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Interoffice Memorandum

To:	Kent Rosenberger	SRR-CWDA-2011-00114 06/29/2011
From:	Barry Lester 6/29/11	
Reviewer:	Steve Hommel 6/29/11	
Subject:	Comparison of a single-porosity shrinking core model with a dual-porosity fractured medium model	

Summary

The PORFLOW Alternative Sensitivity Case K analysis has been developed as part of the response to NRC comment PA-8. As part of the PORFLOW Case K simulation, a shrinking-core technetium K_d model was implemented to approximate the influence of temporal changes of the grout mass from a reducing environment to an oxidized environment as oxygen diffuses from fractures into the intact grout. Additional information pertaining to the shrinking-core K_d model used for technetium transport in the Case K model was developed to support the validity of the model. A comparison between single- and dual-porosity GoldSim models was used to evaluate how well the shrinking-core model implemented in the PORFLOW equivalent single-porosity model could approximate the process of sorption of technetium in a the fractured media transport system. The analysis indicated that the use of the shrinking-core K_d model, in the PORFLOW Case K would produce reasonable results that are likely to underestimate the release of technetium at early times and overestimate the release at later times, when the releases are greater.

Model Comparison

SRR has developed a PORFLOW based sensitivity analysis (Case K) that considers the influence of fracturing on the degradation of the saltstone grout monolith over time, and its influence on the flow of water through the monolith as the grout degrades. In addition to changes reflected in the flow field, a shrinking core model for evaluating time-dependent K_d values based on the degree of oxygen diffused into the grout matrix is being proposed. The shrinking-core model is based on the increased development of fractures over time and the diffusion of oxygen from the fractures into the grout matrix. The following calculations are designed to help evaluate whether, the use of the shrinking core model in an equivalent single porosity radionuclide transport model will acceptably approximate the effects of moving oxidation fronts in the grout matrix between fractures.

GoldSim Models

Two GoldSim models were developed for this analysis. The first model is a one-dimensional single-porosity model that evaluates the release of technetium at the bottom

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of the grout. This model is a simplified version of the PORFLOW model. The second model is a two-dimensional dual-porosity model that evaluates the release of technetium from continuous vertical fractures that traverse grout matrix blocks from which the technetium diffuses into the fractures. Note that the simulation does not consider radionuclide decay, but uses the sorption coefficients for technetium as a basis.

The single porosity model consists of a column of 10 cells through which the water flows at a rate generated by a PORFLOW during the Case K analysis. The flow rates are based on evaluation of the Vault 4 PORFLOW model, for a case where the time-dependent permeabilities are based on the fracturing of the grout over time until the fracture spacing decreases to 0.1 m. Other concrete areas are similarly degraded, but the two GoldSim models represent the behavior of the grout. The model applied an initial K_d value of 1,000 ml/g, representing reduced condition values, and reached a minimum of 10 ml/g, representing oxidized condition values. For the single porosity model, the K_ds used are time dependent with values based upon the shrinking core model values, which are a linearly weighted based on the percent of grout oxidized.

The dual-porosity model consists of 20 rows of cells with each row consisting of 1 fracture cell and 20 matrix cells. The total height of the cell matrix is 7.3 m and each row has the same height 7.3 m/20. The width of the fracture cell is 6.35E-5 m, or half of a 5 mil fracture. The total width of the row of matrix cells is 30.5 m at the start of the simulation, or half the width of Vault 4 grout, taking advantage of the symmetry of the vault. The width of the matrix cells increase by a factor of 1.414 compared to the previous cell, starting at the fracture. This helps to more accurately define the concentration gradient near the fracture. Instead of using the time dependent K_ds from the shrinking core model, the time dependent percent of oxidized grout from the shrinking core model is compared to the normalized width of the matrix zone and the K_ds in each column of matrix cells is changed from 1,000 ml/g to 10 ml/g as the oxygen front passes through. In addition, to more accurately represent the influence of diffusion associated with the increase of fractures over time and the associated increase in diffusive area, the fracture spacing is adjusted over time using the time dependent block-width data from the shrinking core model. Note that the mass within a cell is not adjusted. Because the proportion of the cell that is oxidized does not change when the fracture spacing changes, the model does assume that the oxygen front is at an averaged position for all matrix blocks, allowing the analysis to evaluate a single ½ matrix block. The vertical water flux through the fracture is derived by taking the time dependent Darcy velocities from the PORFLOW simulation and multiplying the Darcy velocity by half of the time-dependent fracture spacing from the shrinking core model and the cell thickness.

Both models assume a matrix bulk density of 1,010 kg/m^3, a porosity of 0.58, and an inventory of 10 g of technetium spread evenly through the grout.

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In addition to a comparison of the single- and dual-porosity model results based upon the data from the Case K simulation, a sensitivity analysis was performed to evaluate how well the single-porosity model can represent a dual-porosity fractured system under different parameter ranges. The parameter changes implemented for the sensitivity analysis are listed in Table 1.

Base Case Results

Figures 1 and 2 can be examined to show a comparison of the results of the single-porosity model and the dual-porosity fracture model which assumes that advective transport through the fractures and matrix diffusion from the blocks of grout to the fractures dominate the transport of radionuclides through the grout monolith. Figure 1 shows a comparison of the technetium release rates from the bottom of the two models. As can be seen from the figure, the single-porosity model does honor the release from a fracture transport model fairly well. Note that because the mass releases from each column of blocks are a step function that includes that whole volume instantaneously instead of progressing through the column over time, a series of spikes form. Figure 2, which presents a comparison of cumulative releases from the two models, shows that there is a greater cumulative release of technetium over time in the early times, and a greater release of technetium at the peak stages of the technetium release.

Sensitivity Analysis

The first set of sensitivity simulations performed in the sensitivity analysis was designed evaluate the influence of the dominantly vertical flow through the grout on the Tc-99 releases from both type models. The time dependent Darcy velocities from the Case K analysis were multiplied by four factors: 0.1, 0.3, 3 and 10, to help determine how sensitive the two systems are to the Darcy velocity, and how well the single-porosity assumption compares to a dual-porosity fractured system. As can be seen, by comparing Figures 3 and 5, to Figure 1 which show the Tc-99 release rates from the grout into the floor using Darcy velocity multipliers of 0.1, 0.3, and 1.0 respectively, the lower the Darcy velocities relative to the base case, the higher the release rates from the dual-porosity model relative to the single-porosity model, accept at peak values. It is expected that since the peaks in the dual-porosity model are remnants of changing the Kds one cell at a time as opposed to over a temporally continuously changing area, that the peaks seen in the single-porosity model will be larger than the peaks in the dual-porosity model. This pattern is also shown more clearly in the cumulative release curves presented in Figures 4, 6, and 2. As the Darcy velocities increase relative to the base case, the greater the releases from the single-porosity model become relative to the dual-porosity model. As shown in Figure 7 and Figure 8 the single porosity model behaves quite similarly to the dual-porosity model when a factor of 3 is used. Figure 9 and Figure 10 show that when a factor of 10 is used, the release of mass from the single-porosity model is greater

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than that of the dual-porosity model until most of the mass has left the system. In addition to evaluating the influence of the Darcy velocities on the two type models, an additional simulation was performed to see how much difference there would be between the dual-porosity model and a dual-permeability model that accounted for vertically downward flow in the oxidized region. As can be seen by comparing Figures 11 and 12 with Figures 1 and 2, respectively, the differences are small.

The second set of sensitivity simulations performed in the sensitivity analysis was designed evaluate the influence of the diffusion coefficient used in the grout on the Tc-99 releases from both type models. The saltstone diffusion coefficient of 1.0E-07 cm^2/sec from the Case K analysis was multiplied by four factors: 0.1, 0.3, 3 and 10, to help determine how sensitive the two systems are to the effective diffusion coefficient, and how well the single-porosity assumption compares to a dual-porosity fractured system with these changes. As can be seen, by comparing Figures 13, 15, 17, and 19, to Figure 1 and Figures 14, 16, 18, and 20, to Figure 2 the main influence of the diffusion coefficient on the dual-porosity system is that the lower the effective diffusion coefficient, the lower the peak that the dual-porosity model reaches, and the longer the mass is released from the matrix (See Figures 13 and 15).

The third set of sensitivity simulations performed in the sensitivity analysis was designed evaluate the influence of fracture spacing on the Tc-99 releases from both type models. For this analysis, the fracture spacings were kept at a constant value throughout the simulation. The fracture spacing considered included: 0.3 m, 0.1 m, 0.3 m, and 1.0 m. The use of constant values was chosen since it allows for an examination of the effects of scale on equilibrium. As can be seen by examining Figures 21 and 22 which are based on the assumption of a 0.03 m fracture spacing and Figures 23 and 24 which are based on the assumption of a 0.1 m fracture spacing, at this small scale, an assumption of equilibrium, holds up quite well as the two models show very similar release rates and cumulative releases. As can be seen by examining Figures 25 and 26 which are based on the assumption of a 0.3 m fracture spacing and Figures 27 and 28 which are based on the assumption of a 1.0 m fracture spacing, at this small scale, an assumption of equilibrium does not hold up as well, and the dual-porosity model shows the influence of the slow diffusion process at the larger scales, with the release at early time being higher for the dual-porosity model relative to the single porosity model and the pattern reversing later in time (near the peak values).

