$$x = \sqrt{(t_{1/2} D_a)}$$

where

$$D_a = \frac{D_e}{\varepsilon + (1-\varepsilon) K_d \rho}$$

$t_{1/2}$ is the half life (year)

D_e is the effective diffusivity (m^2/year)

ε is the porosity (-).

K_d is the distribution coefficient (m^3/kg)

ρ is the density (kg/m^3).

Table 1. Penetration depth (half the initial concentration) after one half-life.

Nuclide	Half life(yr)	Penetration depth (m)
U-238	$4.51 \cdot 10^9$	270
U-234	247000	2
Am-243	7370	0.07
Ni-59	75000	5
Sr-90	28.5	0.21
I-129	$1.60 \cdot 10^7$	537
Cs-135	$2.00 \cdot 10^6$	28
Cs-137	30.2	0.11

It can be seen that Am-243, Cs-137 and Sr-90 have penetration depth less than the shortest diffusion distance in the system, through the 0.35 m bentonite out to Q1. These nuclides will therefore be influenced more than the others when the discretization of block 3 is studied. U-234 and Ni-59 have penetration depth within the dimensions of the systems and will probably be more influenced than the others will when blocks further out in the system are studied.

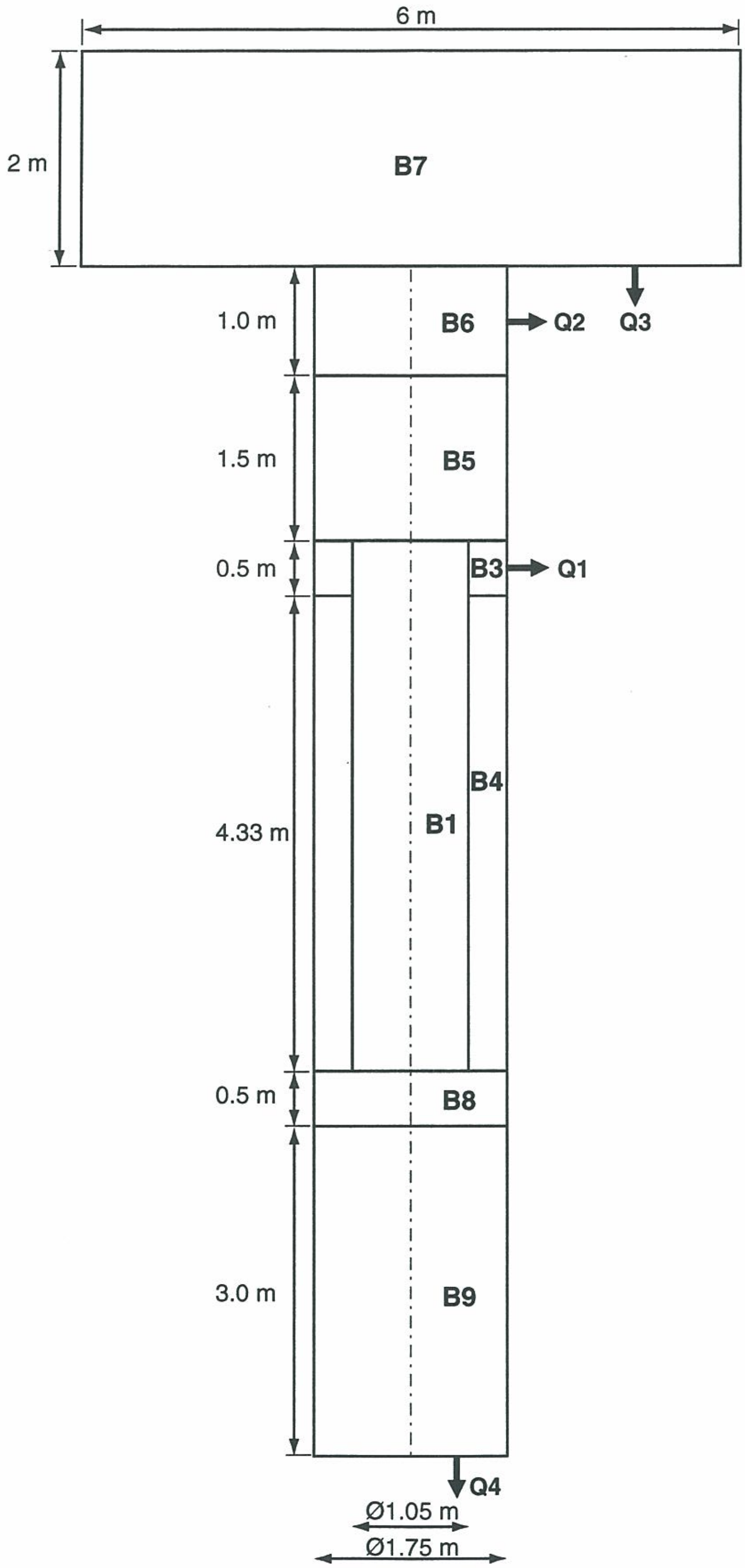

Figure 1. *Division of near-field into model blocks.*

2 CALCULATIONS

2.1 BLOCK 3, BENTONITE OUTSIDE CANISTER HOLE

Block 3 represents the bentonite outside the canister hole and it is connected to a fracture in the rock at the outside, Q1. The dimensions of this bentonite is an inner diameter of 1.05 m, an outer diameter of 1.75 m and a height of 0.5 m. Block 3 has been divided into 3, 6, 9, 12 and 15 compartments of equal thickness to show the effect of the discretization. The model studied is restricted to block 1, 2 and 3, see Figure 2. In Table 1 the dimensions of the compartments in each case are given.

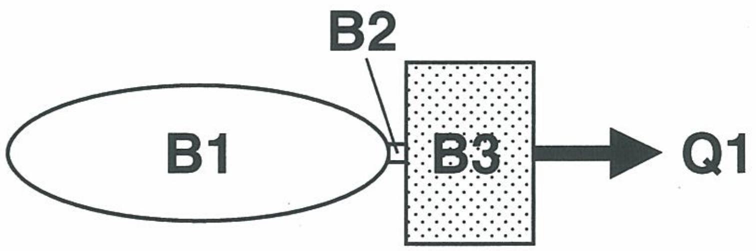

Figure 2. *Schematic illustration of the modelled system, note that the diffusion length are not correctly represented in B1 and B2.*

Table 1. Discretization of block 3, with 3, 6, 9, 12 and 15 compartments.

		Z_LENGTH	Z_AREA	R_LENGTH	R_AREA
3 Compartments					
	1	0.500	0.428	0.117	1.833
	2	0.500	0.513	0.117	2.199
	3	0.500	0.599	0.117	2.566
6 Compartments					
	1	0.500	0.203	0.058	1.741
	2	0.500	0.224	0.058	1.924
	3	0.500	0.246	0.058	2.107
	4	0.500	0.267	0.058	2.291
	5	0.500	0.289	0.058	2.474
	6	0.500	0.310	0.058	2.657
9 Compartments					
	1	0.500	0.133	0.039	1.710
	2	0.500	0.143	0.039	1.833
	3	0.500	0.152	0.039	1.955
	4	0.500	0.162	0.039	2.077
	5	0.500	0.171	0.039	2.199
	6	0.500	0.181	0.039	2.321
	7	0.500	0.190	0.039	2.443
	8	0.500	0.200	0.039	2.566
	9	0.500	0.209	0.039	2.688

12 Compartments					
	1	0.500	0.099	0.029	1.695
	2	0.500	0.104	0.029	1.787
	3	0.500	0.110	0.029	1.878
	4	0.500	0.115	0.029	1.970
	5	0.500	0.120	0.029	2.062
	6	0.500	0.126	0.029	2.153
	7	0.500	0.131	0.029	2.245
	8	0.500	0.136	0.029	2.337
	9	0.500	0.142	0.029	2.428
	10	0.500	0.147	0.029	2.520
	11	0.500	0.152	0.029	2.611
	12	0.500	0.158	0.029	2.703
15 Compartments					
	1	0.500	0.079	0.023	1.686
	2	0.500	0.082	0.023	1.759
	3	0.500	0.086	0.023	1.833
	4	0.500	0.089	0.023	1.906
	5	0.500	0.092	0.023	1.979
	6	0.500	0.096	0.023	2.053
	7	0.500	0.099	0.023	2.126
	8	0.500	0.103	0.023	2.199
	9	0.500	0.106	0.023	2.272
	10	0.500	0.109	0.023	2.346
	11	0.500	0.113	0.023	2.419
	12	0.500	0.116	0.023	2.492
	13	0.500	0.120	0.023	2.566
	14	0.500	0.123	0.023	2.639
	15	0.500	0.127	0.023	2.712

The results of the calculations with different number of compartments in block 3 is shown in Figure 3 as release rates at Q1 as a function of time. The calculation times are given in Table 2.

Table 2. Calculation times for different discretizations in block 3.

