Appendix B
Memo from Rebecca L. Blaine
Illustrating Linearity of SECO-TRANSPORT Calculations

ECODYNAMICS MEMORANDUM

TO: Jon Helton
FROM: Rebecca L. Blaine /rlb
DATE: January 30, 1996
RE: Source Term Study

The following calculations were performed to verify the linear behavior of the source term in the SECOTP2D code. The problems were run on the standard local grid, 46x53 elements measuring 125 m on each side. Dual porosity was modeled. Median values from the 1992 PA were used for most parameters with the exception of fracture spacing and chemical retardation. The values for the parameters used are as follows: matrix porosity = .139, matrix tortuosity = .12, fracture spacing = 2 m, fracture porosity = .001, longitudinal dispersivity = 100, and transverse dispersivity = 10. Three radioisotopes were transported, ^{240}PU, ^{241}AM, and ^{233}U. The amount of chemical retardation applied was very small, R = 2.74678, for ^{240}PU and ^{233}U, and no retardation, R = 1, for ^{241}AM. This value of retardation for ^{241}AM was chosen because of the very short half-life of this isotope. If any retardation is used, all of the injected mass is retained in the grid or decays before it reaches the boundary chosen for integration. A constant velocity field was used with a value for Darcy velocity of 1.0E-09 m/sec. (The average Darcy velocity along the path of a particle released from the site to the 2.5km boundary for the 70 transmissivity fields used in the 1992 PA ranges from 1.0E-09 to 9.0E-10.) The duration of each problem was 10,000 years starting at t = 0.0 and with a time step of 5 years.

Six runs were made varying only the source function. The first, baseline case duplicated the "unit source" used for the DCCA calculations. This consisted of a square pulse beginning at t = 0.0 years and ending at t = 50 years with at constant injection rate of 2.0E-09 kg/sec. The total amount of mass injected in this case for each radioisotope was 3.15569 kg. The second case simply doubled the rate to 4.0E-09 kg/sec (which of course doubles the amount of mass injected). The third through sixth cases all used more complicated functions. Figure 1 shows all six source functions used for all three isotopes. Table 1 shows the total amount of mass injected for each isotope in each of the six runs.

Table 1 - Total mass (kg) injected for each isotope in each case

Case number	Total Mass (kg)
1	3.15569
2	6.31138
3	17.356295
4	6.31138
5	315.569
6	757.3656

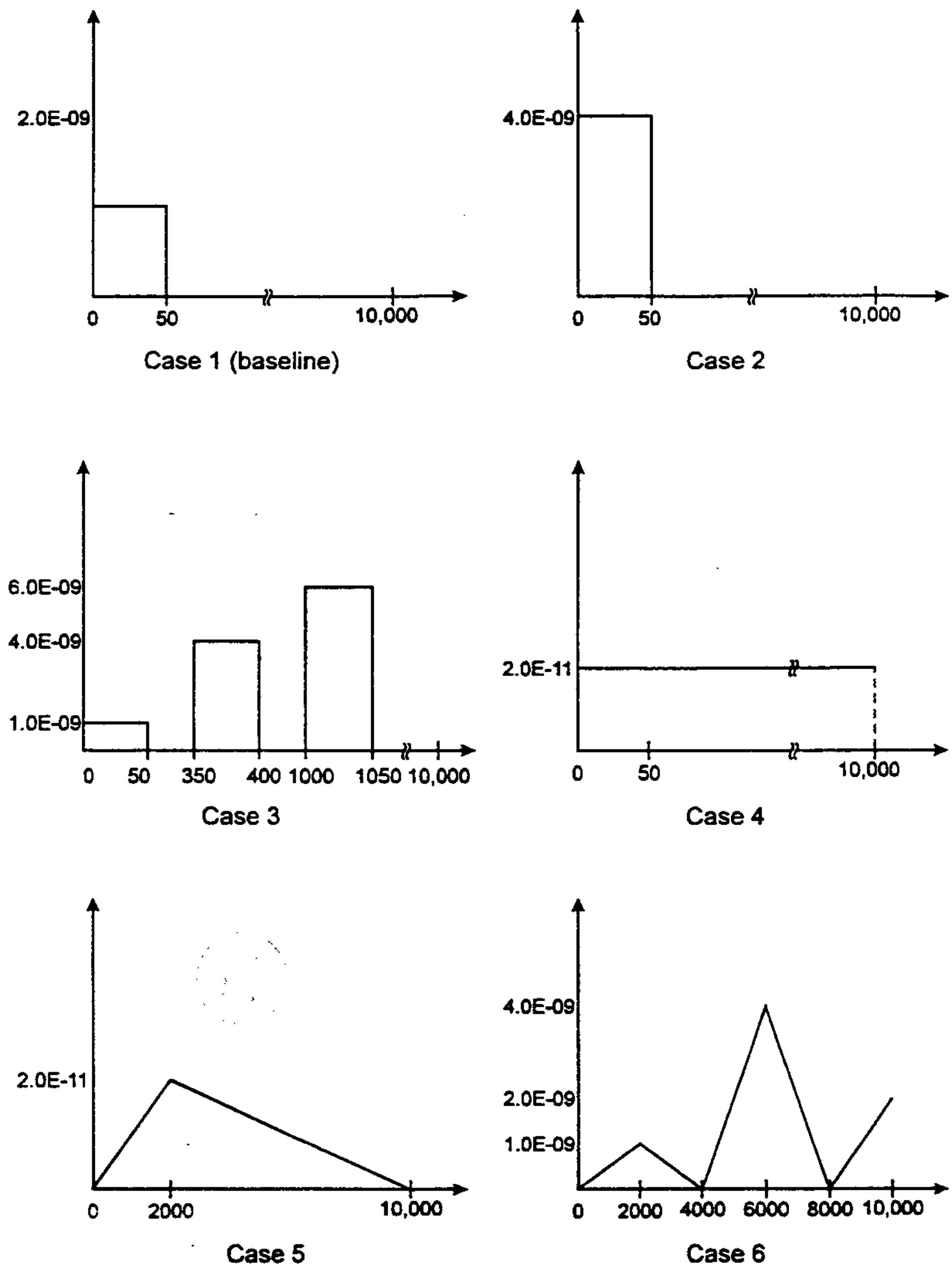


Figure 1 - Input source function for for the six cases

The purpose of running case 2 was to see if doubling the amount of mass injected doubles the amount of mass discharged. The discharge is calculated by summing the mass around a rectangular boundary with the southern edge 2.5 km from the injection point. (The flow was set to be directly south so all of the mass that crosses the discharge boundary crosses the southern edge.) This discharge is calculated by the code at each time step. The total discharge calculated is the integral of this curve over time. Table 2 shows the amount of each radioisotope that crossed the boundary set at 2.5 km from the release point over the entire 10,000 year time period for cases 1 and 2. As the amount injected for each radioisotope was doubled, the amount that crossed the 2.5 km boundary should show a factor of 2 when the results of case 2 are divided by the results of case 1. The values shown in Table 2 verify that the factor is indeed 2.