The fourth set of sensitivity simulations performed in the sensitivity analysis was designed evaluate the influence of K_ds on the Tc-99 releases from both type models. For this analysis, the reducing zone and oxidized zones were varied based on values considered for the saltstone. The base case (see Figures 1 and 2) represents a system with a reducing zone K_d of 1,000 ml/g and an oxidized zone K_d of 10 ml/g. The other three

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cases represent systems with: 1) a reducing zone K_d of 1,000 ml/g and an oxidized zone K_d of 0.8 ml/g (see Figures 29 and 30), 2) a reducing zone K_d of 500 ml/g and an oxidized zone K_d of 10 ml/g (see Figures 31 and 32), and 3) a reducing zone K_d of 500 ml/g and an oxidized zone K_d of 0.8 ml/g (see Figures 33 and 34). As can be seen by examining Figures 29, 31, 33, and 1, as expected, there is a longer release (or tail) once all of the zones are oxidized when the oxidized region K_d is 10 ml/g. It can also be seen that seen by examining Figures 30, 32, 34, and 2, as expected, the earlier cumulative single-porosity releases are closer to dual-porosity cumulative releases when the reducing region K_d is 500 ml/g as opposed to 1,000 ml/g.

Table 1: Simulations Performed in the Sensitivity Analysis

Case	Parameter(s) Updated	Figures
Base	-----	1 and 2
1	Darcy velocities × 0.1	3 and 4
2	Darcy velocities × 0.3	5 and 6
3	Darcy velocities × 3.0	7 and 8
4	Darcy velocities × 10.0	9 and 10
5	Effective diffusion coefficients × 0.1	11 and 12
6	Effective diffusion coefficients × 0.3	13 and 14
7	Effective diffusion coefficients × 3.0	15 and 16
8	Effective diffusion coefficients × 10.0	17 and 18
9	Vertical flow through the oxidized zone	19 and 20
10	Fracture spacing = 0.03 m	21 and 22
11	Fracture spacing = 0.01 m	23 and 24
12	Fracture spacing = 0.3 m	25 and 26
13	Fracture spacing = 1.0 m	27 and 28
14	Oxidized region K_d = 0.8 ml/g	29 and 30
15	Reduced region K_d = 500 ml/g	31 and 32
16	Reduced region K_d = 500 ml/g Oxidized region K_d = 0.8 ml/g	33 and 34

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Figure 1: Comparison of Single- and Dual-Porosity Model Releases of Technetium for the Base Case

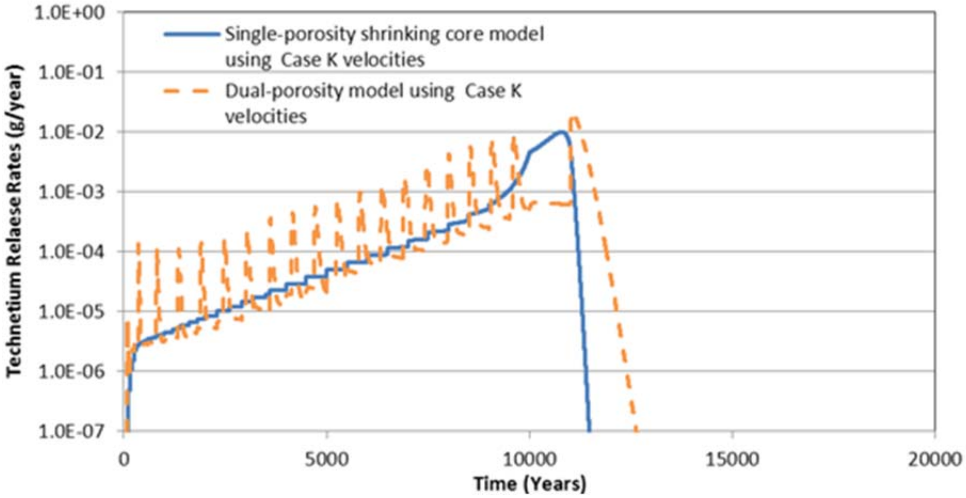

Figure 2: Comparison of Single- and Dual-Porosity Model Cumulative Releases of Technetium for the Base Case

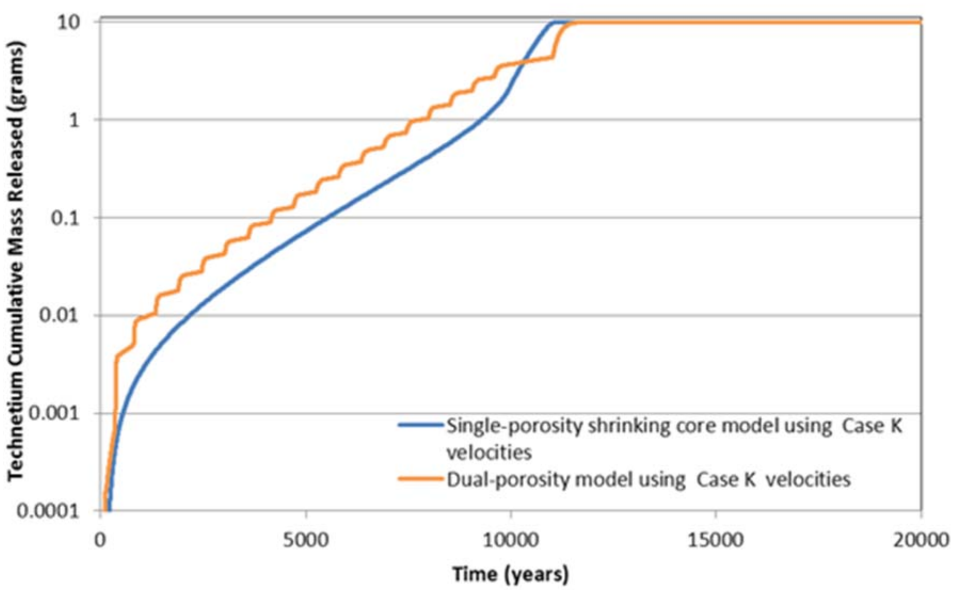

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Figure 3: Comparison of Single- and Dual-Porosity Model Releases of Technetium when the Darcy Velocity is Multiplied by 0.1

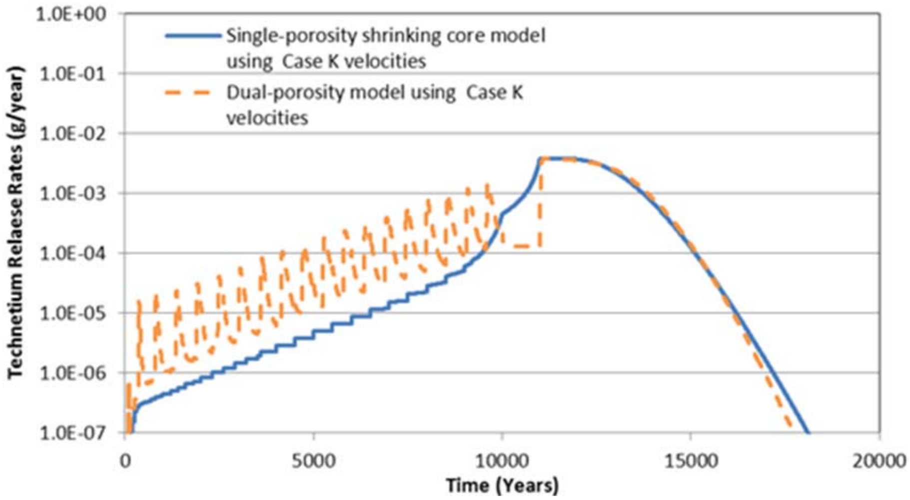

Figure 4: Comparison of Single- and Dual-Porosity Model Cumulative Releases of Technetium when the Darcy Velocity is Multiplied by 0.1

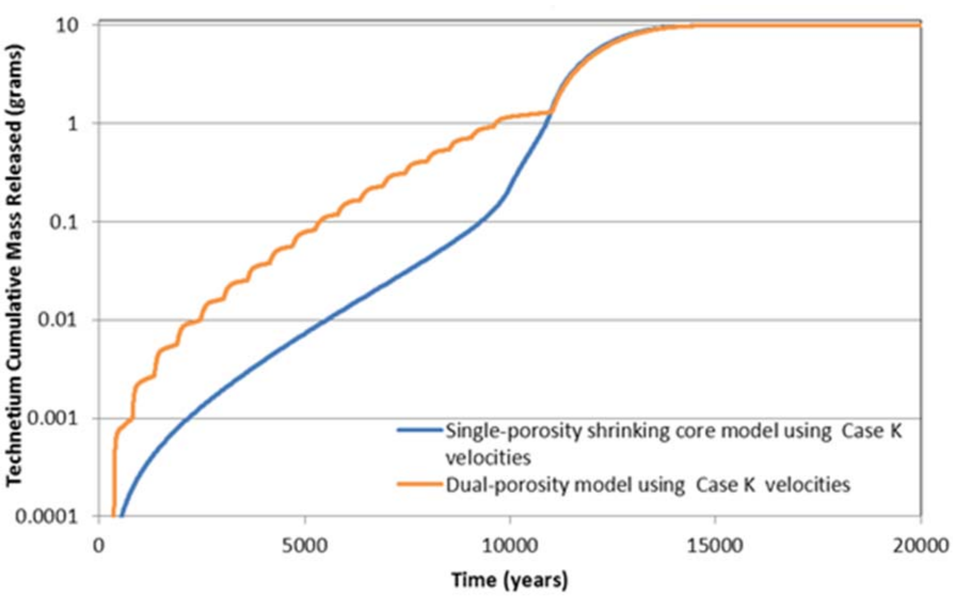

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Figure 5: Comparison of Single- and Dual-Porosity Model Releases of Technetium when the Darcy Velocity is Multiplied by 0.3