Number of compartments in block 3	Total number of compartments	CPU-time
3	5	0:34
6	8	0:38
9	11	0:45
12	14	0:55
15	17	1:12

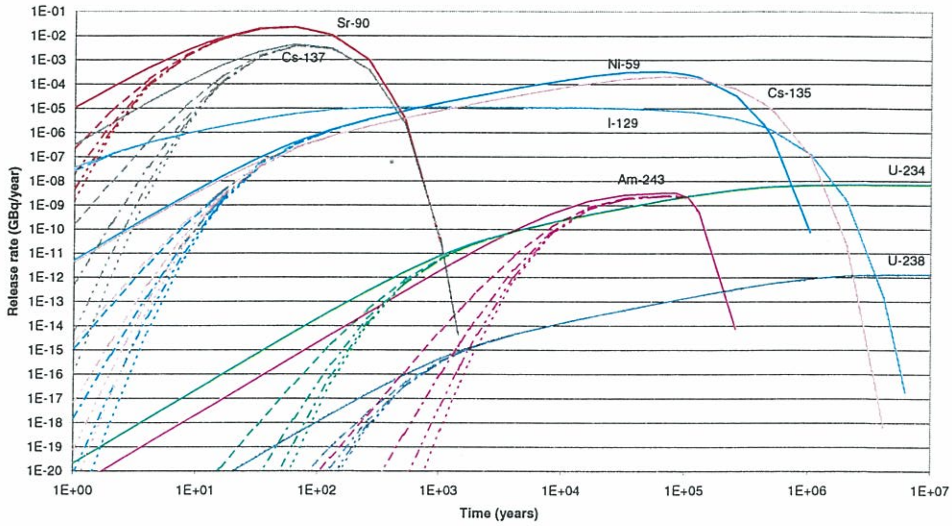

Figure 3. Release rates (GBq/year) at Q1 as a function of time in the case with different number of compartments in block 3. The continuous line is the case with 3 compartments, the cases with 6, 9, 12 and 15 compartments are indicated with smaller and smaller dots in their lines.

The different release rate curves show differences in the transient phase between the cases with different number of compartments. For Am-243 the maximum release is also influenced, more than three compartments result in somewhat lower maximum release. The differences are sufficiently small that using more than 3 or perhaps 6 compartments is not necessary in block 3.

2.1.1 Increased K_d-value for Sr and Cs

The influence of the discretization of block 3 may be of larger importance for the short-lived nuclides if different K_d-values are used. The effect of K_d-values has been studied by increasing the K_d-value for Sr-90, Cs-135 and Cs-137. Three different discretizations where studied, 3, 6 and 9 compartments. In Figure 4 the release rates as a function of time is shown.

In the introduction it was shown that the penetration depth after one half-life for Sr-90 and Cs-137 was 0.2 m and 0.1 m, respectively. With the increased K_d-values the penetration depths are decreased to 0.02 and 0.01 m. Calculation of the number of half lives passes during the transport through the 0.35 m bentonite it results in over 200 for Sr-90 and 1000 for Cs-137. For Cs-135 the penetration depth after one half life is 3 m, i.e. longer than the bentonite barrier. This check of the penetration depth is a good help when evaluating the discretization.

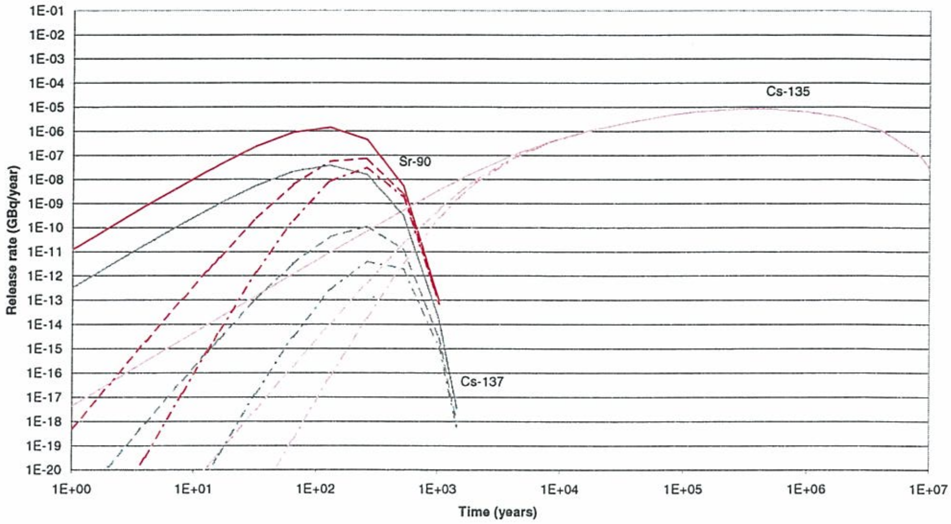

Figure 4. *Release rates (GBq/year) at Q1 as a function of time in the case with different number of compartments in block 3 and 100 times increased K_d-value. The continuous line is the case with 3 compartments, the cases with 6 and 9 compartments are indicated with smaller and smaller dots in their lines.*

The release rates for the different discretizations show a large influence for both Sr-90 and Cs-137. Based on these differences the discretization for block 3 was chosen to be 6 compartments. In the following calculations block 3 is therefore divided into 6 compartments.

2.2 BLOCK 5, BENTONITE ABOVE CANISTER

2.2.1 Investigation of short circuit effects

Since block 5 is connected to all compartments in block 3 there is a possibility of a short circuit effect, i.e. nuclides may diffuse from the first compartment in block 3 up to block 5 and back to block 3 in the last compartment. To study this effect block 5 was added to the studied model, see Figure 5. The effect of block 5 as a sink will also affect the release. Block 5 was divided into 1, 2, 4, 7 and 8 compartments in the horizontal direction, the dimensions are given in Table 3. In the case with 2 compartments the division was one above block 3 and beside. In the case with 4 compartments the division was three equally thick above block 3 and one beside. In the case with 7 compartments the division six equally thick above block 3 and one beside. In the case with 8 compartments the division was six equally thick above block 3 and two beside (a small close to the six).

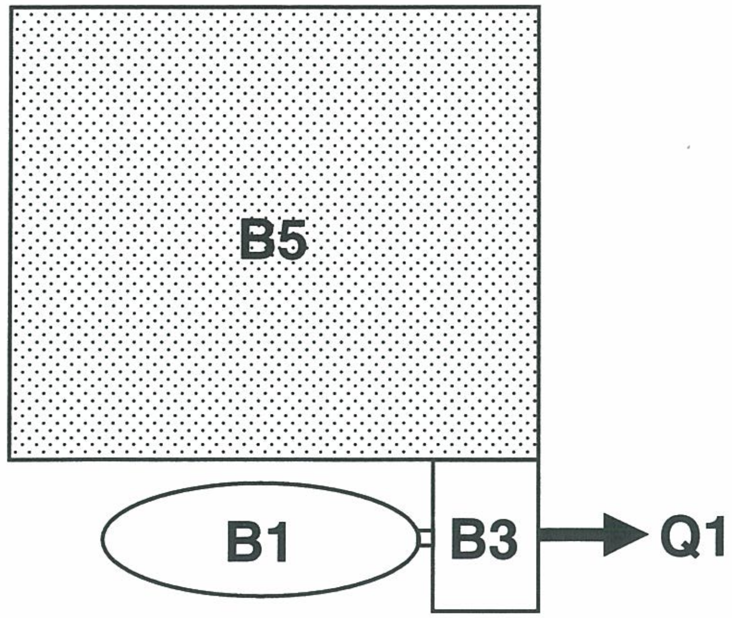

__Figure 5__. Schematic illustration of the modelled system, note that the diffusion length are not correctly represented.

Table 3. Discretization of block 5, with 1, 2, 4, 7 and 8 compartments in the horizontal direction.

		Z_LENGTH	Z_AREA	R_LENGTH	R_AREA
1 Compartment					
	1	1.500	2.405	0.000	1.000
2 Compartments					
	1	1.500	0.866	0.525	2.474
	2	1.500	1.539	0.350	6.597
4 Compartments					
	1	1.500	0.866	0.525	2.474
	2	1.500	0.428	0.117	5.498
	3	1.500	0.513	0.117	6.597
	4	1.500	0.599	0.117	7.697
7 Compartments					
	1	1.500	0.866	0.525	2.474
	2	1.500	0.203	0.058	5.223
	3	1.500	0.224	0.058	5.773
	4	1.500	0.246	0.058	6.322
	5	1.500	0.267	0.058	6.872
	6	1.500	0.289	0.058	7.422
	7	1.500	0.310	0.058	7.972
8 Compartments					
	1	1.500	0.567	0.425	2.003
	2	1.500	0.298	0.100	4.477
	3	1.500	0.203	0.058	5.223
	4	1.500	0.224	0.058	5.773
	5	1.500	0.246	0.058	6.322
	6	1.500	0.267	0.058	6.872
	7	1.500	0.289	0.058	7.422
	8	1.500	0.310	0.058	7.972

The result of the calculations with different discretizations of block 5 in the horizontal direction is shown in Figure 6 and 7 as release rates at Q1 as a function of time. The calculation times are given in Table 4.

Table 4. Calculation times for different discretizations in the horizontal direction in block 5. In all cases block 3 is divided into 6 compartments.