Table 2 - Comparison of Integrated Discharge for Cases 1 and 2

Radioisotope	Case 1 (kg)	Case 2 (kg)	Factor (case 2/case 1)
^{240}PU	0.185048	0.370095	1.99999
^{241}AM	3.174245E-04	6.348490E-05	2.0
^{233}U	2.033126E-03	4.066235E-03	1.99999

The purpose of running case 3 was to see if the results of this case are a linear combination of the results of case 1. This case is of interest as it represents multiple intrusions at different times. As in case 2, both the total discharge for each radioisotope were compared. The total discharge of each radioisotope in case 3 should be a linear combination of the discharge in case 1 described by the relationship $D = 2D_1 + 3D_2 + 0.5D_3$, where D_1 is the discharge in case 1 integrated over 10,000 years, D_2 is the discharge in case 1 integrated over 9650 years, and D_3 is the discharge in case 1 integrated over 9000 years. Table 3 shows the discharge calculated by running case 3, the value calculated from the discharge in case 1 (using the equation shown), and the percent error between the two values.

Table 3 - Comparison of Integrated Discharge in Case 3 to Calculated Values

Radioisotope	Case 3 (kg)	Calculated (kg)	Percent error
^{240}PU	0.973453	0.966098	.76%
^{241}AM	1.751912E-03	1.745407E-03	.37%
^{233}U	9.318708E-03	9.343115-03	.26%

Cases 4 through 6 were run to verify that the source term calculation maintains its linear behavior with more complicated input functions that would take into account diffusion into and out of the matrix material. Tables 4 - 6 show for cases 4 - 6 respectively the comparison of the discharge calculated with the SECOTP run and the discharge calculated from linear combinations of the results of case 1. The discharge calculated for case 4 was obtained by the equation $D = .01 \sum D_i$, i = 1,200, where D_i is the discharge of case 1 integrated over 10,000 - (i-1)50 years. The sum is multiplied by .01 as the constant rate of the source function of case 4 was .01 of the rate of the source function of case 1. The discharge for cases 5 and 6 was obtained by the equation $D = \sum R_i D_i$, i = 1,200, where R_i is the rate of the ith 50 year interval divided by the rate of the 50 year pulse in case 1 and D_i is the discharge of case 1 integrated over 10,000 - (i-1)50 years.

Table 4- Comparison of Integrated Discharge in Case 4 to Calculated Values

Radioisotope	Case 4 (kg)	Calculated (kg)	Percent error
^{240}PU	0.119528	0.120146	0.52%
^{241}AM	4.053027E-04	4.067540E-04	0.36%
^{233}U	5.402719E-04	5.568291-04	3.06%

Table 5 - Comparison of Integrated Discharge in Case 5 to Calculated Values

Radioisotope	Case 5 (kg)	Calculated (kg)	Percent error
^{240}PU	7.402370	7.441312	0.53%
^{241}AM	2.571217E-02	2.579650E-02	0.33%
^{233}U	2.550871E-02	2.646831E-02	3.76%

Table 6 - Comparison of Integrated Discharge in Case 6 to Calculated Values

Radioisotope	Case 6 (kg)	Calculated (kg)	Percent error
^{240}PU	4.438583	4.461932	0.53%
^{241}AM	3.313131E-05	3.354456E-05	1.25%
^{233}U	1.326739E-02	1.376989E-02	3.79%

In addition to the tables presented here showing the percent error in the calculated answer as compared to the answer obtained by running the SECOTP code, Figures 2 - 13 show graphically the comparisons of the cumulative discharge all the isotopes in cases 3 - 6.