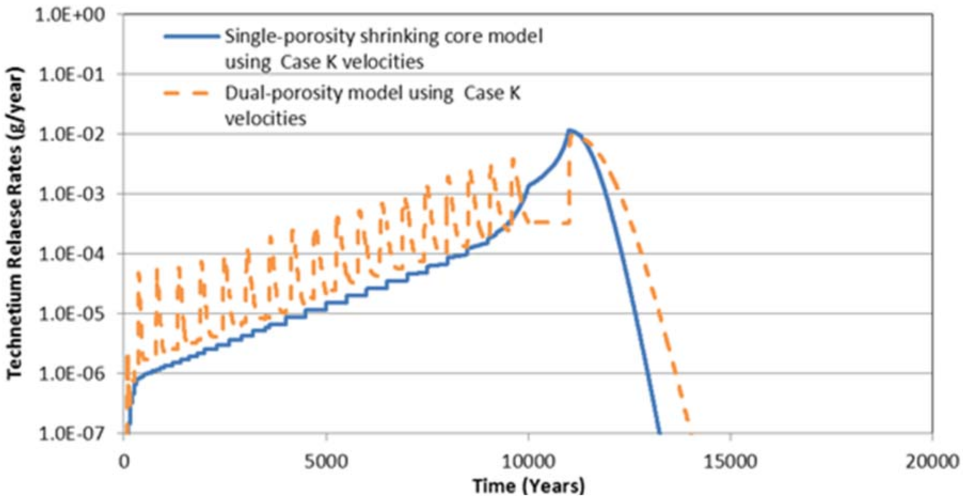

Figure 6: Comparison of Single- and Dual-Porosity Model Cumulative Releases of Technetium when the Darcy Velocity is Multiplied by 0.3

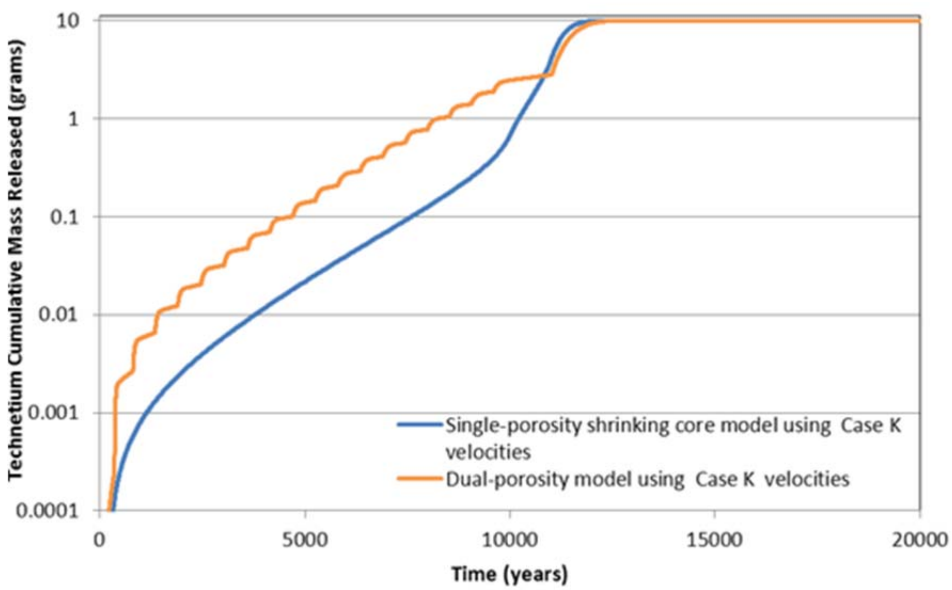

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Figure 7: Comparison of Single- and Dual-Porosity Model Releases of Technetium when the Darcy Velocity is Multiplied by 3

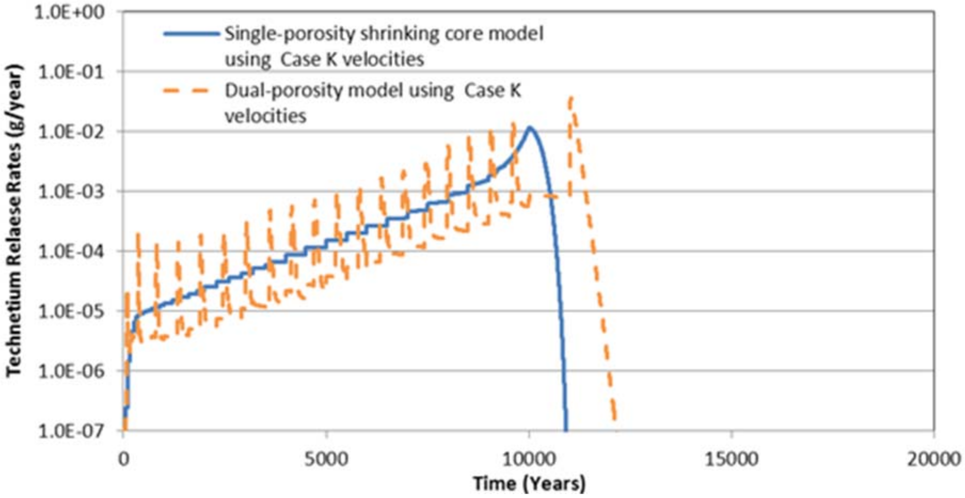

Figure 8: Comparison of Single- and Dual-Porosity Model Cumulative Releases of Technetium when the Darcy Velocity is Multiplied by 3

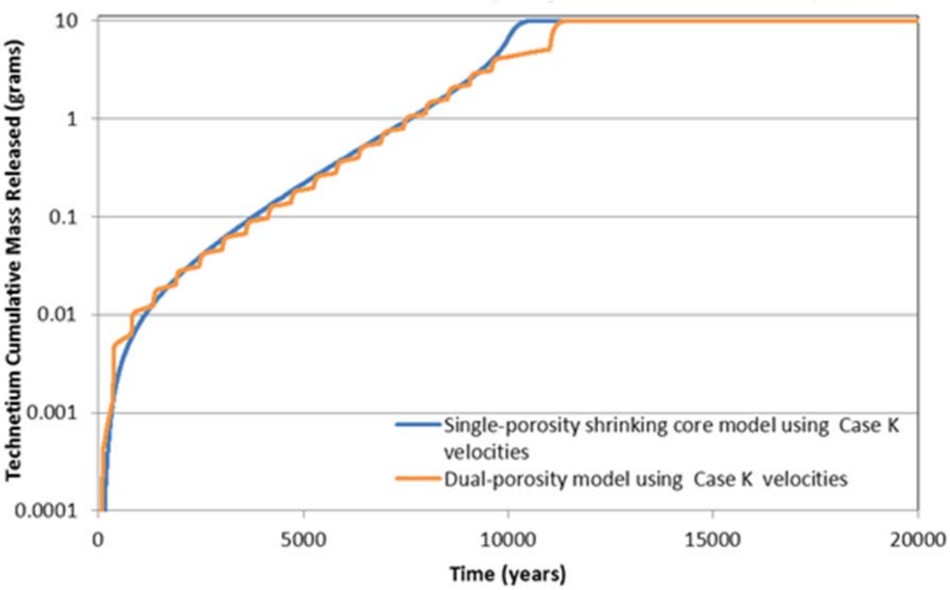

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Figure 9: Comparison of Single- and Dual-Porosity Model Releases of Technetium when the Darcy Velocity is Multiplied by 10

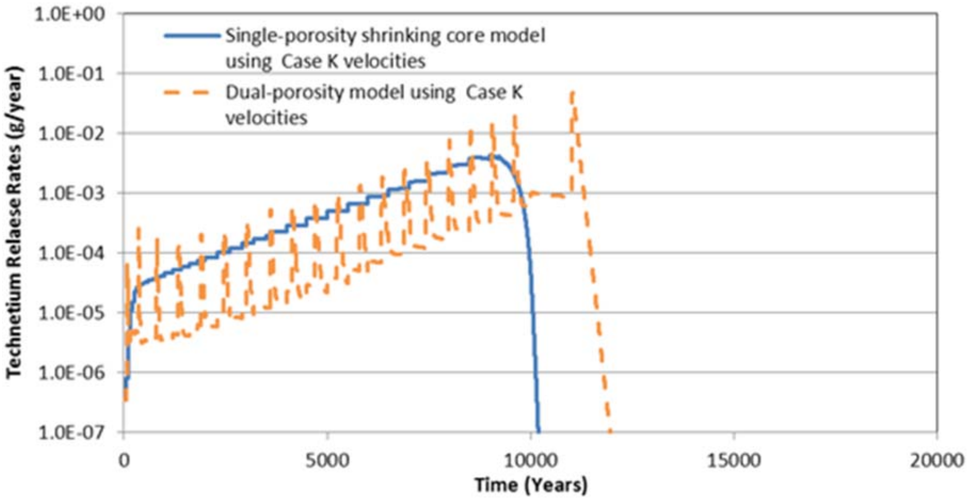

Figure 10: Comparison of Single- and Dual-Porosity Model Cumulative Releases of Technetium when the Darcy Velocity is Multiplied by 10