Number of compartments in block 5	Total number of compartments	CPU-time
1	9	0:40
2	10	0:42
4	12	0:48
7	15	0:58
8	16	1:03

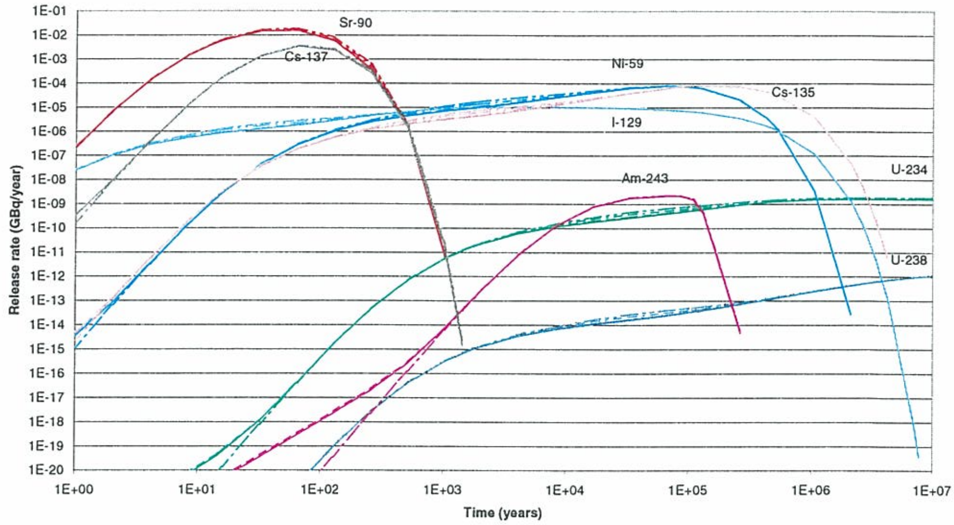

Figure 6. *Release rates (GBq/year) at Q1 as a function of time in the case with different number of compartments in the horizontal direction in block 5. The continuous line is the case with 1 compartment, the cases with 2, 4, 7 and 8 compartments are indicated with smaller and smaller dots in their lines.*

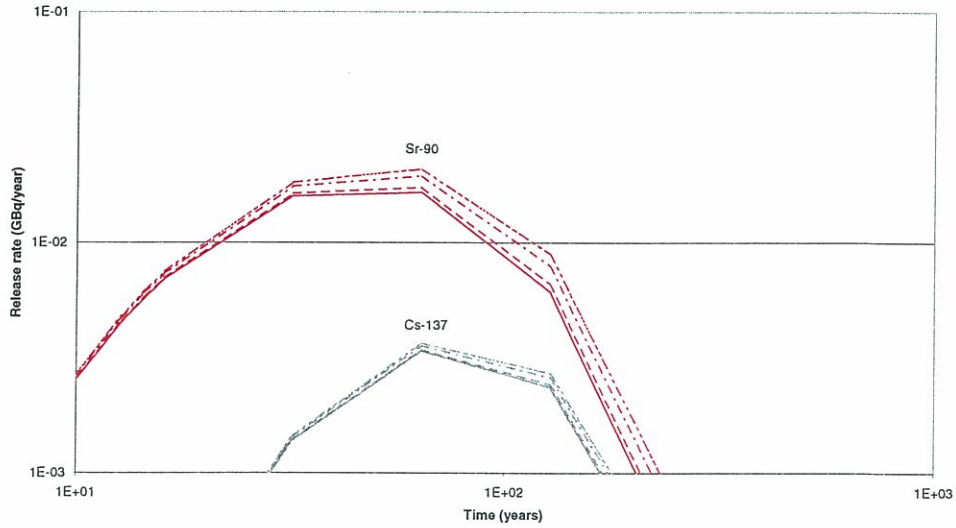

Figure 7. *(Detail of Figure 6) Release rates (GBq/year) at Q1 as a function of time in the case with different number of compartments in the horizontal direction in block 5. The continuous line is the case with 1 compartment, the cases with 2, 4, 7 and 8 compartments are indicated with smaller and smaller dots in their lines.*

The two different phenomena of block 5: short circuit and sink-effect can be identified in the figures. At short times the release rates for 1 and 2 compartments are clearly higher, due to short circuit effects. The effect of block 5 as a sink is rather large (see also next section) but the effect is smaller when more compartments are used as can be seen in figure 7.

Shorter diffusion length to block 5

The small short circuit effect may be due to the long diffusion length to block 5. Calculations with one compartment in block 5 with a height of only 1 dm was performed. The release rates are shown in Figure 8.

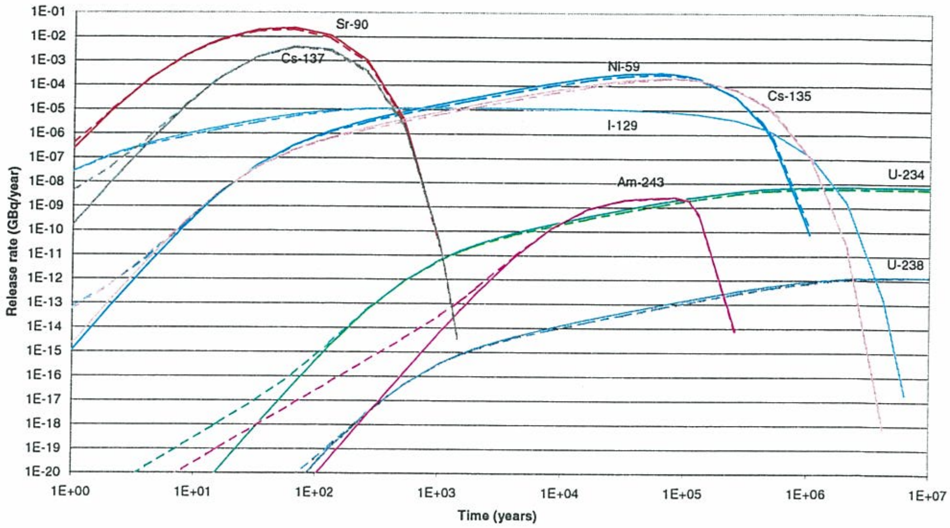

Figure 8. Release rates (GBq/year) at Q1 as a function of time in the case with one compartments in block 5, only 1 dm high. The continuous line is the case without block 5 and the dashed line is with block 5.

The figure shows the short circuit effects at the instationary phase, but the maximum release is lower due to the effect of block 5 as a sink. The conclusion is that it is not needed to divide block 5 into several compartments in the horisontal direction and that a discretization in the vertical direction can allow compartments as small as 1 dm and still not have short circuit effects influencing the system too much. In the following calculations block 5 will have only one compartment in the horisontal direction.

2.2.2 Discretization in the vertical direction

Division into 3 and 6 compartments investigates the discretization in block 5 in the vertical direction. The model is in this case including block 1, 2, 3, 5 and 6, see Figure 9. The dimensions of the compartments are given in Table 5.

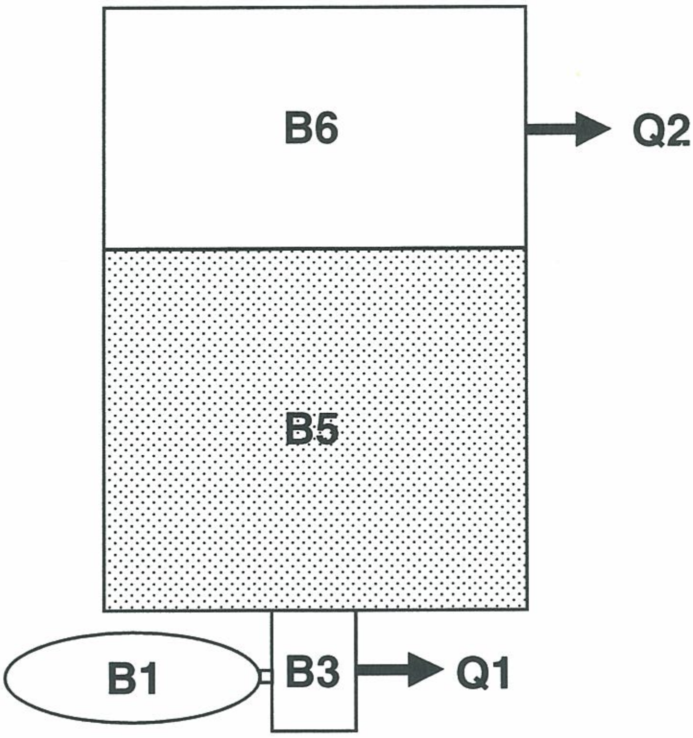

Figure 9. Schematic illustration of the modelled system, note that the diffusion length are not correctly represented.

Table 5. Discretization of block 5 with 1, 3, 6 compartments in the vertical direction.

		Z_LENGTH	Z_AREA	R_LENGTH	R_AREA
1 Compartment					
	1	1.500	2.405	0.000	1.000
3 Compartments					
	1	0.500	2.405	0.000	1.000
	2	0.500	2.405	0.000	1.000
	3	0.500	2.405	0.000	1.000
6 Compartments					
	1	0.250	2.405	0.000	1.000
	2	0.250	2.405	0.000	1.000
	3	0.250	2.405	0.000	1.000
	4	0.250	2.405	0.000	1.000
	5	0.250	2.405	0.000	1.000
	6	0.250	2.405	0.000	1.000

The release rates at Q1, Q2 and the total release rates are given in Figure 10, 11 and 12. The calculation times are given in Table 6.

Table 6. Calculation times for different discretizations in the vertical direction in block 5. In all cases block 3 is divided into 6 compartments and block 6 into one compartment.