Case 3 - Cumulative Discharge for ^{240}PU

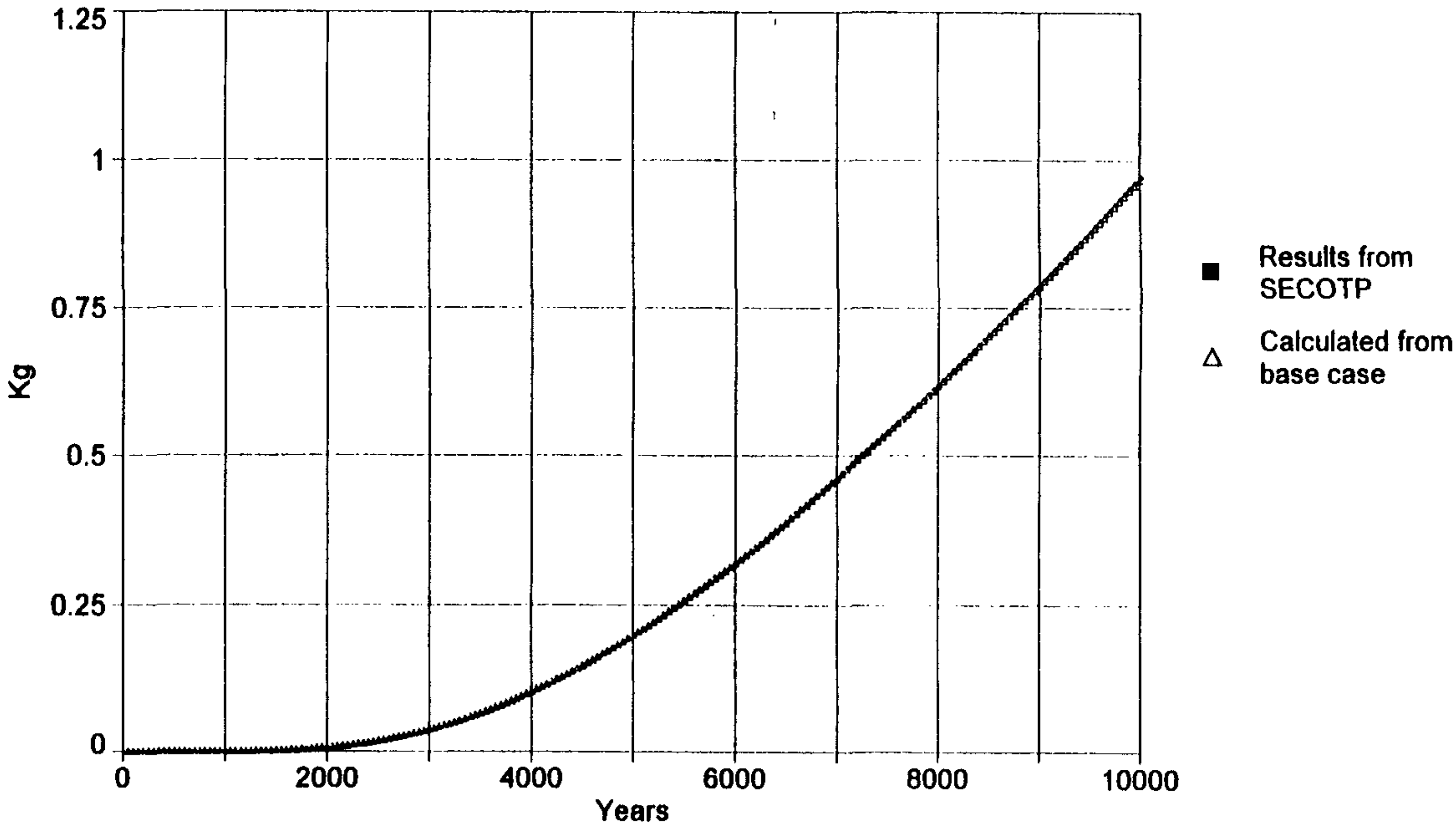
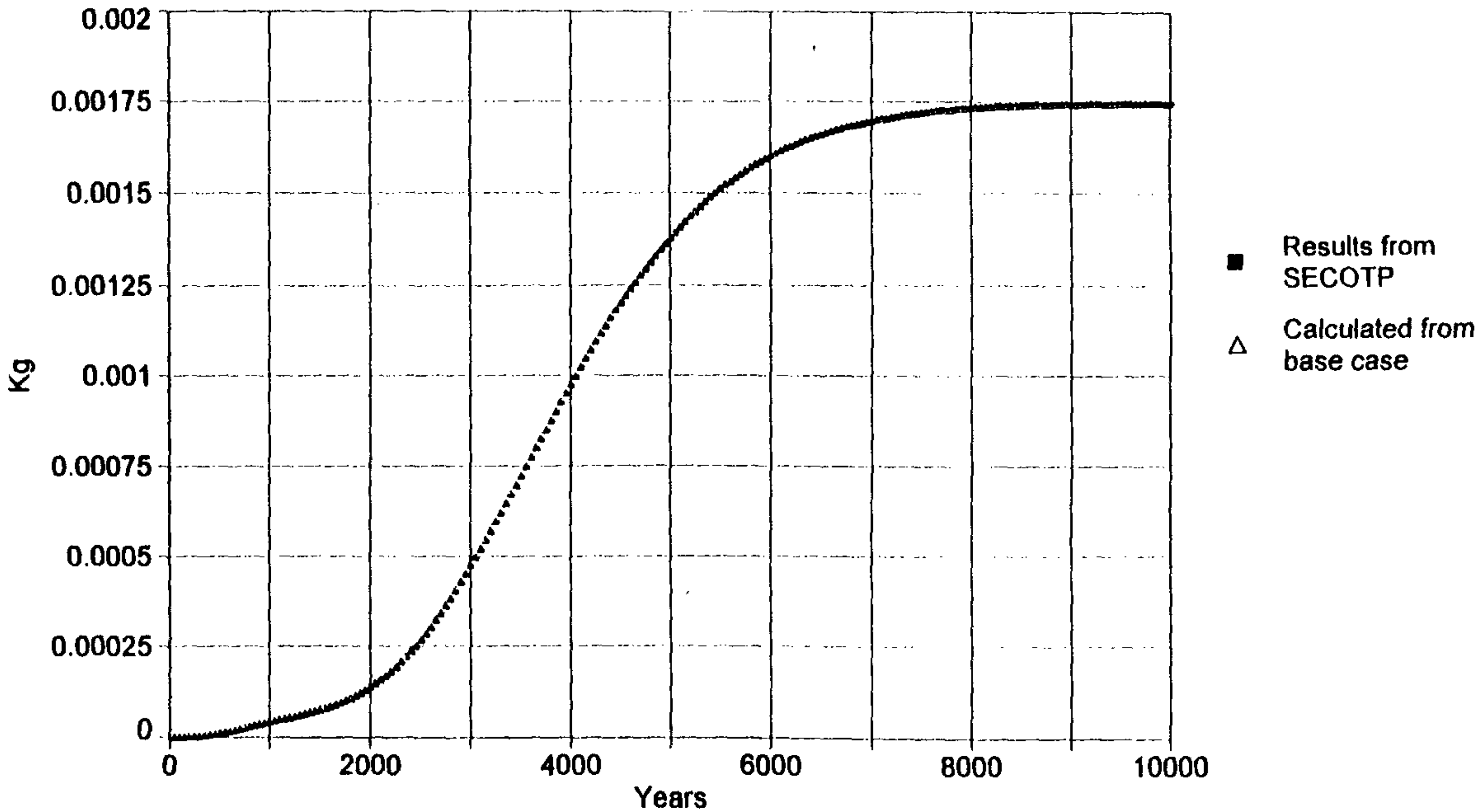
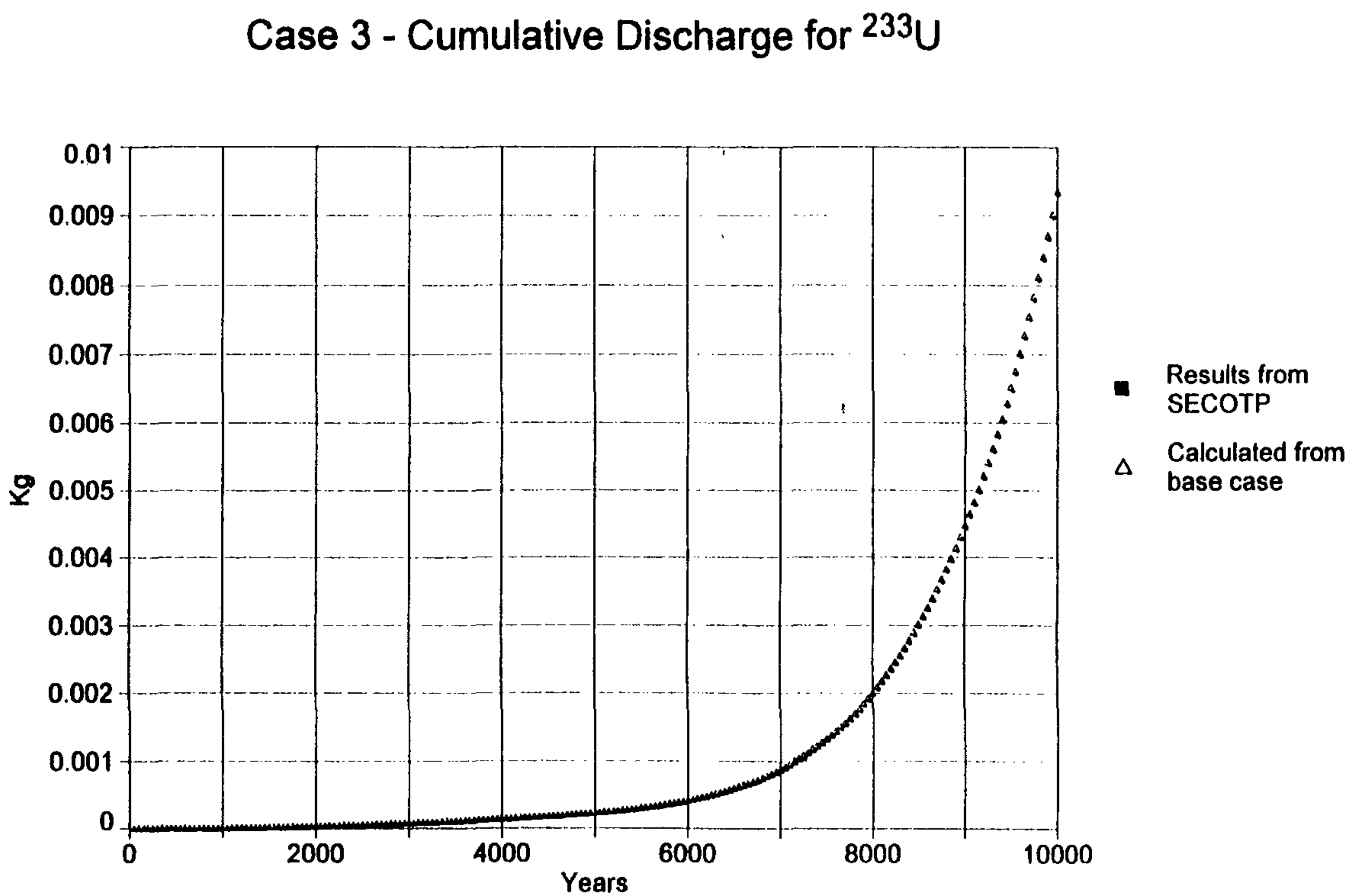