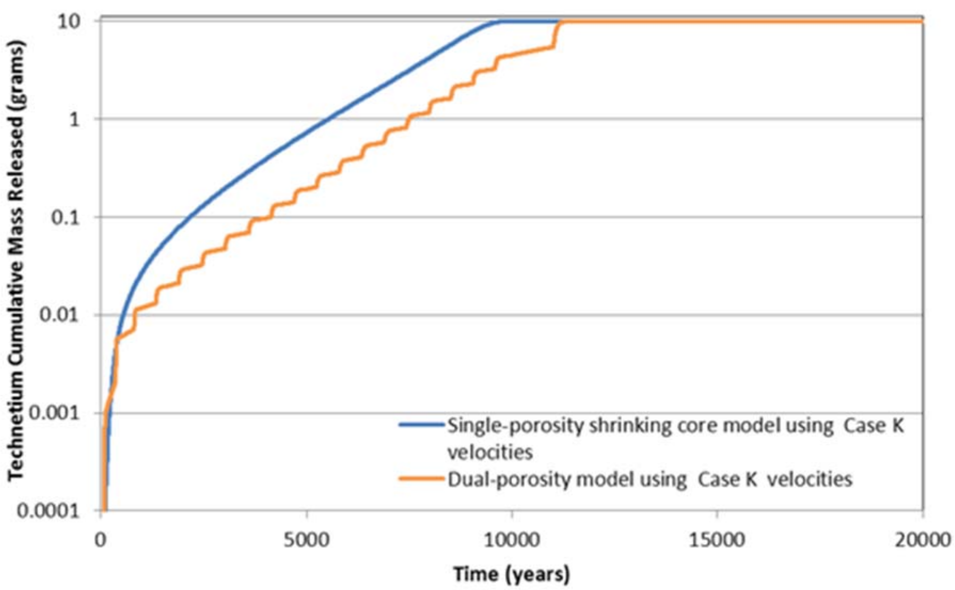

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Figure 11: Comparison of Single- and Dual-Porosity Model Releases of Technetium when there is Flow through Oxidized Zones

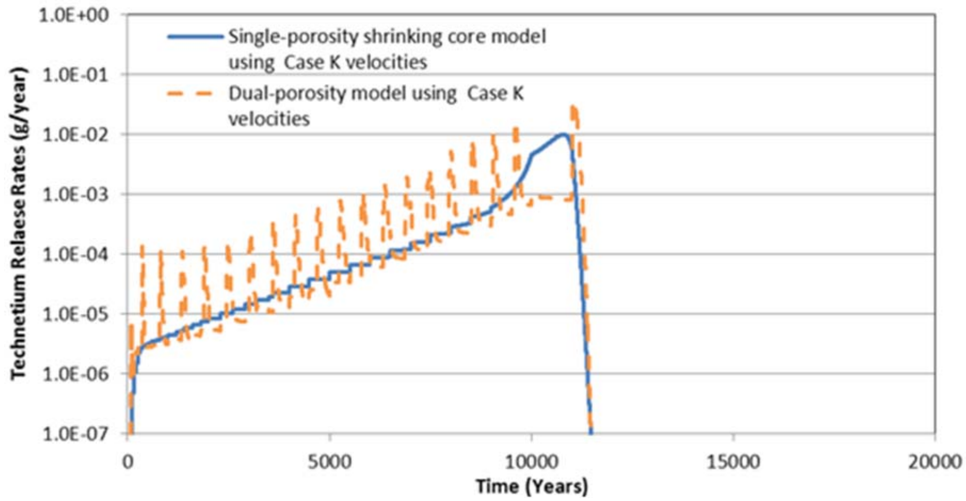

Figure 12: Comparison of Single- and Dual-Porosity Model Cumulative Releases of Technetium when there is Flow through Oxidized Zones

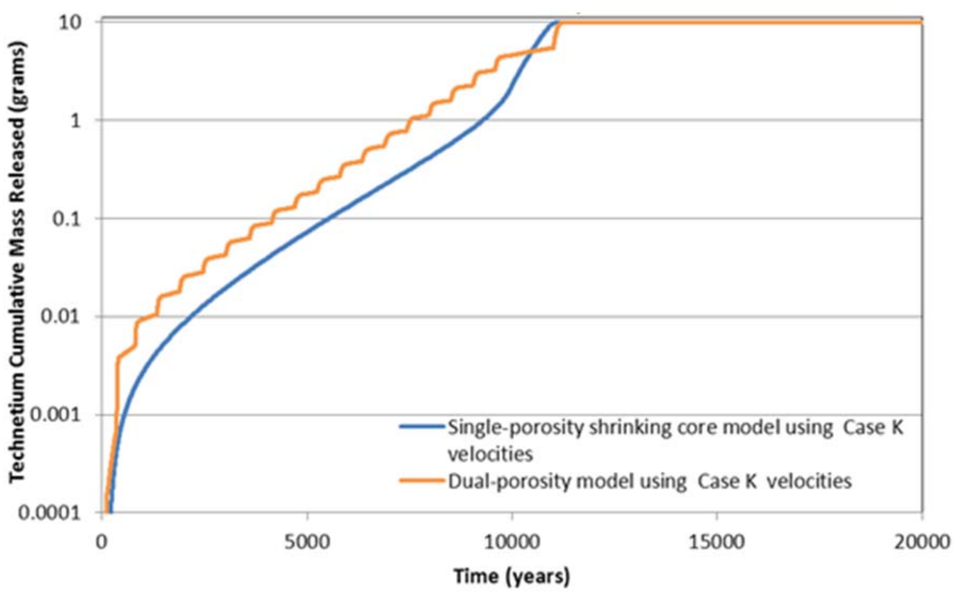

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Figure 13: Comparison of Single- and Dual-Porosity Model Releases of Technetium when the Effective Diffusion Coefficient is Multiplied by 0.1

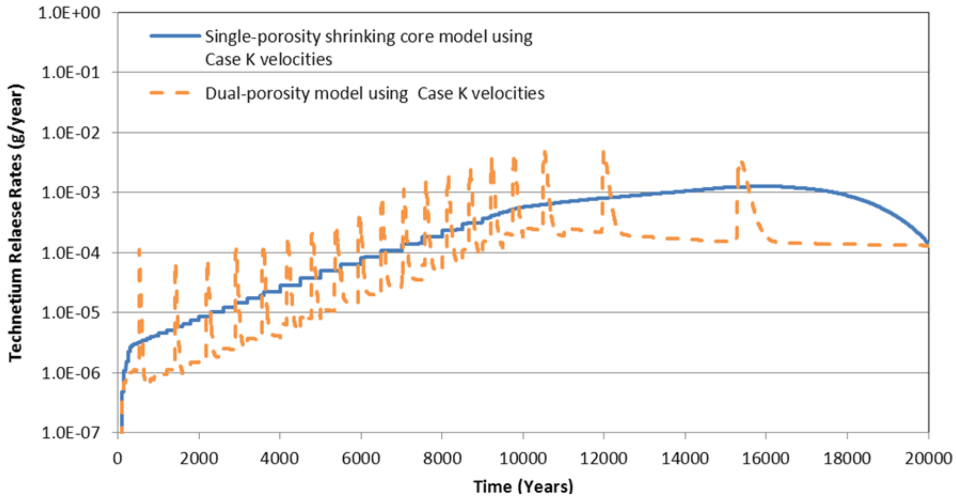

Figure 14: Comparison of Single- and Dual-Porosity Model Cumulative Releases of Technetium when the Initial Fracture Spacing Is Set to 61 Meters (Deff × 0.1)

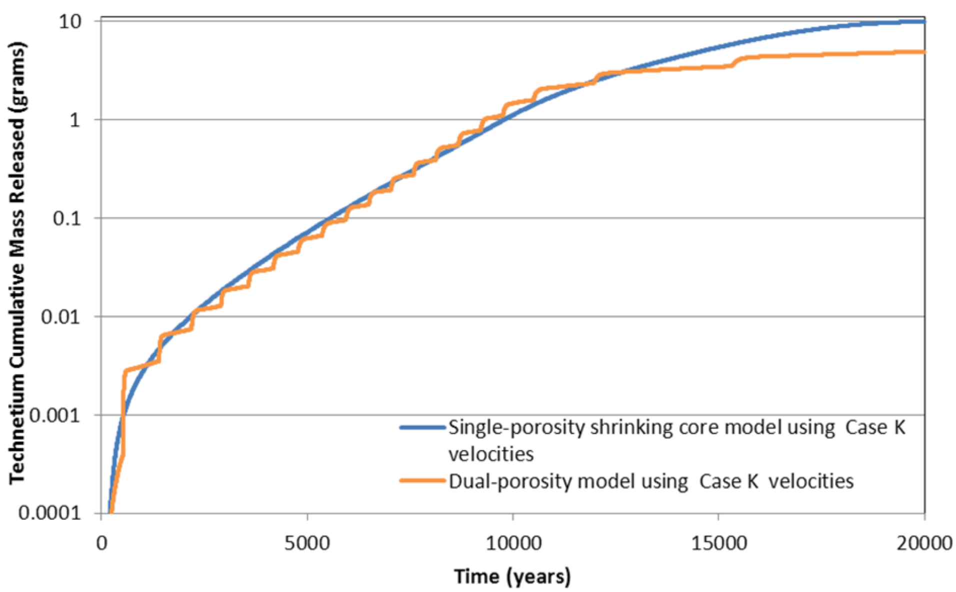

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Figure 15: Comparison of Single- and Dual-Porosity Model Releases of Technetium when the Effective Diffusion Coefficient is Multiplied by 0.3