Number of compartments in block 5	Total number of compartments	CPU-time
1	10	0:44
3	12	0:51
6	15	1:03

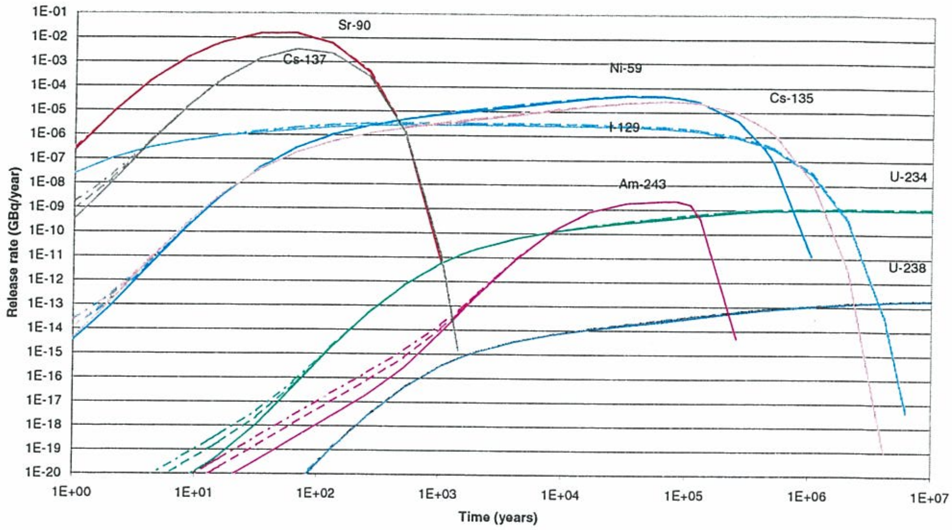

Figure 10. *Release rates (GBq/year) at Q1 as a function of time in the cases with 1, 3 and 6 compartments in the vertical direction in block 5. The continuous line is the case with one compartment, dashed line is the case with 3 compartments and the dashed-doted line is the case with 6 compartments.*

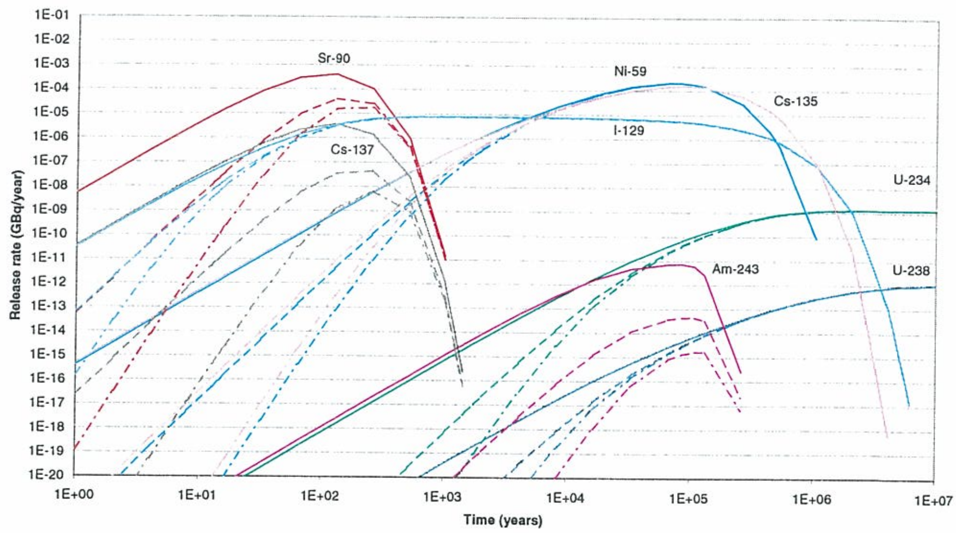

Figure 11. *Release rates (GBq/year) at Q2 as a function of time in the cases with 1, 3 and 6 compartments in the vertical direction in block 5. The continuous line is the case with one compartment, dashed line is the case with 3 compartments and the dashed-doted line is the case with 6 compartments.*

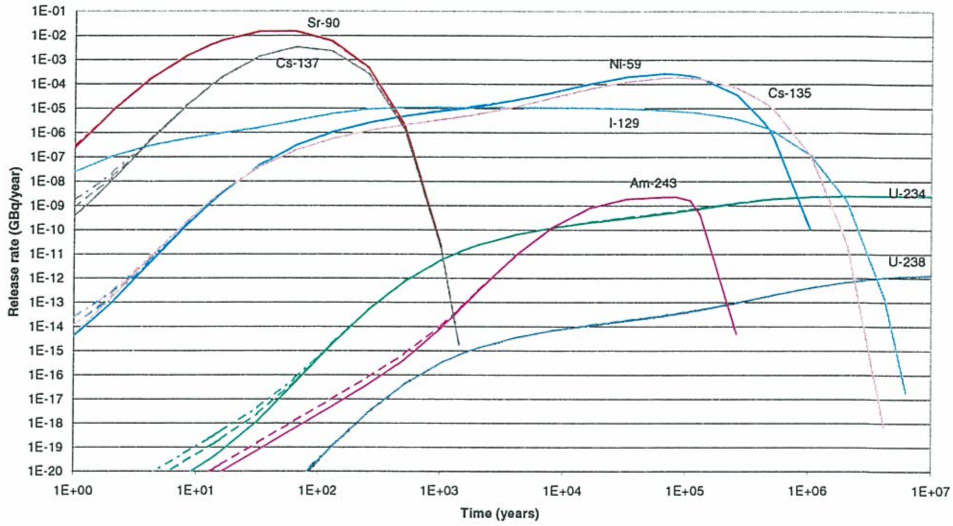

__Figure 12.__ Total release rates (GBq/year) (Q1 and Q2) as a function of time in the cases with 1, 3 and 6 compartments in the vertical direction in block 5. The continuous line is the case with one compartment, dashed line is the case with 3 compartments and the dashed-doted line is the case with 6 compartments.

The total release rates show small effects due to different discretizations of block 5. The effect at Q2 is large for Sr-90, Cs-137 and Am-243. The conclusion is that if only the total release rate is studied, one compartment in block 5 is sufficient for the studied nuclides. If however the release through Q2 is of interest, more compartments are necessary to give accurate results.

Block 6 is not divided into more compartments in this study. Division into smaller compartments than in block 5 is not defensible, since it is smaller and it consists of sand-bentonite, which has higher diffusivity and hence the concentration profiles will be developed faster in this block than in block 5.

2.3 BLOCK 7, SAND-BENTONITE IN TUNNEL

The sand-bentonite in the tunnel above is divided into 3 compartments in the original model, here the two compartments at the side are divided into 3 compartments each resulting in 7 compartments. The dimensions of the compartments are given in Table 7. The modelled system consists of block 1, 2, 3, 5, 6 and 7 and release path through Q1, Q2 and Q3, see Figure 13.

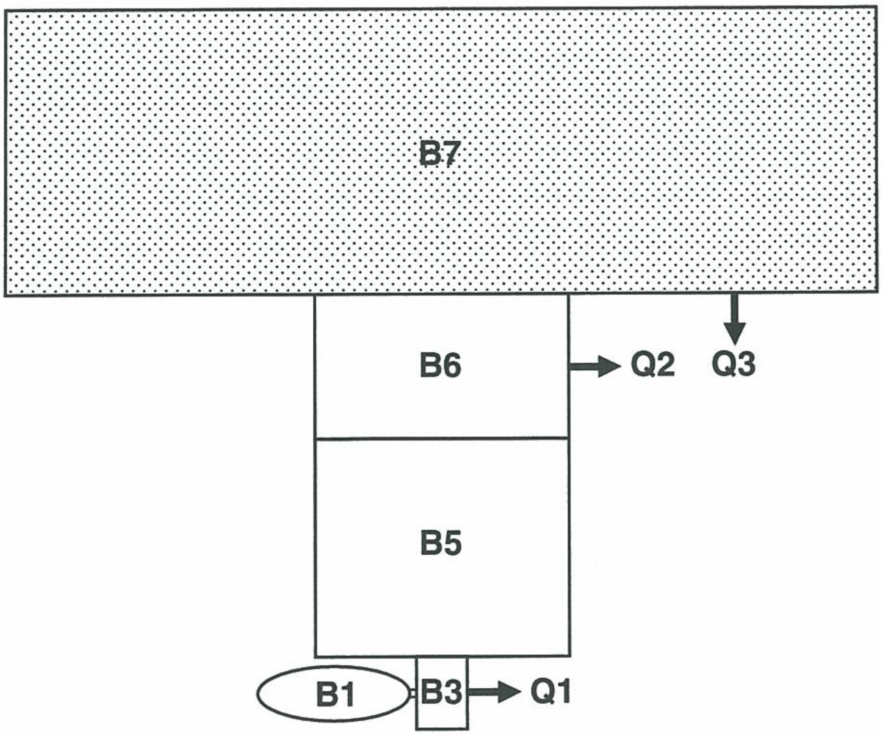

Figure 13. *Schematic illustration of the modelled system, note that the diffusion length are not correctly represented.*

Table 5. Discretization of block 7 with 3 and 7 compartments.

		Z_LENGTH	Z_AREA	R_LENGTH	R_AREA
3 Compartments					
	1	2.125	12.240	2.000	26.400
	2	1.750	12.240	2.000	21.700
	3	2.125	12.240	2.000	26.400
7 Compartments					
	1	0.708	12.240	2.000	8.768
	2	0.708	12.240	2.000	8.768
	3	0.708	12.240	2.000	8.768
	4	1.750	12.240	2.000	21.700
	5	0.708	12.240	2.000	8.768
	6	0.708	12.240	2.000	8.768
	7	0.708	12.240	2.000	8.768

The release rates through Q1, Q2, Q3 and the total release rates are shown in Figure 14, 15, 16 and 17. The calculation times are given in Table 6.

Table 6. Calculation times for different discretizations in block 7. In all cases block 3 is divided into 6 compartments and block 5 and 6 into one compartment each.