Figure 2

Figure 3

Case 3 - Cumulative Discharge for ^{241}AM





Case 3 - Cumulative Discharge for 233U
0.01
0.009
0.008
0.007
0.006
0.005
0.004
0.003
0.002
0.001
0
Kg
0
2000
4000
6000
8000
10000
Years
Results from SECOTP
Calculated from base case

Figure 4

Case 4 - Cumulative Discharge for ^{240}PU

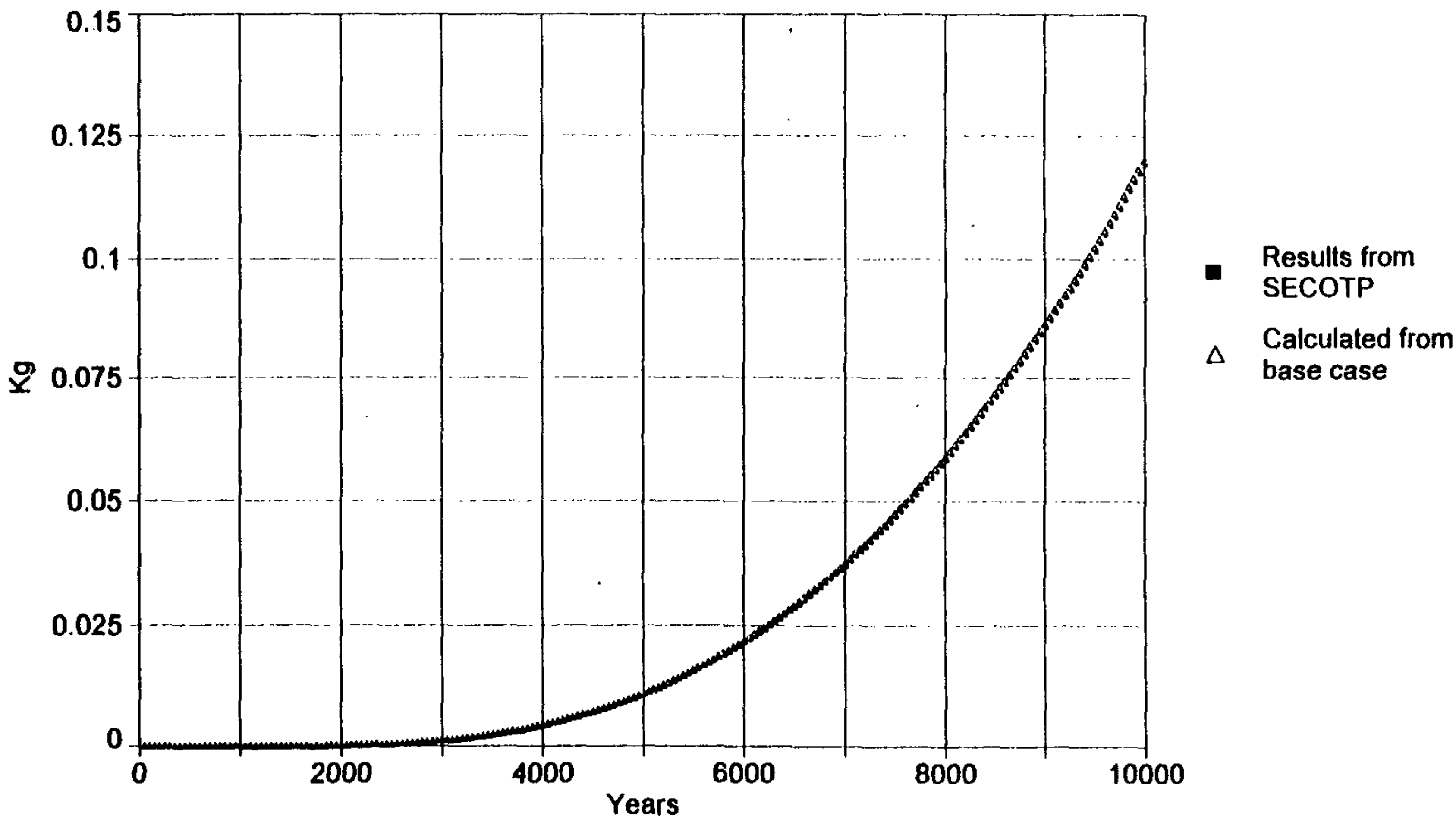


Figure 5

Case 4 - Cumulative Discharge for ^{241}AM

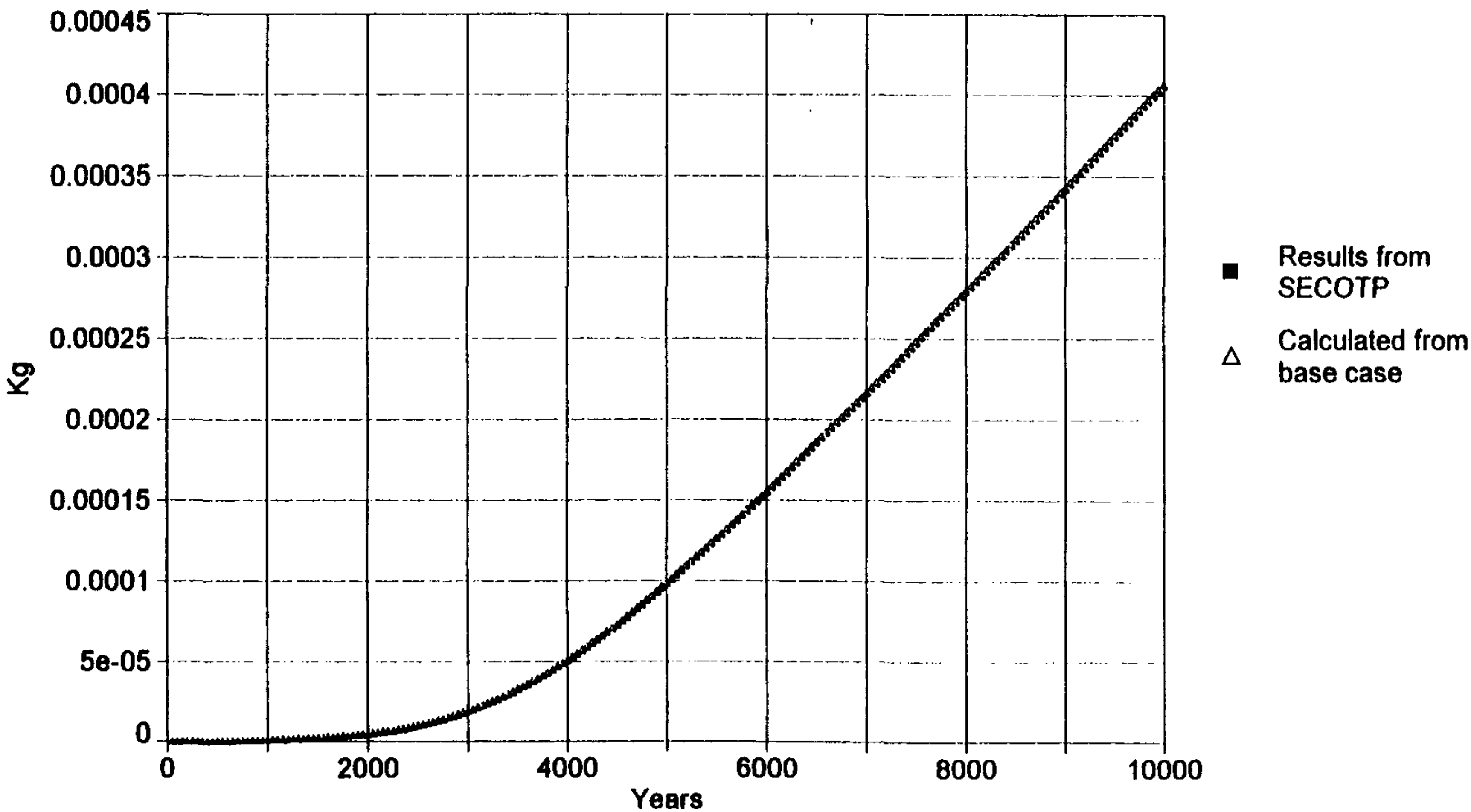


Figure 6

Case 4 - Cumulative Discharge for ^{233}U

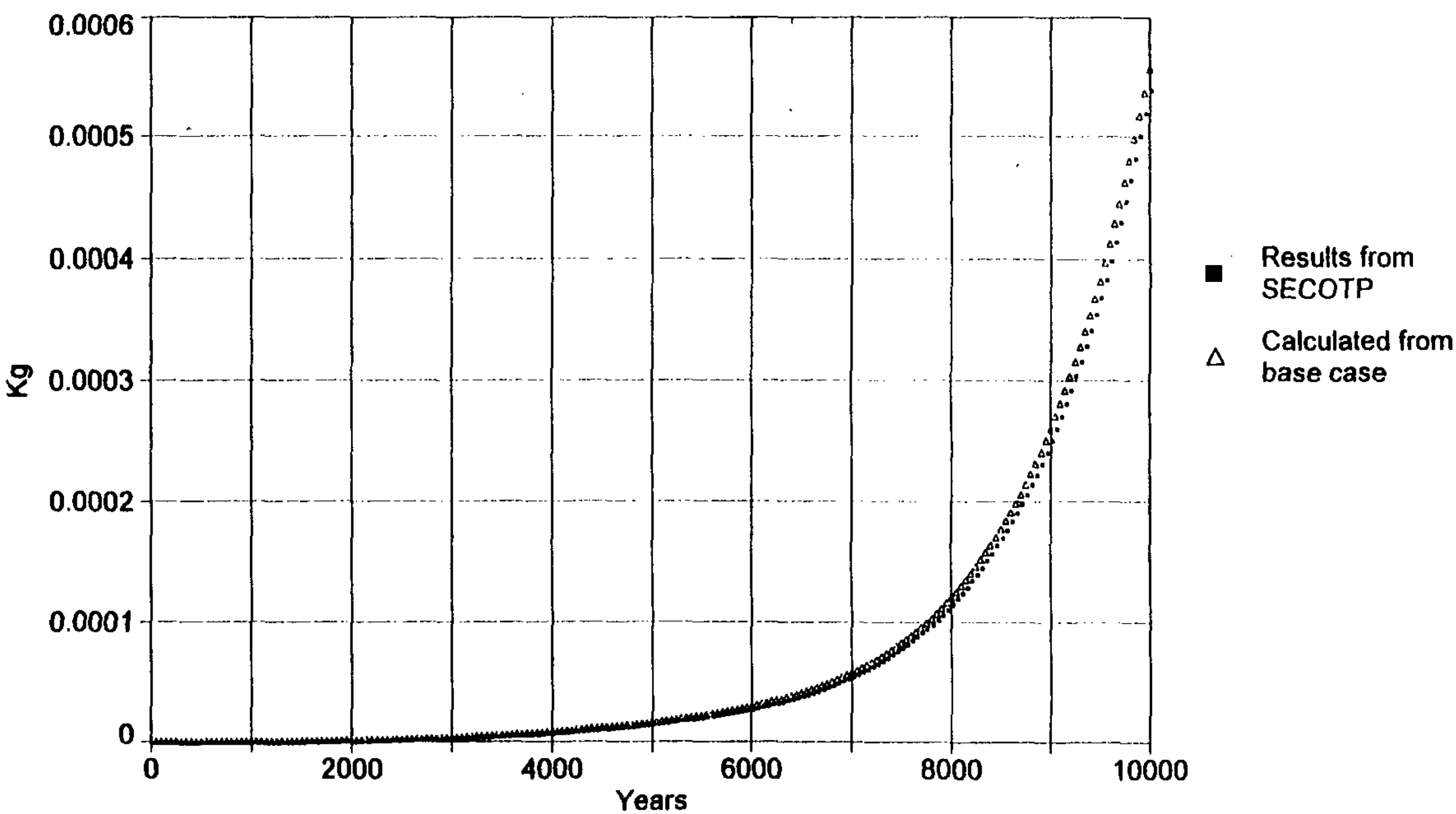
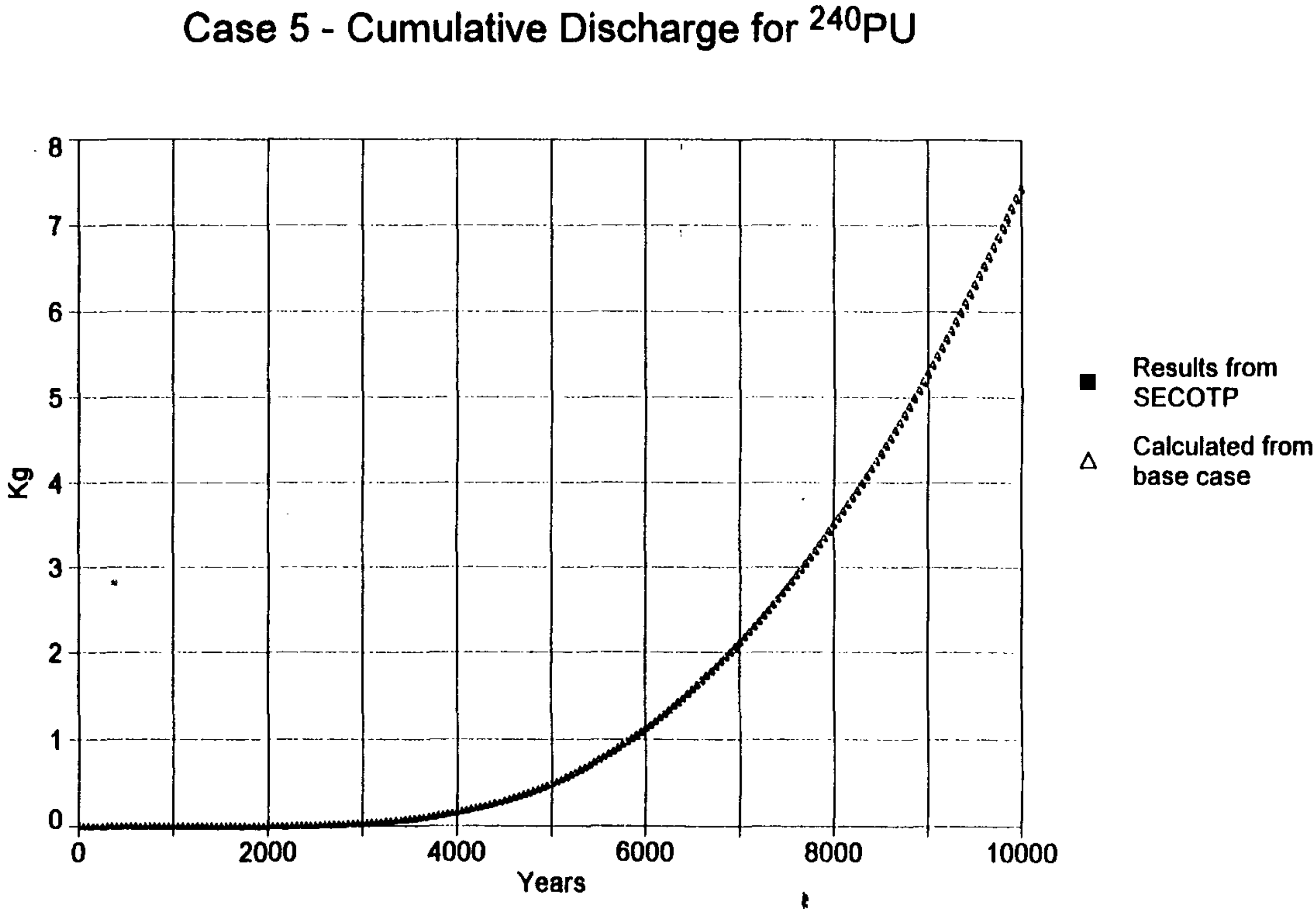