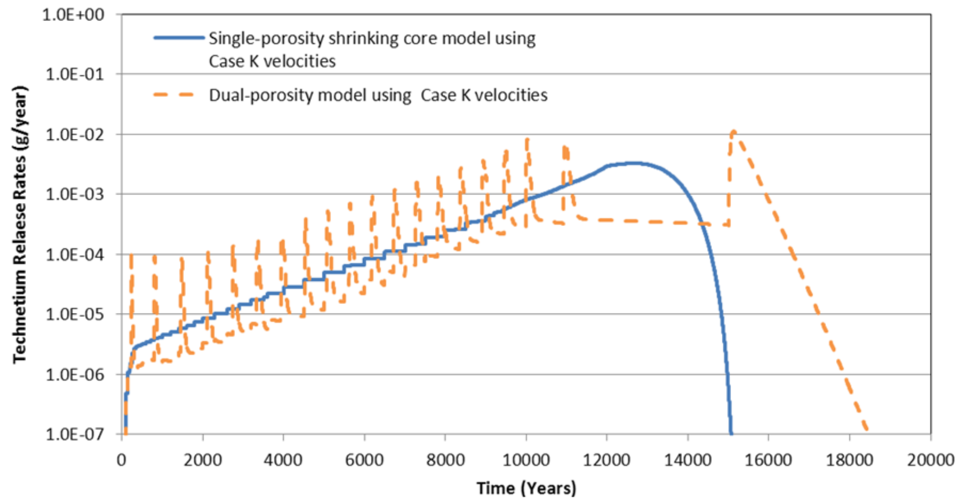

Figure 16: Comparison of Single- and Dual-Porosity Model Cumulative Releases of Technetium when the Effective Diffusion Coefficient is Multiplied by 0.3

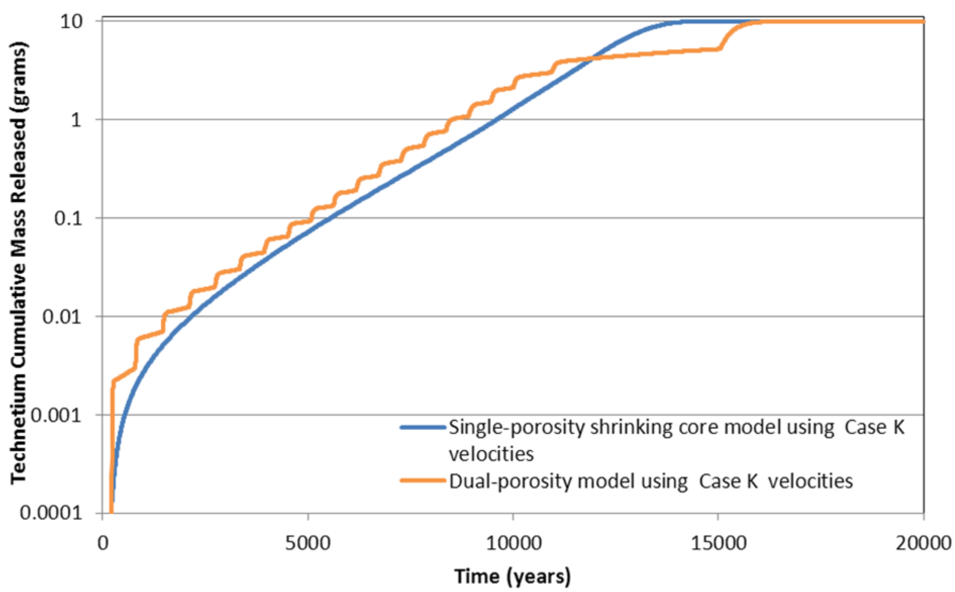

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Figure 17: Comparison of Single- and Dual-Porosity Model Releases of Technetium when the Effective Diffusion Coefficient is Multiplied by 3

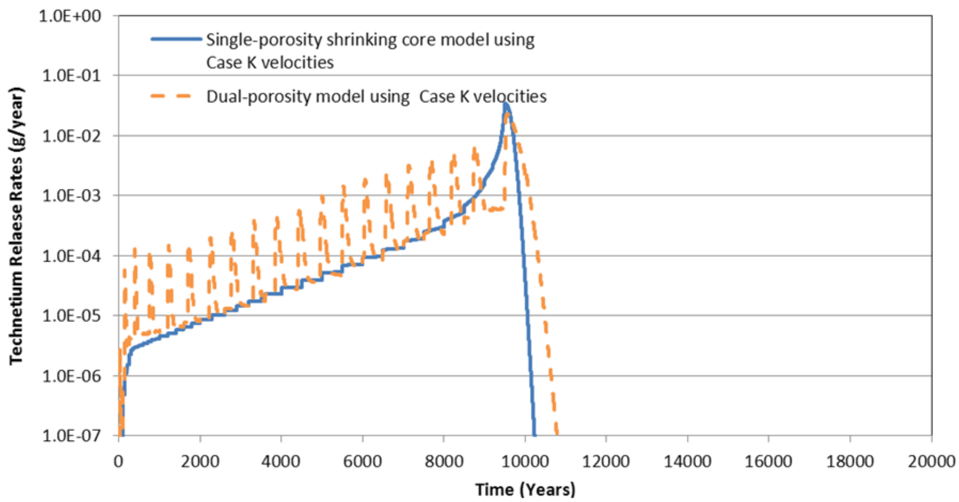

Figure 18: Comparison of Single- and Dual-Porosity Model Cumulative Releases of Technetium when the Effective Diffusion Coefficient is Multiplied by 3

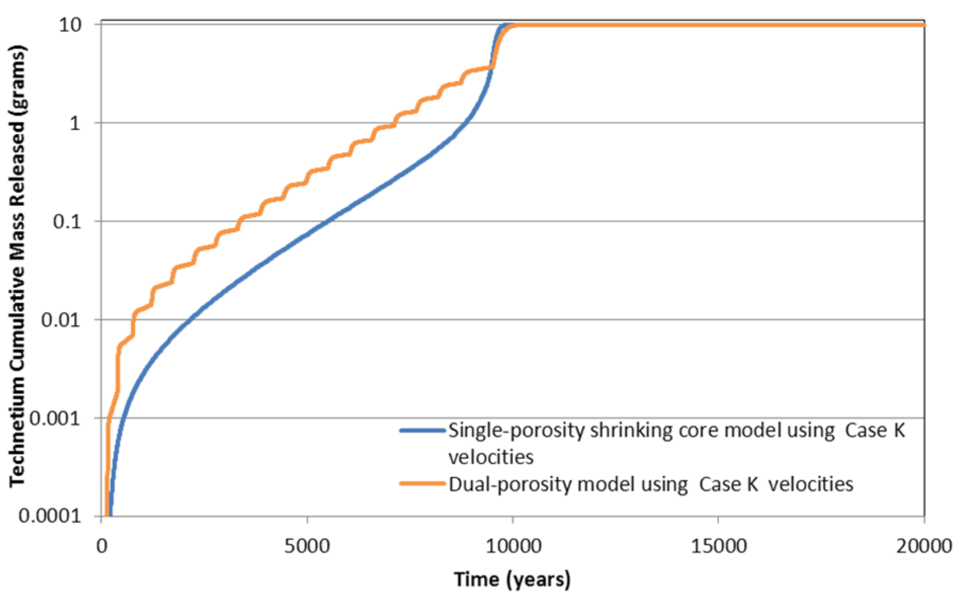

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Figure 19: Comparison of Single- and Dual-Porosity Model Releases of Technetium when the Effective Diffusion Coefficient is Multiplied by 10

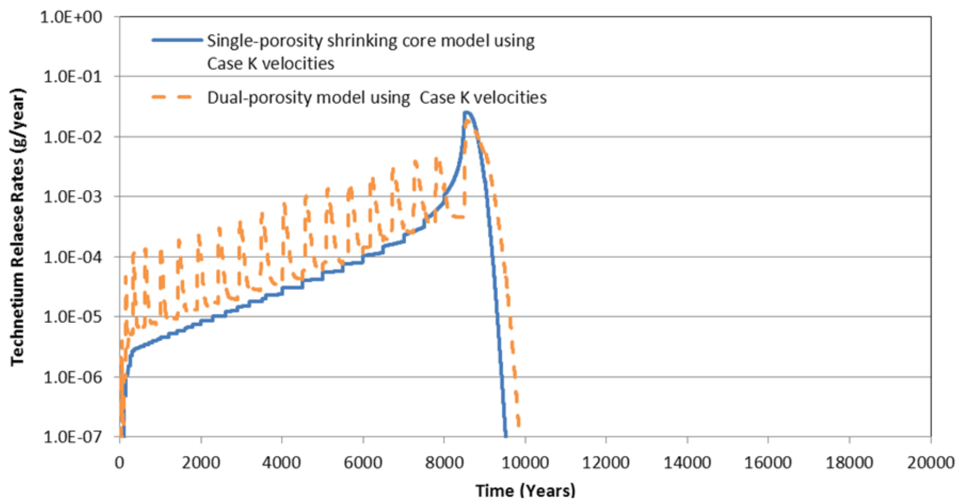

Figure 20: Comparison of Single- and Dual-Porosity Model Cumulative Releases of Technetium when the Effective Diffusion Coefficient is Multiplied by 10