Number of compartments in block 7	Total number of compartments	CPU-time
3	13	0:42
7	17	1:12

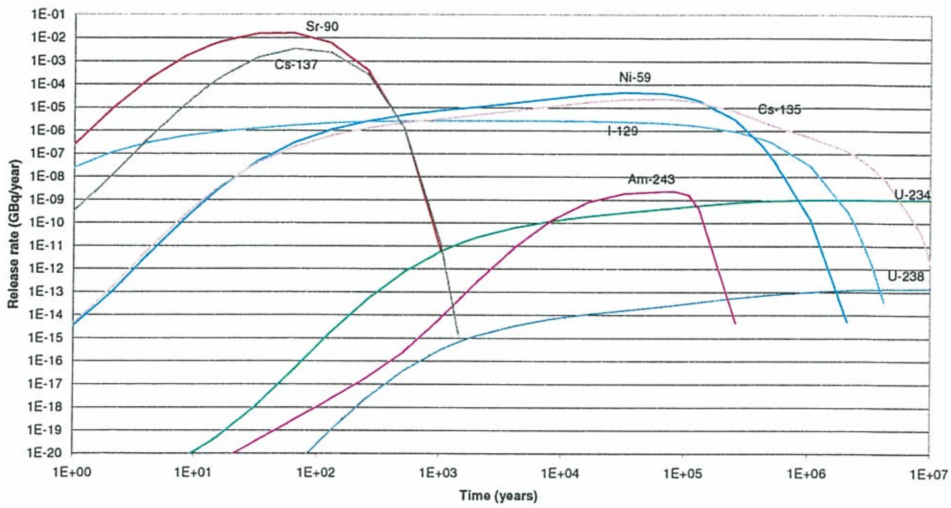

Figure 14. *Release rates (GBq/year) at Q1 as a function of time in the cases with 3 and 7 compartments in block 7. The continuous line is the case with 3 compartments and dashed line is the case with 7 compartments.*

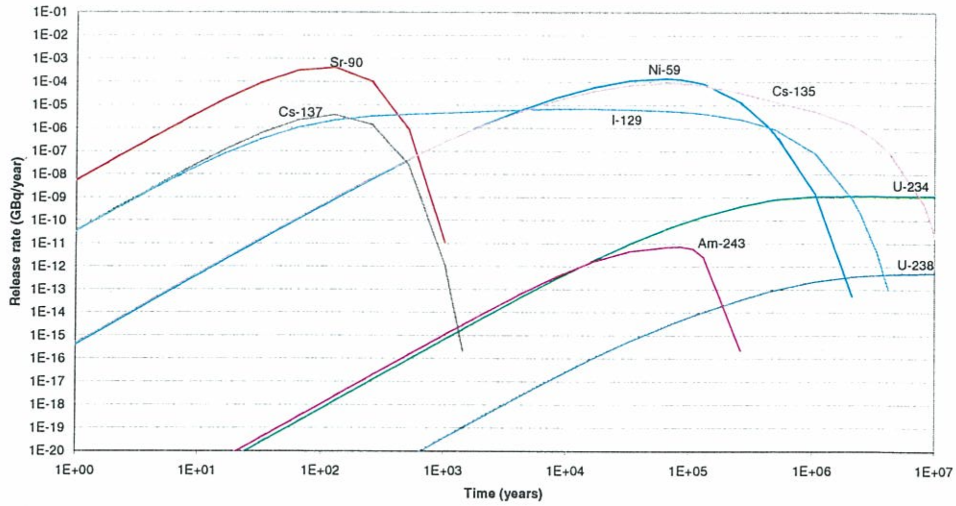

Figure 15. *Release rates (GBq/year) at Q2 as a function of time in the cases with 3 and 7 compartments in block 7. The continuous line is the case with 3 compartments and dashed line is the case with 7 compartments.*

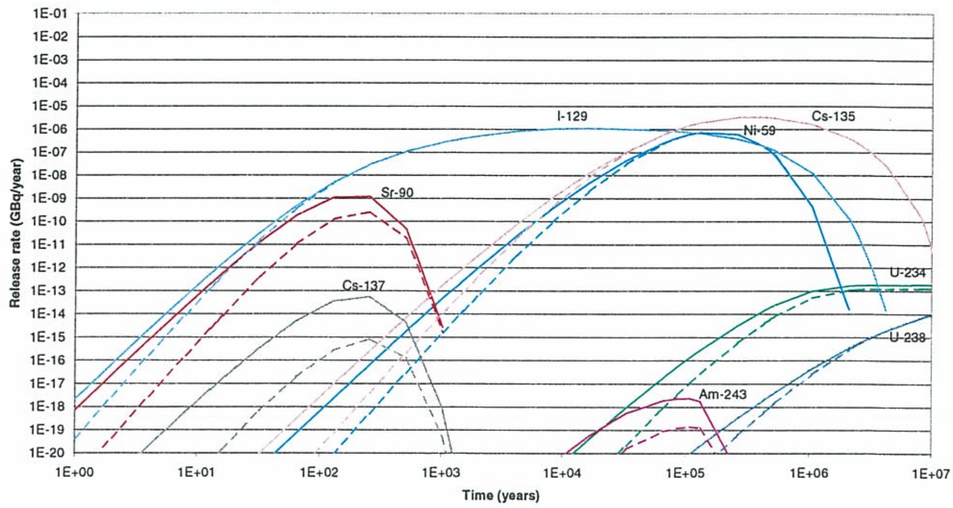

Figure 16. *Release rates (GBq/year) at Q3 as a function of time in the cases with 3 and 7 compartments in block 7. The continuous line is the case with 3 compartments and dashed line is the case with 7 compartments.*

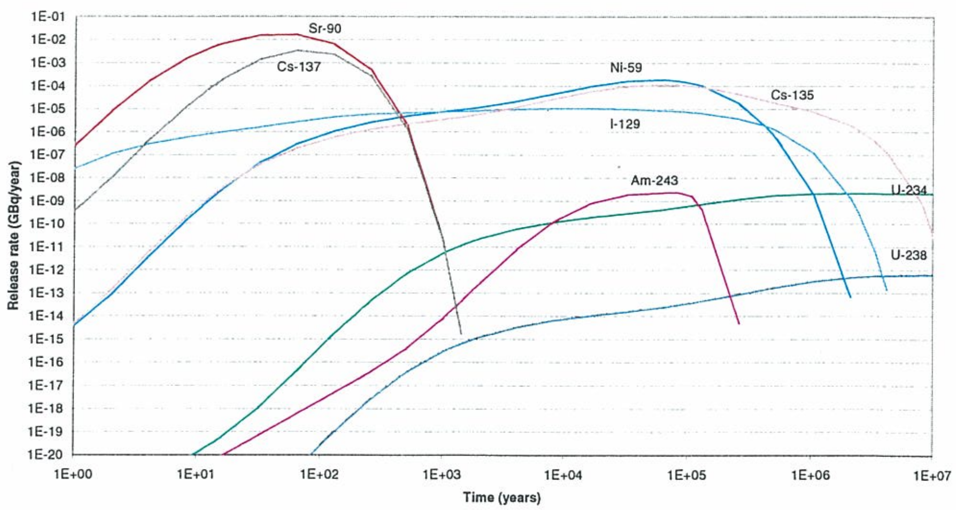

Figure 17. *Total release rates (GBq/year) (Q1, Q2 and Q3) as a function of time in the cases with 3 and 7 compartments in block 7. The continuous line is the case with 3 compartments and dashed line is the case with 7 compartments.*

The figures show that there are differences only in the release rates at Q3, which constitute a minor part of the total release. The conclusion is hence that the original division into 3 compartment is sufficient to describe the total release rates. If the release through Q3 will be studied, more compartments are necessary to give good representation of the release.

2.4 BLOCK 4, BENTONITE SURROUNDING CANISTER

The discretization in block 4, the bentonite surrounding the canister, has been studied by division into five compartments compared to the two in the original model. The release down through block 4, 8 and 9 out through Q4 has been shown to be small in previous studies. The effect as a sink is dependent on the discretization and hence the total release may be influenced by the discretization. Four compartments close to the source were made 0.5 m high and the fifth compartment was made 2.33 m high. The dimensions of the compartments are further described in Table 7. The modelled system is now the total system including all nine blocks and all four release paths, see Figure 18.

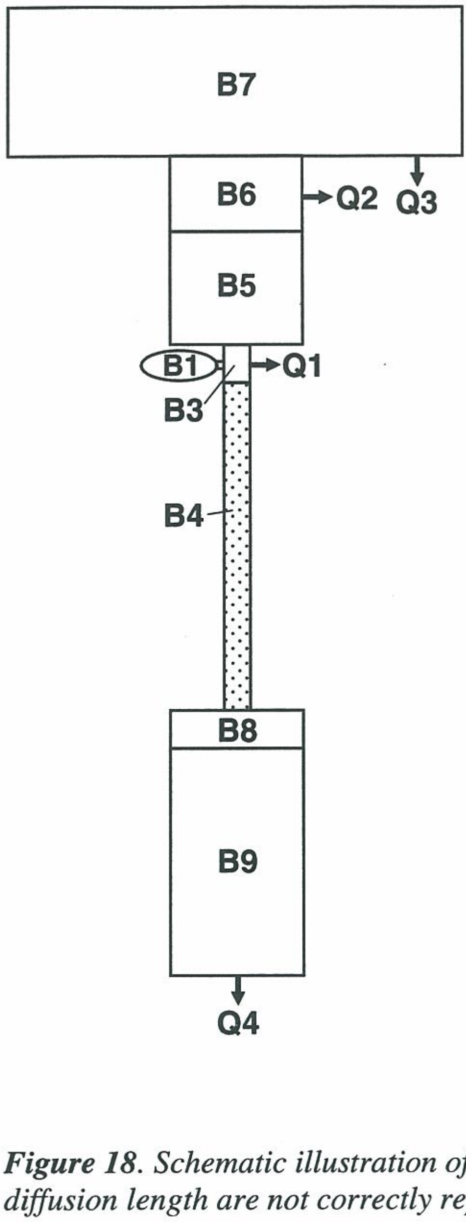

Figure 18*. Schematic illustration of the modelled system, note that the diffusion length are not correctly represented.*

Table 7. Discretization of block 4 with 2 and 5.