Figure 7

Figure 8



Case 5 - Cumulative Discharge for 240PU
Kg
Years
0
1
2
3
4
5
6
7
8
0
2000
4000
6000
8000
10000
Results from SECOTP
Calculated from base case

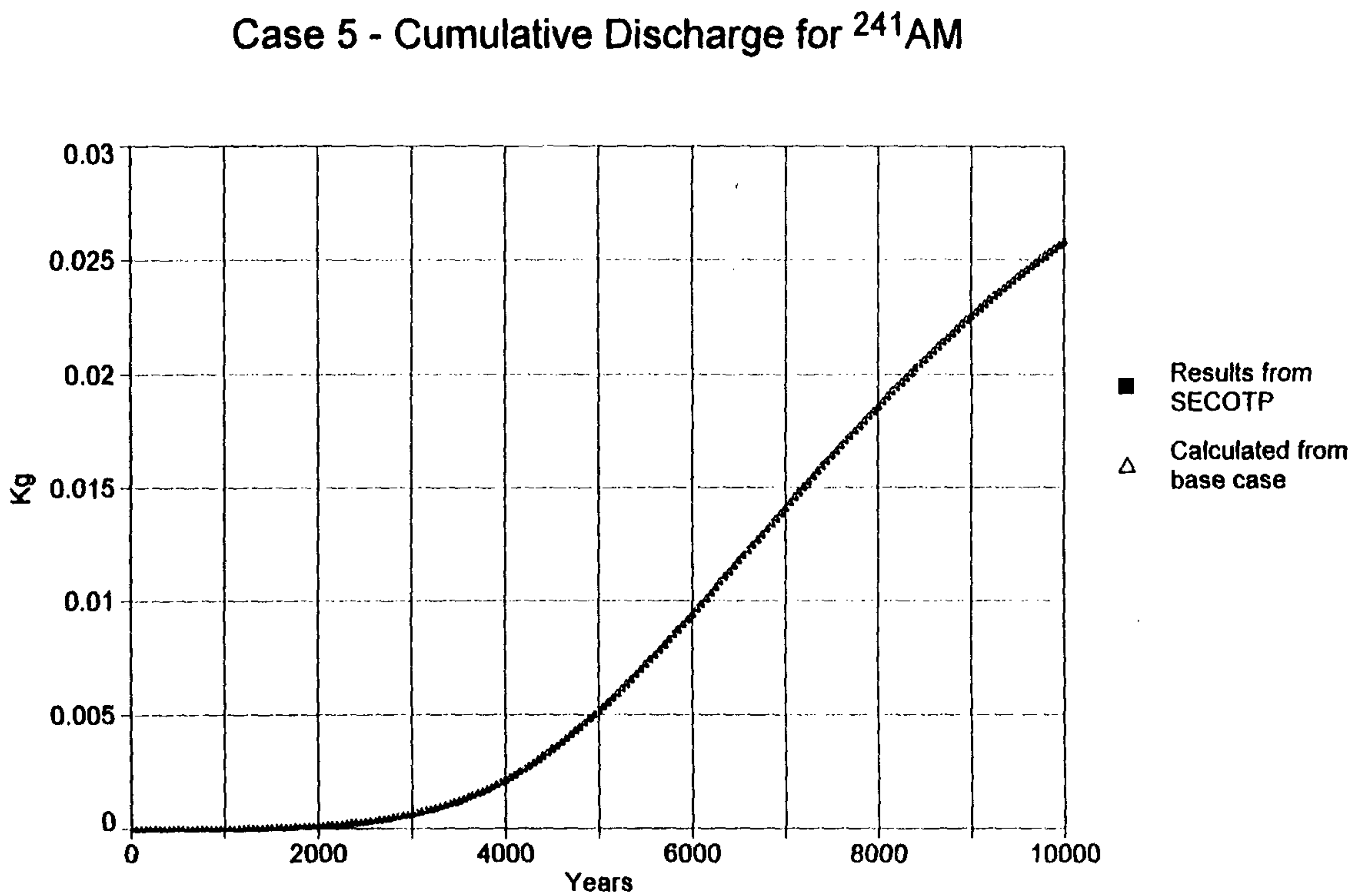

Case 5 - Cumulative Discharge for 241AM
0.03
0.025
0.02
0.015
0.01
0.005
0
Kg
0
2000
4000
6000
8000
10000
Years
Results from SECOTP
Calculated from base case