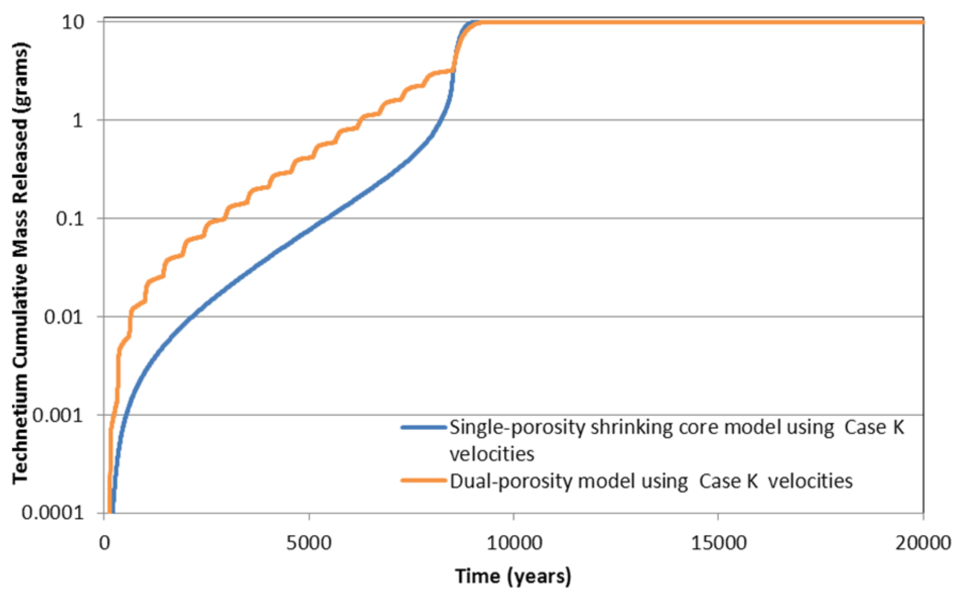

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Figure 21: Comparison of Single- and Dual-Porosity Model Releases of Technetium when the Fracture Spacing Is Set to 0.03m

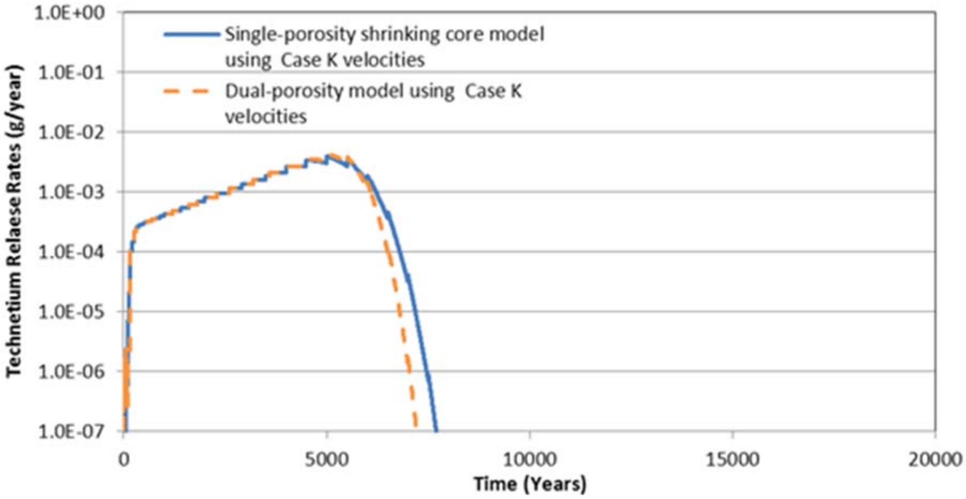

Figure 22: Comparison of Single- and Dual-Porosity Model Cumulative Releases of Technetium when the Fracture Spacing Is Set to 0.03m

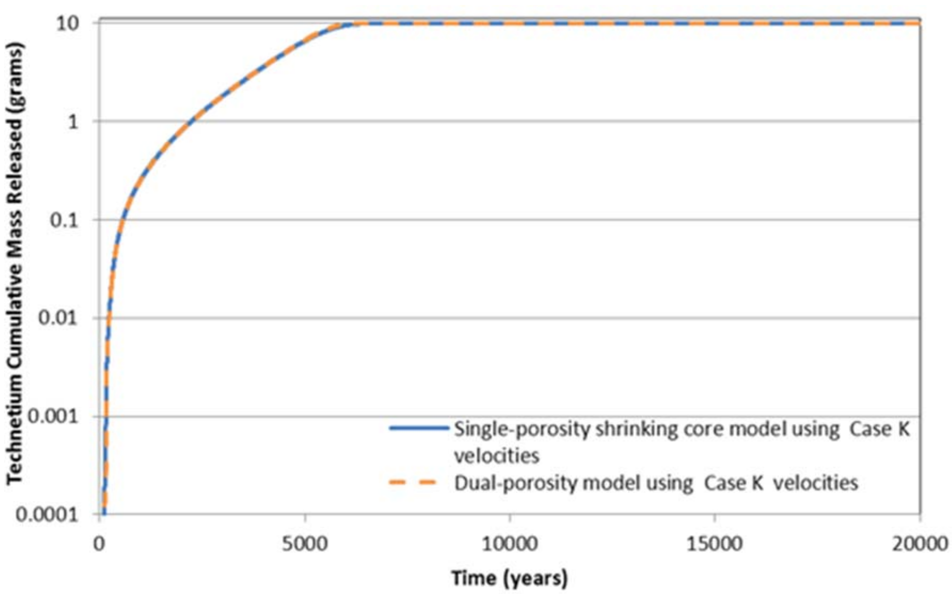

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Figure 23: Comparison of Single- and Dual-Porosity Model Releases of Technetium when the Fracture Spacing Is Set to 0.1m

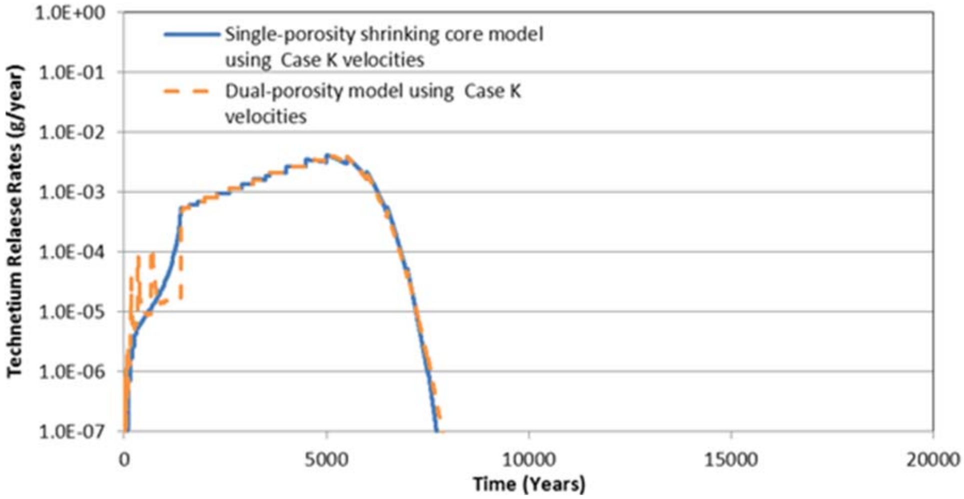

Figure 24: Comparison of Single- and Dual-Porosity Model Cumulative Releases of Technetium when the Fracture Spacing Is Set to 0.1m

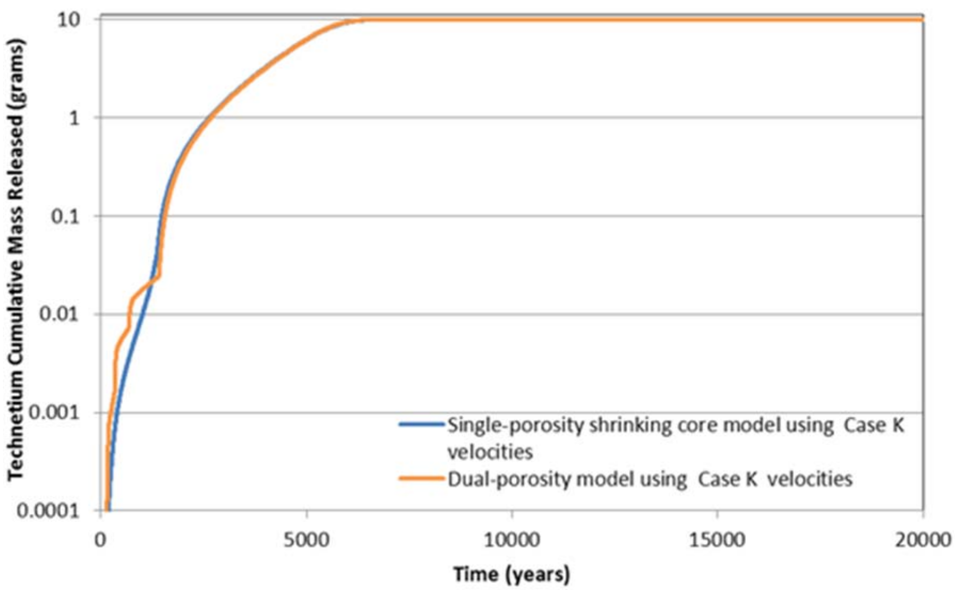

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Figure 25: Comparison of Single- and Dual-Porosity Model Releases of Technetium when the Fracture Spacing Is Set to 0.3 Meters