		Z_LENGTH	Z_AREA	R_LENGTH	R_AREA
2 Compartments					
	1	2.165	1.539	0.000	1.000
	2	2.165	1.539	0.000	1.000
5 Compartments					
	1	0.500	1.539	0.000	1.000
	2	0.500	1.539	0.000	1.000
	3	0.500	1.539	0.000	1.000
	4	0.500	1.539	0.000	1.000
	5	2.330	1.539	0.000	1.000

The release rates through Q1, Q2, Q3, Q4 and the total release rates are shown in Figure 19, 20, 21, 22 and 23. The calculation times are given in Table 8.

Table 8. Calculation times for different discretizations in block 4. In all cases block 3 is divided into 6 compartments, block 5, 6, 8 and 9 into one compartment each and block 7 into 3 compartments.

Number of compartments in block 4	Total number of compartments	CPU-time
2	17	1:20
5	20	1:32

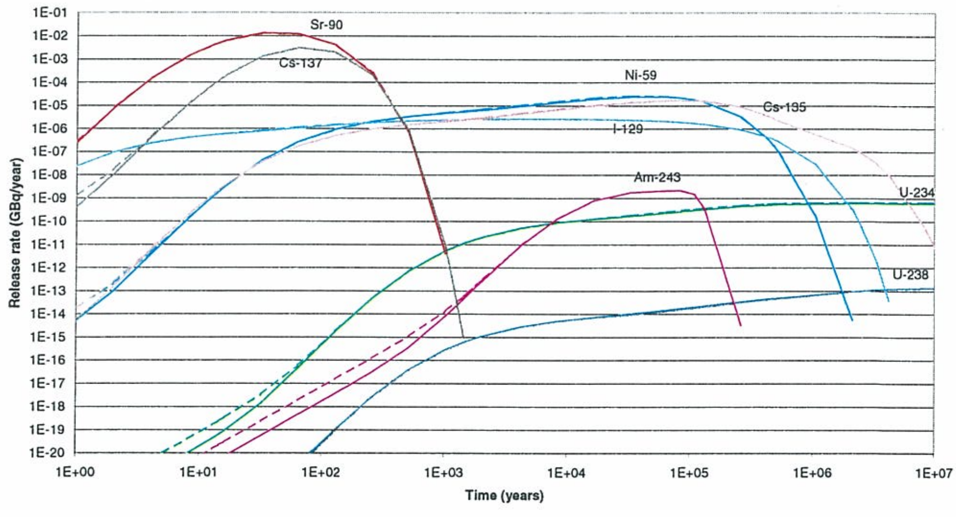

Figure 19. Release rates (GBq/year) at Q1 as a function of time in the cases with 2 and 5 compartments in block 4. The continuous line is the case with 2 compartments and dashed line is the case with 5 compartments.

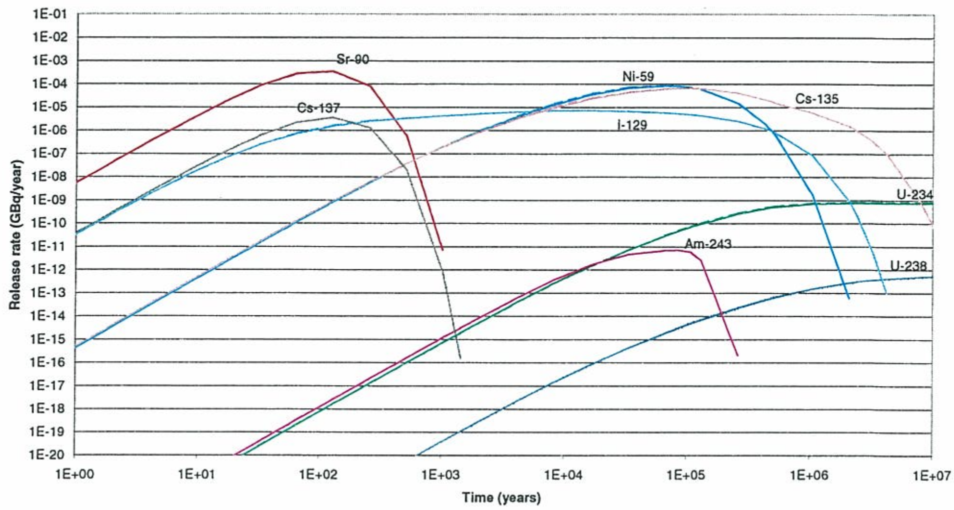

Figure 20. Release rates (GBq/year) at Q2 as a function of time in the cases with 2 and 5 compartments in block 4. The continuous line is the case with 2 compartments and dashed line is the case with 5 compartments.

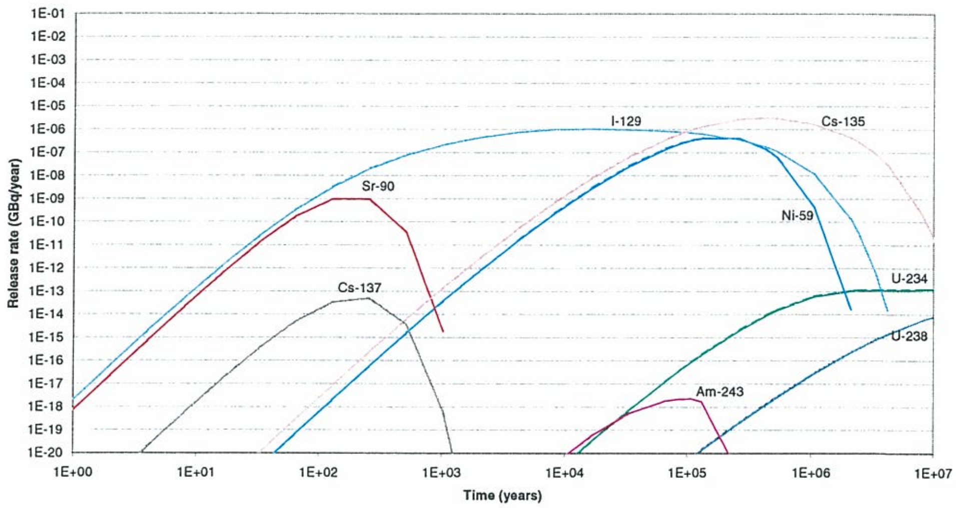

Figure 21. Release rates (GBq/year) at Q3 as a function of time in the cases with 2 and 5 compartments in block 4. The continuous line is the case with 2 compartments and dashed line is the case with 5 compartments.

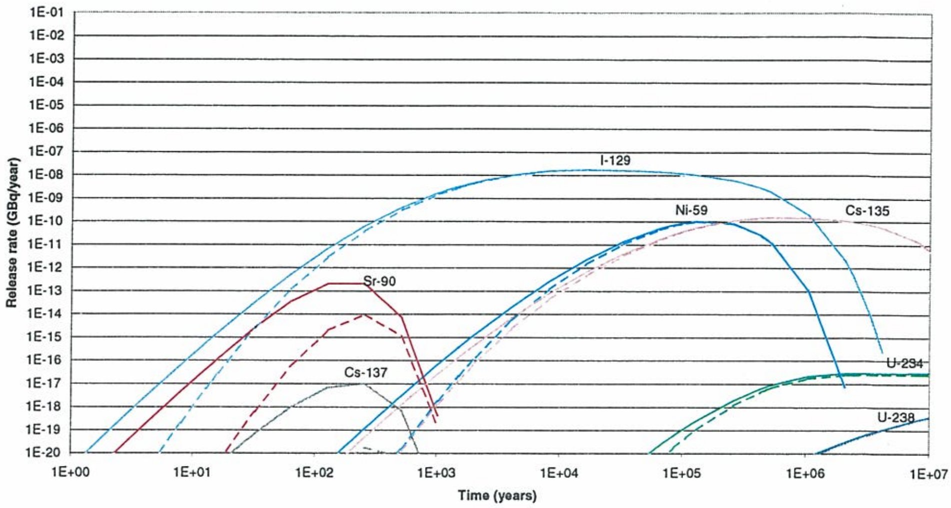

Figure 22. *Release rates (GBq/year) at Q4 as a function of time in the cases with 2 and 5 compartments in block 4. The continuous line is the case with 2 compartments and dashed line is the case with 5 compartments.*

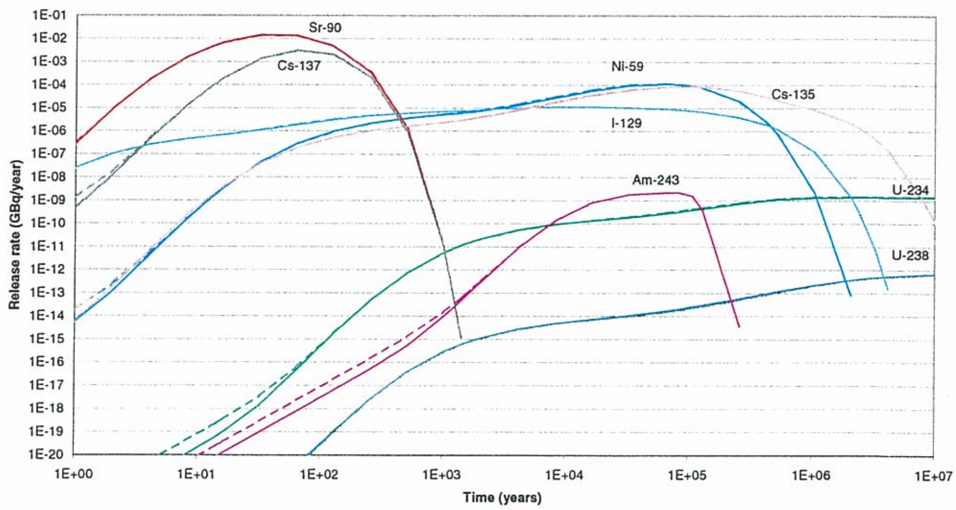

Figure 23. *Total release rates (GBq/year) (Q1, Q2, Q3 and Q4) as a function of time in the cases with 2 and 5 compartments in block 4. The continuous line is the case with 2 compartments and dashed line is the case with 5 compartments.*

It can be concluded from the figures that the total release is only influenced to a little extent if block 4 is divided into 5 instead of 2 compartments. The original 2 compartments are hence sufficient to describe the total release rates. The release through the bottom path, Q4, is however influence more and if this release will be studied a finer discretization is necessary.