Figure 9

Case 5 - Cumulative Discharge for ^{233}U

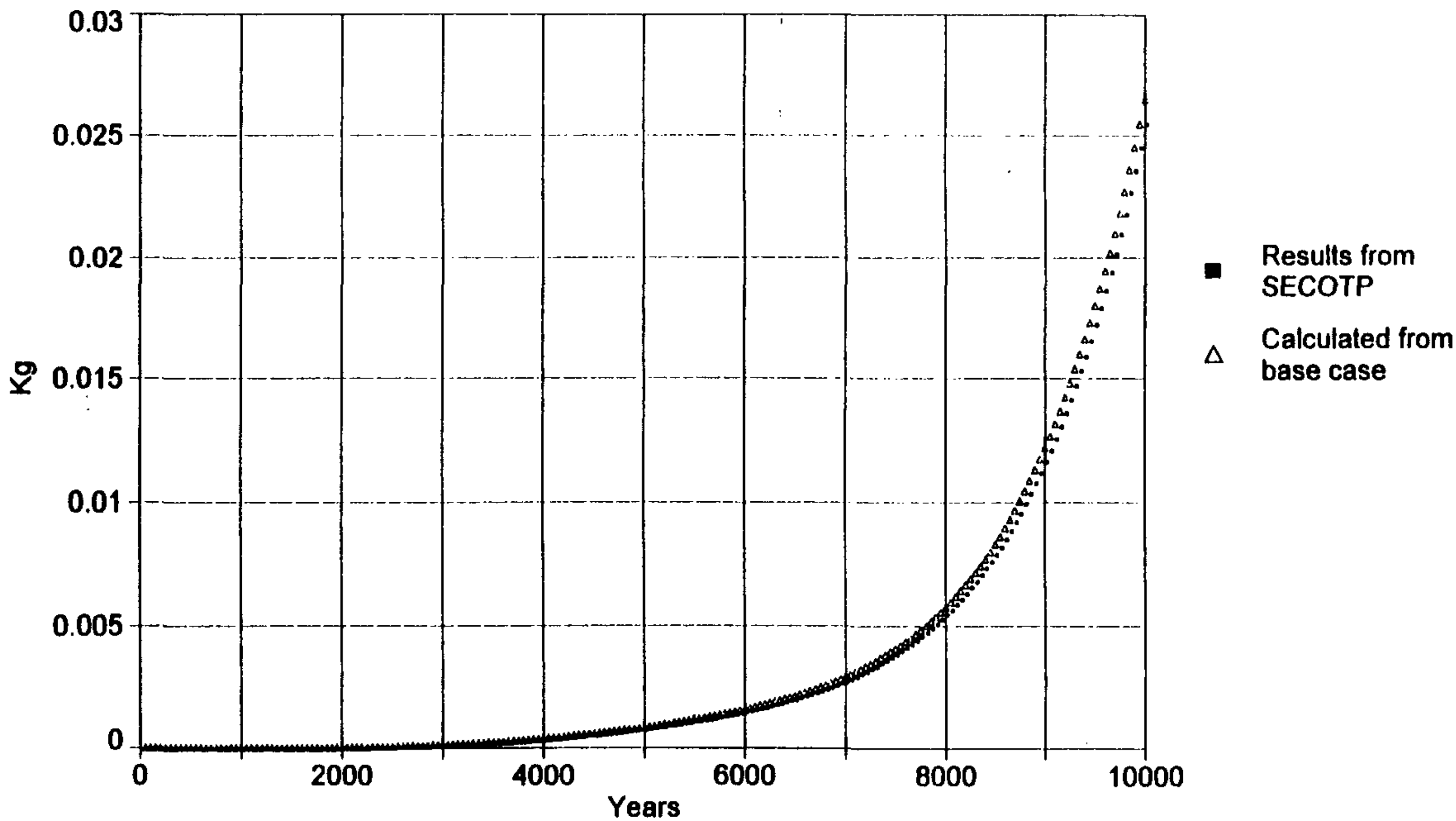
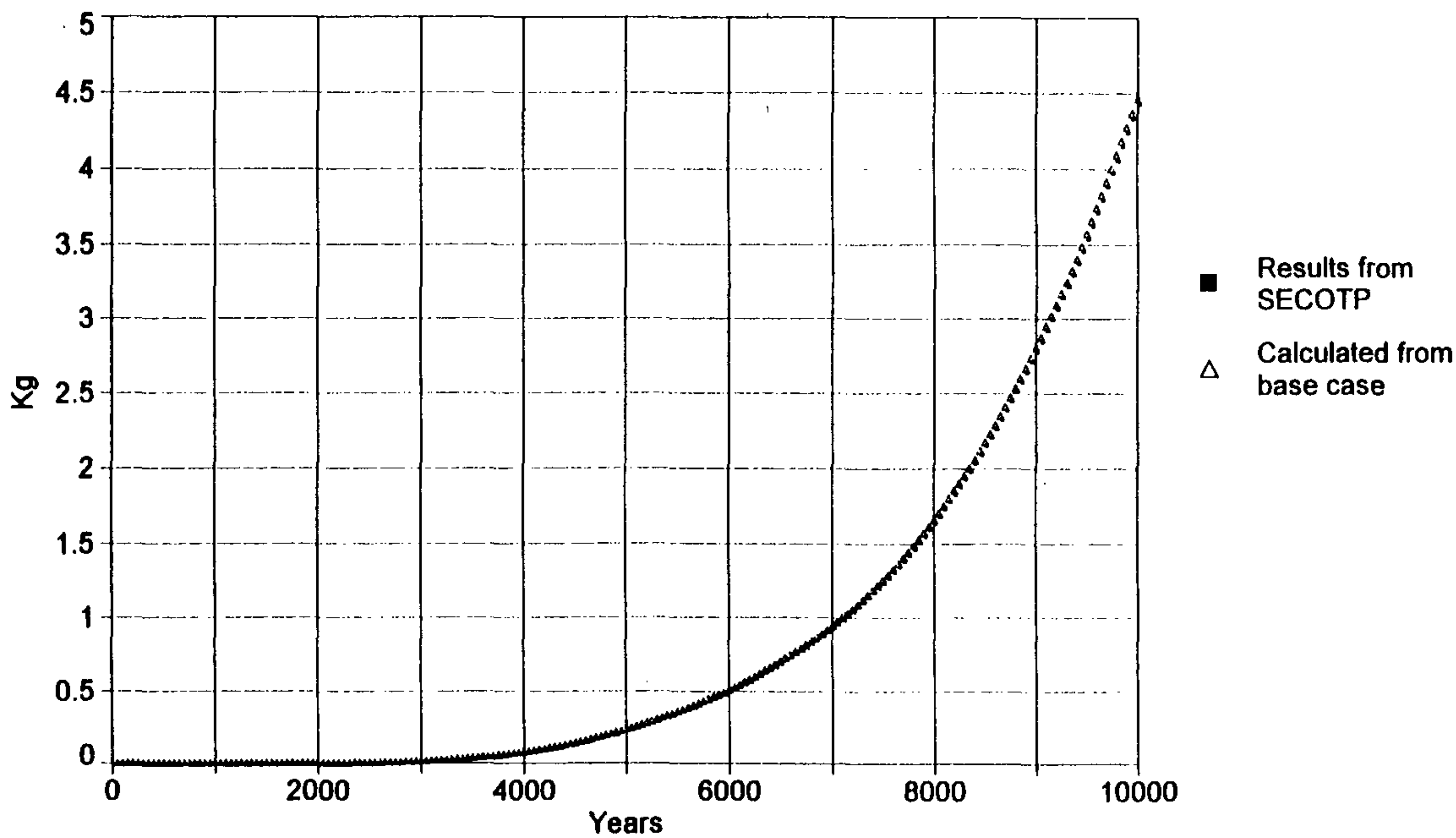
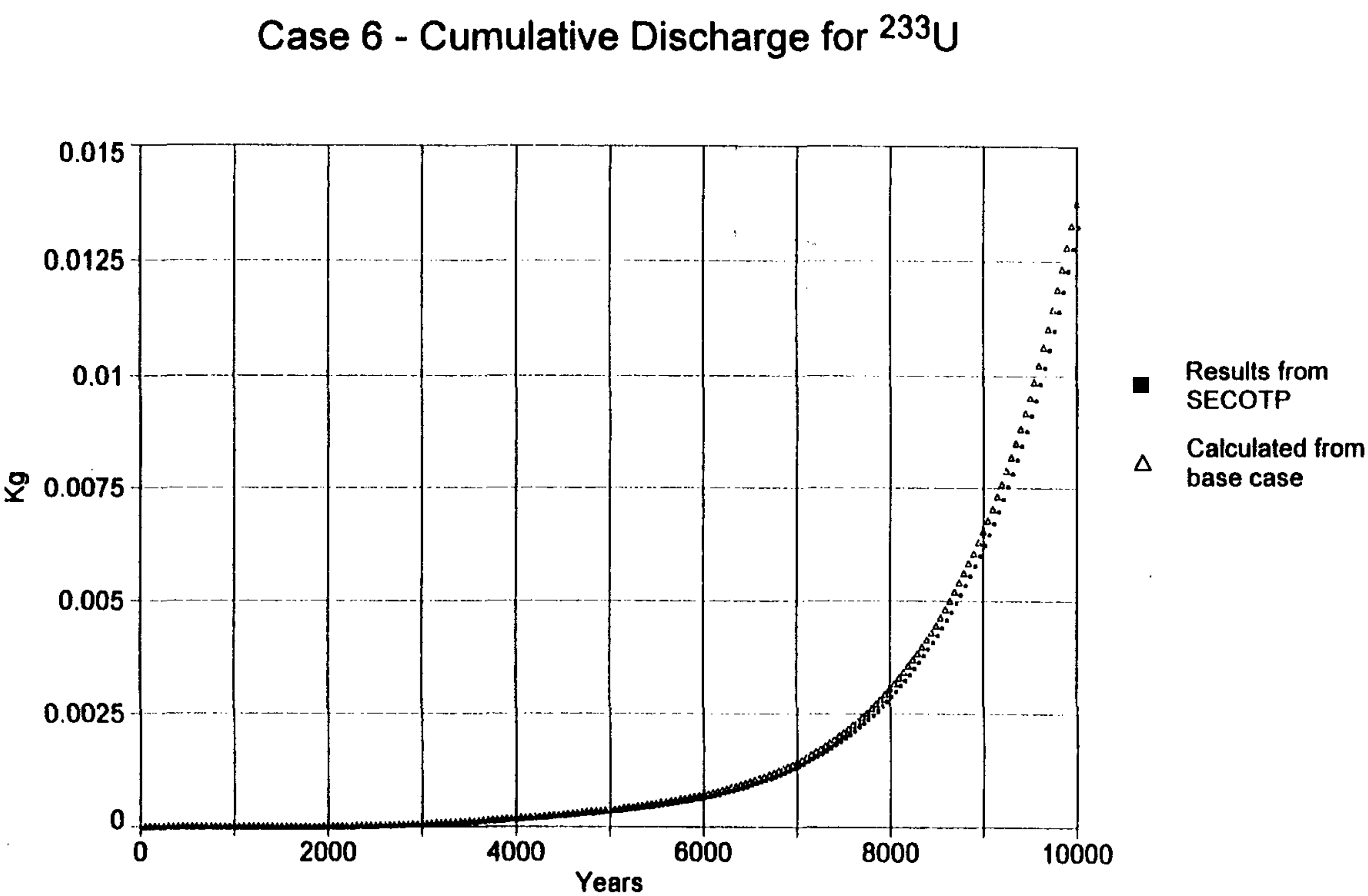