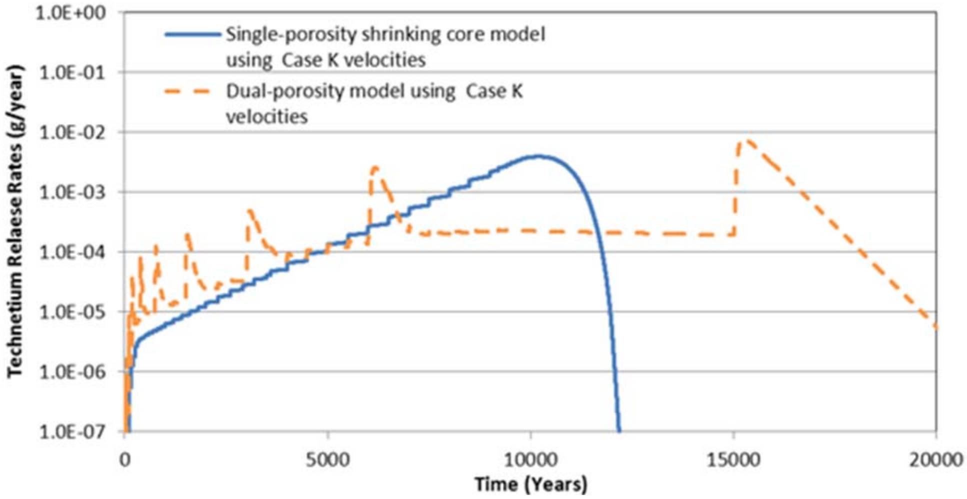

Figure 26: Comparison of Single- and Dual-Porosity Model Cumulative Releases of Technetium when the Fracture Spacing Is Set to 0.3m

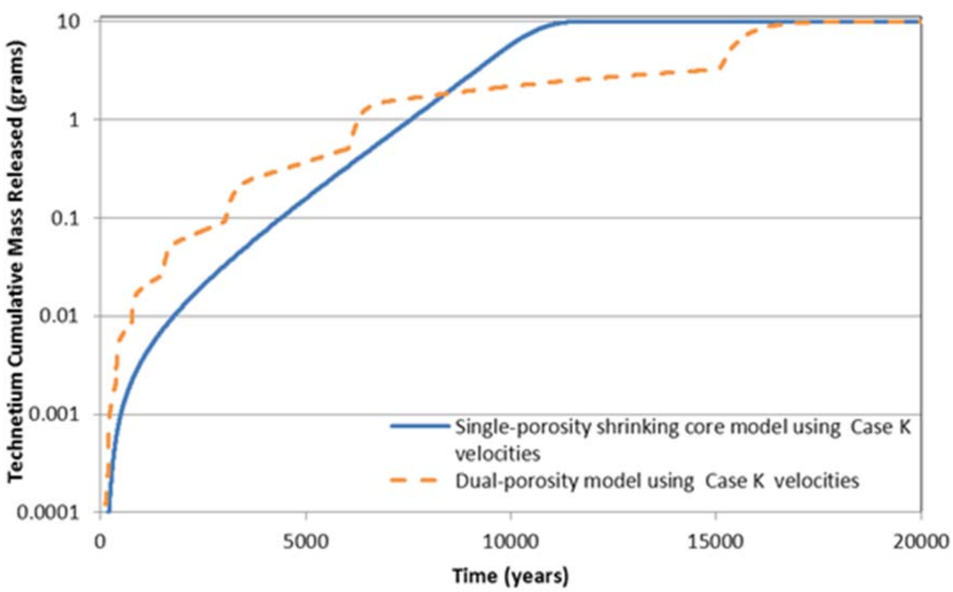

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Figure 27: Comparison of Single- and Dual-Porosity Model Releases of Technetium when the Fracture Spacing Is Set to 1m

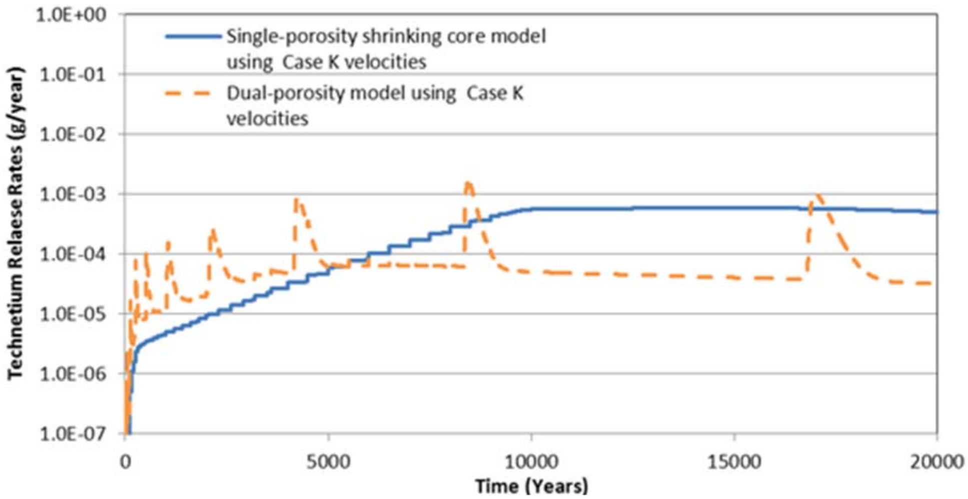

Figure 28: Comparison of Single- and Dual-Porosity Model Cumulative Releases of Technetium when the Fracture Spacing Is Set to 1m

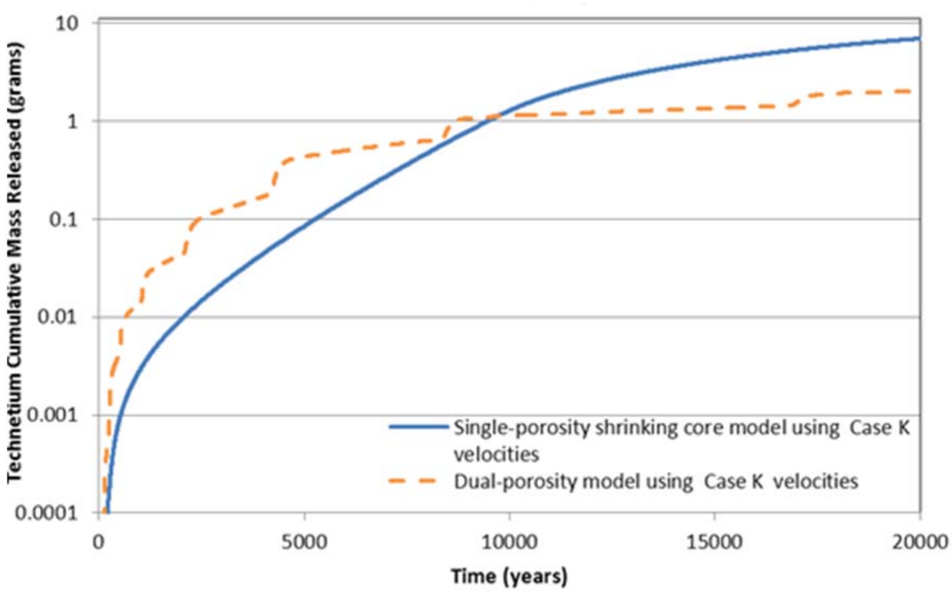

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Figure 29: Comparison of Single- and Dual-Porosity Model Releases of Technetium when the Oxidized Region K_d Is Set to 0.8 ml/g

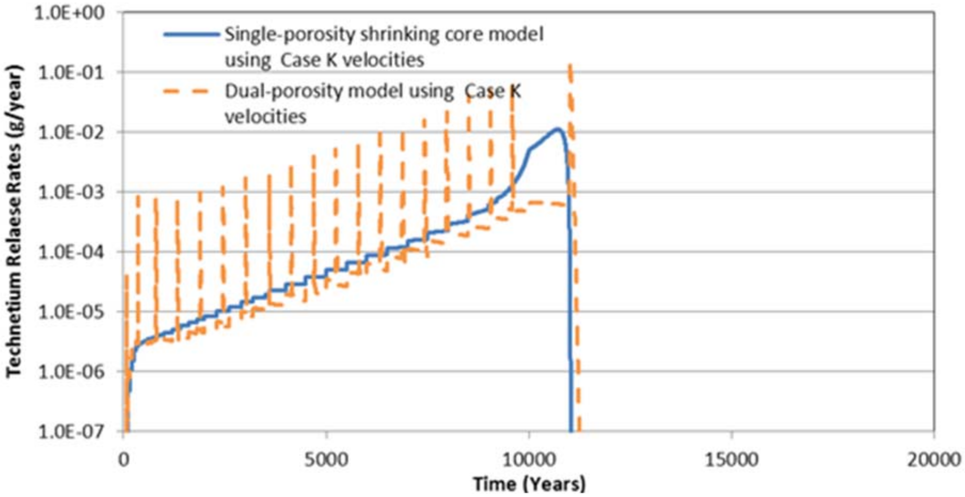

Figure 30: Comparison of Single- and Dual-Porosity Model Cumulative Releases of Technetium when the Oxidized Region K_d Is Set to 0.8 ml/g