2.5 FINAL DISCRETIZATION

The calculations performed have shown that the original discretization modified only to content 6 compartment in block 3 is sufficient to describe the total release rates for the studied nuclides. The release of the studied nuclides was totally dominated by release through either Q1 or Q2. Other nuclides or other parameter combinations may exhibit release rates more equally divided between Q1 and Q2 and may therefore be more influenced by the discretization close to block 3. The proposed final discretization is therefore three equal compartments in block 5 and 2 compartments in block 4, one 1 m high close to block 3 and the other 3.33 m high. The dimensions for all compartments in the final discretization are given in Table 9. The final discretization is shown in Figure 24.

Table 9. Dimensions for all compartments in the final discretization.

	Compartment number	Z_LENGTH	Z_AREA	R_LENGTH	R_AREA
Block 1	1	0.000	1.000	0.000	1.000
Block 2	1	0.050	5.00E-06	0.000	1.000
Block 3	1	0.500	0.203	0.058	1.741
	2	0.500	0.224	0.058	1.924
	3	0.500	0.246	0.058	2.107
	4	0.500	0.267	0.058	2.291
	5	0.500	0.289	0.058	2.474
	6	0.500	0.310	0.058	2.657
Block 4	1	1.000	1.539	0.000	1.000
	2	3.330	1.539	0.000	1.000
Block 5	1	0.500	2.405	0.000	1.000
	2	0.500	2.405	0.000	1.000
	3	0.500	2.405	0.000	1.000
Block 6	1	1.000	2.405	1.750	5.500
Block 7	1	2.125	12.240	2.000	26.400
	2	1.750	12.240	2.000	21.700
	3	2.125	12.240	2.000	26.400
Block 8	1	0.500	2.405	0.000	1.000
Block 9	1	3.000	2.405	0.000	1.000

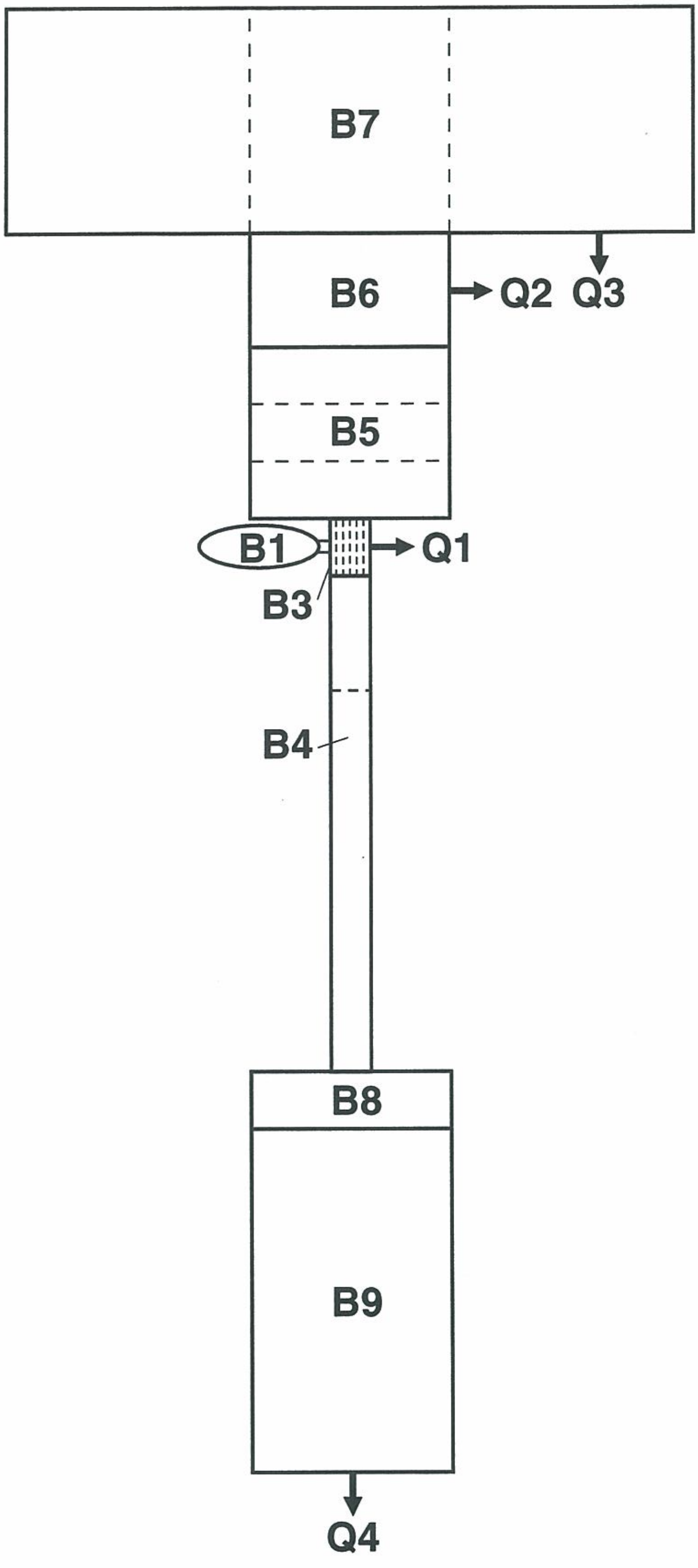

Figure 24. *Final discretization.*

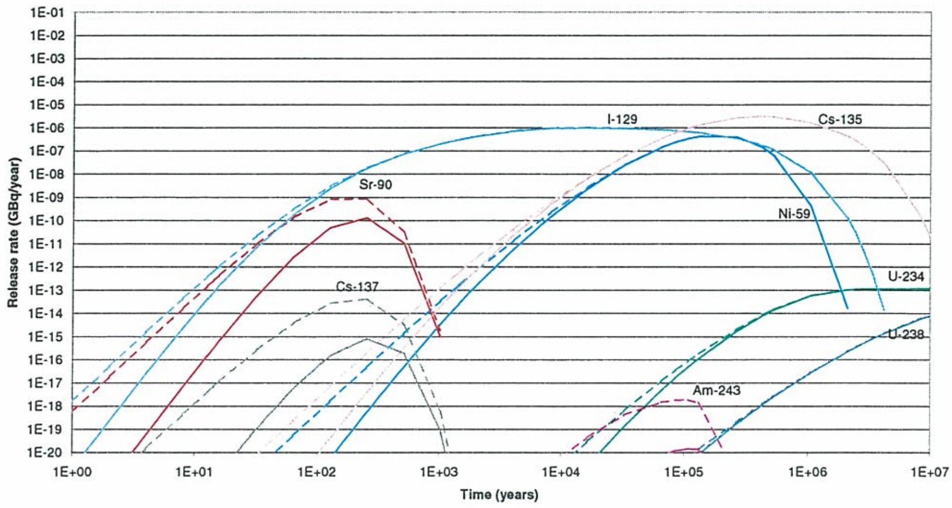

Figure 27. Release rates (GBq/year) at Q3 as a function of time in the case with the final discretization (continuous lines) compared to the original discretization (dashed lines).

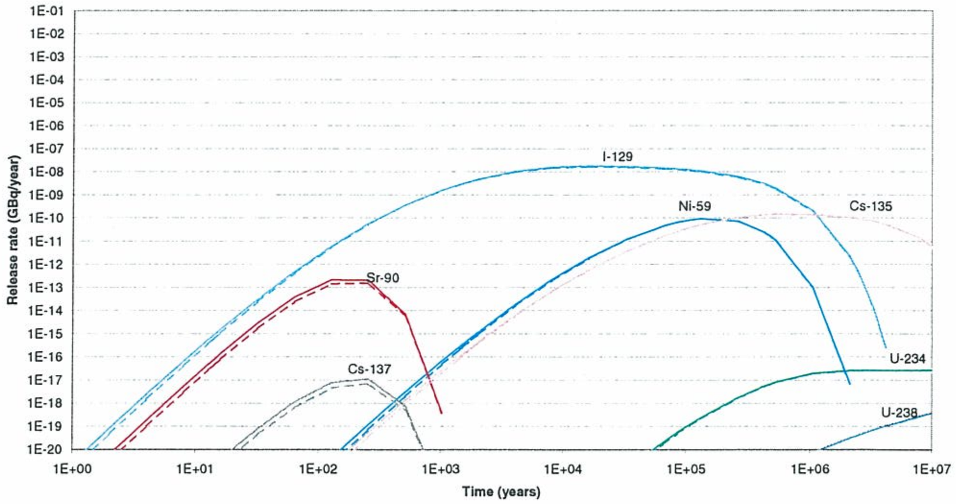

Figure 28. Release rates (GBq/year) at Q4 as a function of time in the case with the final discretization (continuous lines) compared to the original discretization (dashed lines).