Figure 10

Figure 11

Case 6 - Cumulative Discharge for ^{240}PU





Case 6 - Cumulative Discharge for 233U
Kg
0.015
0.0125
0.01
0.0075
0.005
0.0025
0
0
2000
4000
6000
8000
10000
Years
Results from SECOTP
Calculated from base case

Figure 12

Case 6 - Cumulative Discharge for ^{241}AM

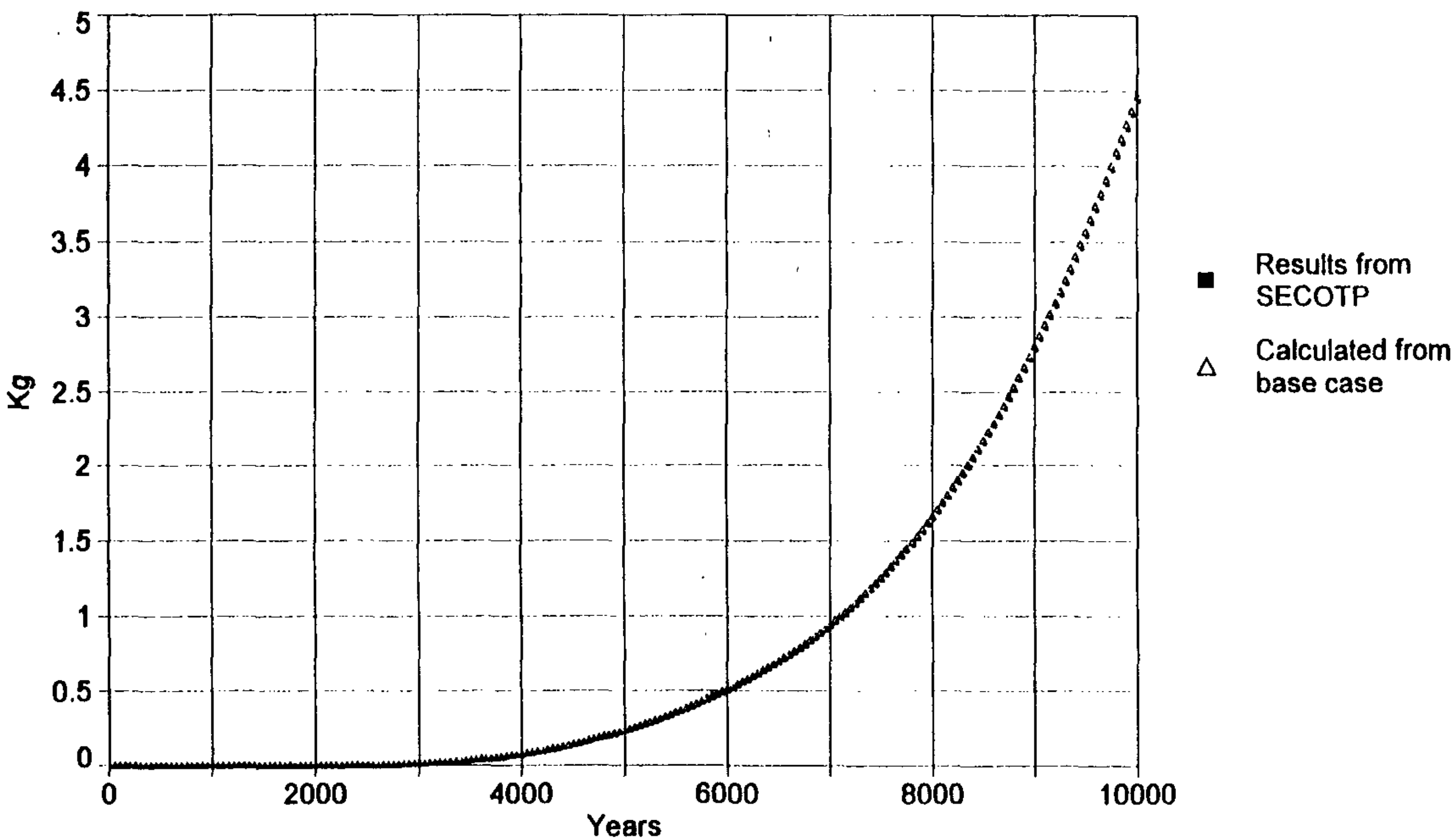


Figure 13