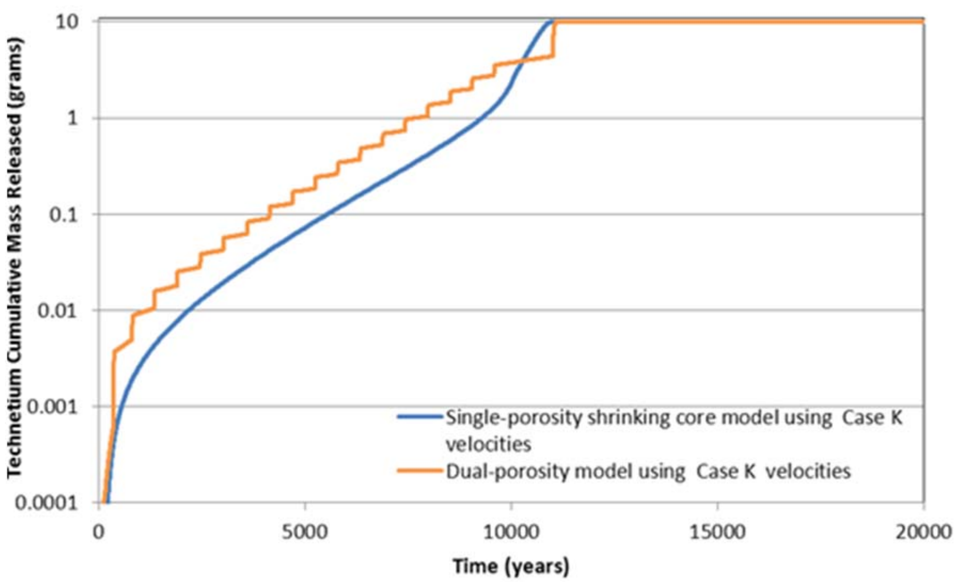

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Figure 31: Comparison of Single- and Dual-Porosity Model Releases of Technetium when the Reducing Region K_d Is Set to 500 ml/g

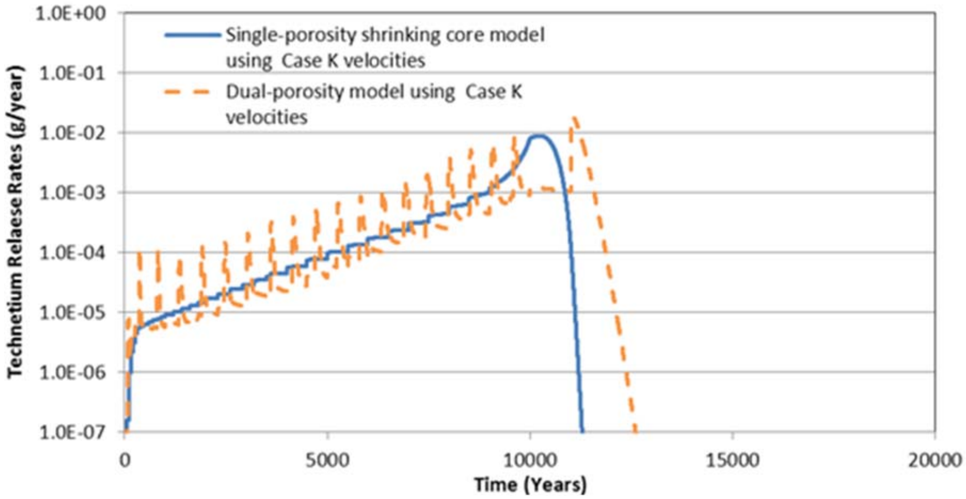

Figure 32: Comparison of Single- and Dual-Porosity Model Cumulative Releases of Technetium when the Reducing Region K_d Is Set to 500 ml/g

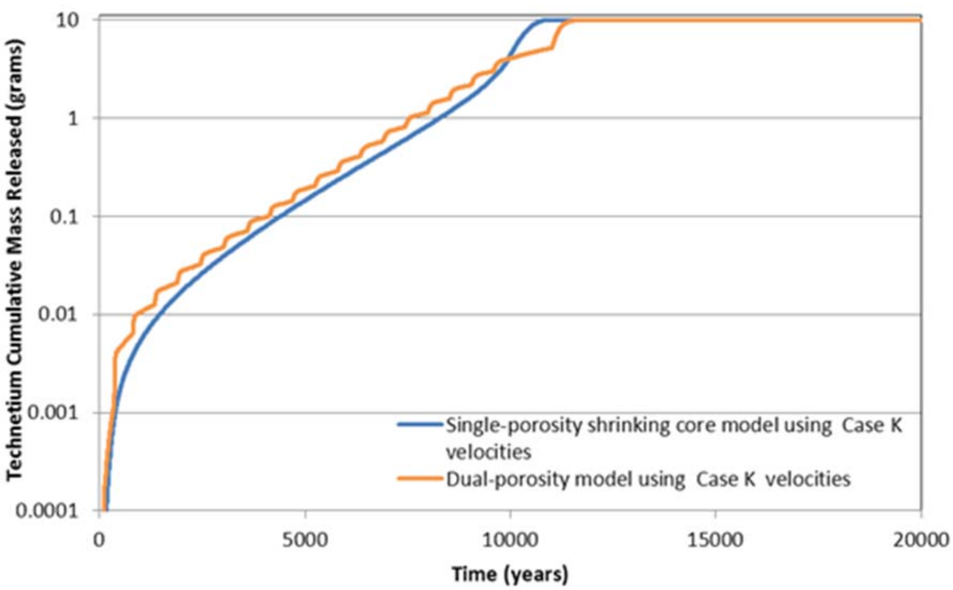

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Figure 33: Comparison of Single- and Dual-Porosity Model Releases of Technetium when the the Reducing Region K_d Is Set to 500 ml/g and the Oxidized Region K_d Is Set to 0.8 ml/g

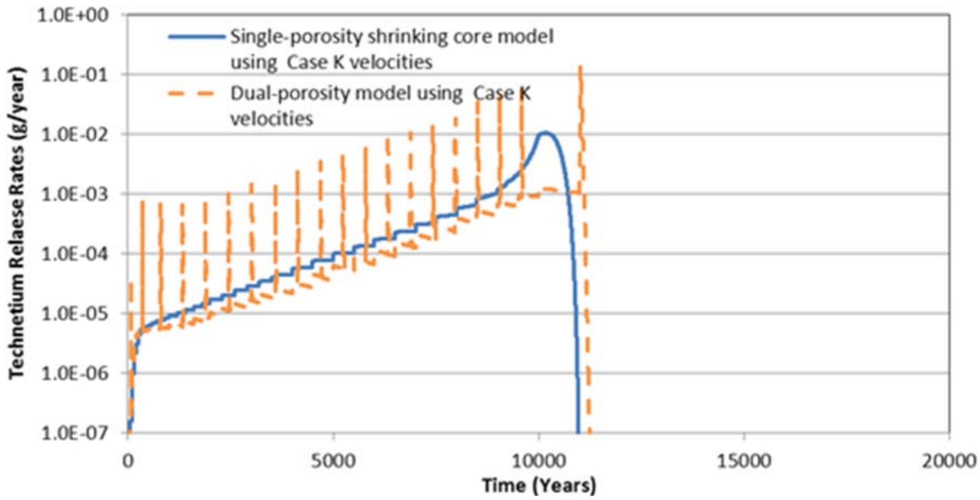
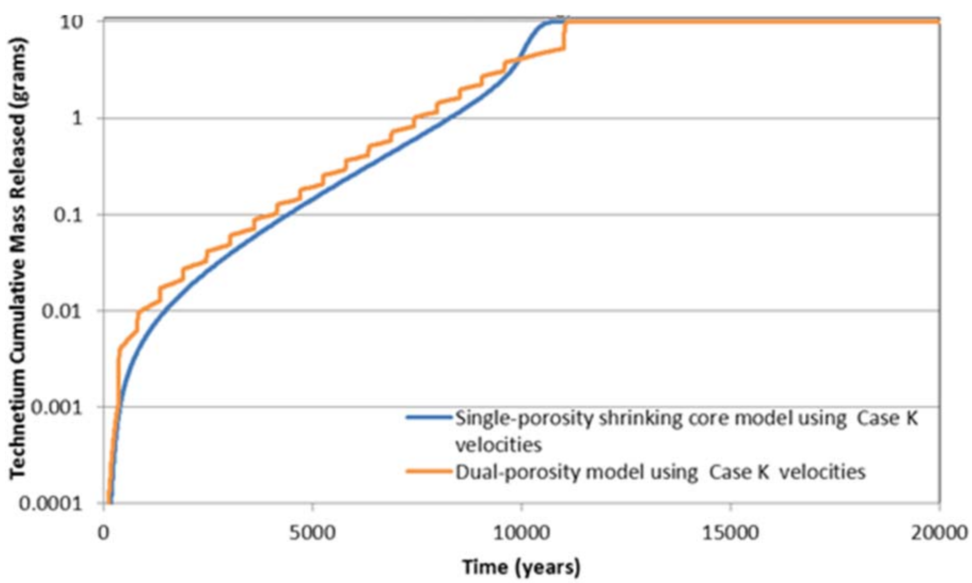


Figure 34: Comparison of Single- and Dual-Porosity Model Cumulative Releases of Technetium when the Reducing Region K_d Is Set to 500 ml/g and the Oxidized Region K_d Is Set to 0.8 ml/g



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