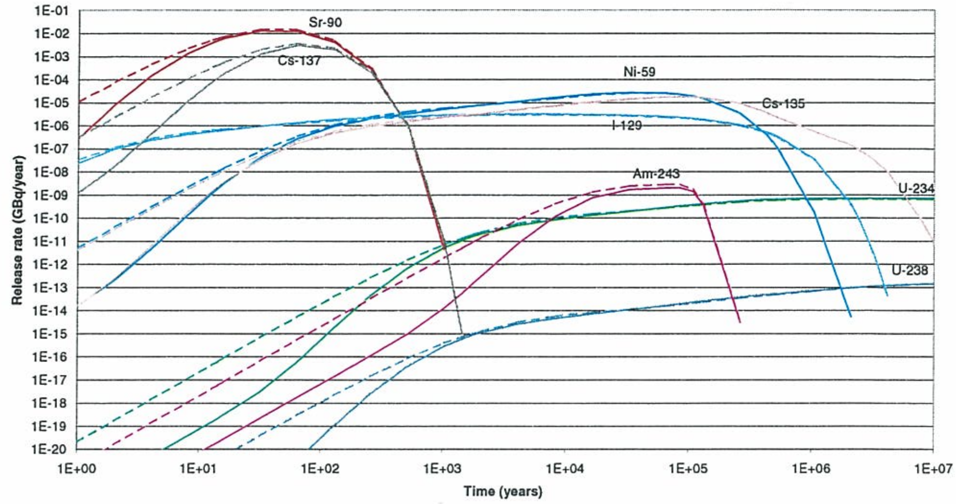

Figure 25. *Release rates (GBq/year) at Q1 as a function of time in the case with the final discretization (continuous lines) compared to the original discretization (dashed lines).*

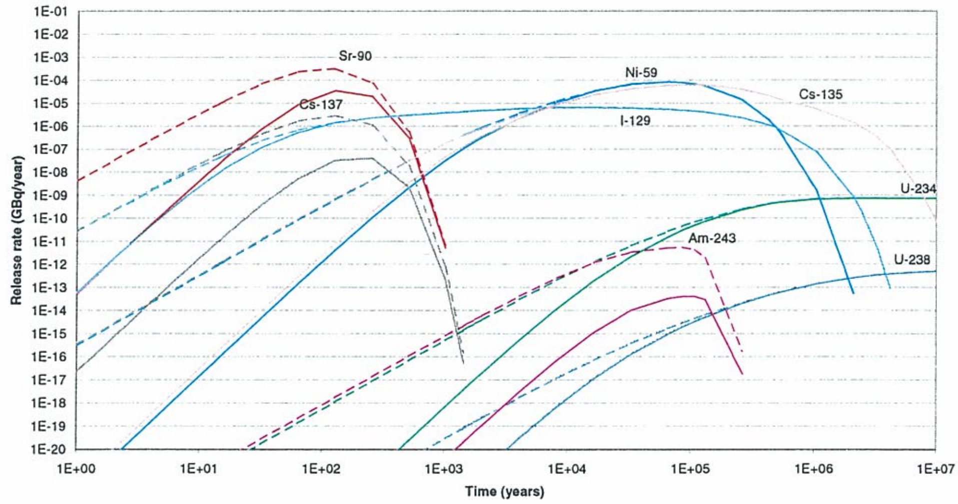

Figure 26. *Release rates (GBq/year) at Q2 as a function of time in the case with the final discretization (continuous lines) compared to the original discretization (dashed lines).*

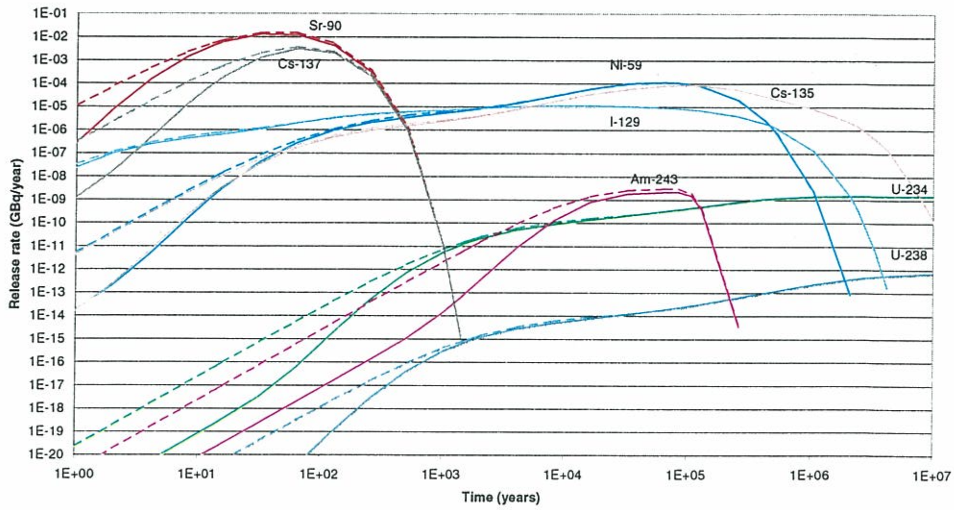

Figure 29. Total release rates (GBq/year) (Q1, Q2, Q3 and Q4) as a function of time in the case with the final discretization (continuous lines) compared to the original discretization (dashed lines).

2.6 CALCULATION TIMES

The calculation time is an important criterion when optimising the discretization. The calculation time was recorded for each calculation case. The calculation times are in all cases short, but it should be noted that this is only one realisation with few nuclides, one stream tube and one canister. The real calculations comprise several additional nuclides, many realisations, many stream tubes and canisters. The calculation times will then be some hundred times longer than the one recorded here. The calculation time is roughly dependent on the square of the total number of compartments. The calculation time as a function of the square of the total number of compartments is shown in Figure 30. The final discretization with 19 instead of 14 compartments require about 20 % more calculation time.

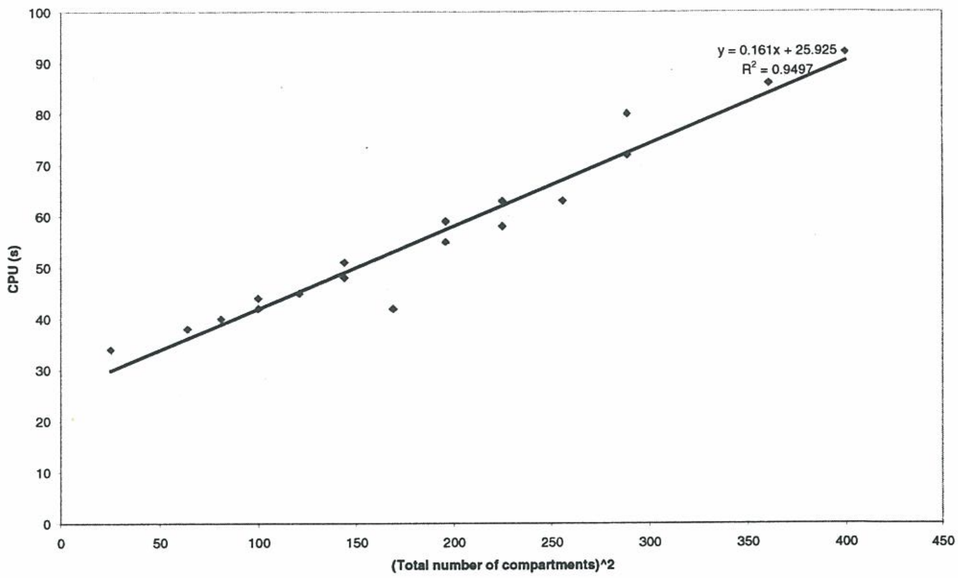

***Figure 30**. Calculation time (CPU) as a function of the square of the total number of compartments.*

3 DISCUSSION AND CONCLUSIONS

The original discretization used for the near field in COMP23 is shown to give a good representation in most cases. The release rates are always overestimated with the original discretization, especially in the early instationary phase. In some cases, for example for the short-lived nuclides Sr-90 and Cs-137, with increased K_d-values, the overestimation of the maximum release rates is large. A finer discretization is shown to give less overestimated release.

If one block with several compartments is connected to a block with fewer compartments than in the first block there may be a potential short circuit effect. This means that the nuclides may go from the first compartment through a connected block and back to the last compartment instead of through all compartments. This effect may be present between block 3 and 5 and also between block 3 and 4. The effect was shown to be of minor importance in the calculations with different number of compartments in the horizontal direction in block 5.

Some general conclusion of the function of the studied system can be drawn. For example the correlation between different nuclides and the dominating release path. The release rates for the short-lived nuclides, Sr-90 and Cs-137, and also Am-243 are totally dominated by release through Q1. The release rates for the other nuclides, U-238, U-234, Ni-59, Cs-135 and I-129 are totally dominated by release through Q2. Another conclusion is that since the total releases are dominated by release through Q1 and Q2, the release paths up through block 7 and down through block 4, 8 and 9 mainly act as sinks.

The discretization proposed comprises 6 compartments in the horisontal direction in block 3, 2 compartments in block 4 (one 1 m high and the other 3.33 m high), 3 compartments in the vertical direction in block 5 and all other blocks are unchanged. This increase from 14 to 19 compartments also gives a margin for other nuclides and/or transport parameters than those studied. If the release rates through individual paths are to be studied in more detail a finer discretization is necessary.

The calculation time is another optimisation criterion when the discretization is studied. The calculation time was found to increase in proportion to the square of the number of compartments. The calculation time increaces about 20 % with the proposed increase from 14 to 19 compartments.

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