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# PFLOTRAN-RepoTREND Source Term Comparison Summary

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# PFLOTRAN-RepoTREND Source Term Comparison Summary

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## Abstract

Code inter-comparison studies are useful exercises to verify and benchmark independently developed software to ensure proper function, especially when the software is used to model high-consequence systems which cannot be physically tested in a fully representative environment. This summary describes the results of the first portion of the code inter-comparison between PFLOTRAN and RepoTREND, which compares the radionuclide source term used in a typical performance assessment.

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# 4 NOMENCLATURE

| | |
|---|---|
| PWR | pressurized water reactor |
| GW-d/MTHM | gigawatt-days per metric ton of heavy metal |

# 5 INTRODUCTION

Code inter-comparison studies are useful exercises to verify and benchmark independently developed software to ensure proper function, especially when the software is used to model high-consequence systems which cannot be physically tested in a fully representative environment.

PFLOTRAN and RepoTREND are two suites of software used to model nuclear waste repository performance assessment. PFLOTRAN, partially developed at Sandia National Laboratories, is an open source, massively parallel subsurface simulator that solves systems of generally nonlinear partial differential equations describing multiphase, multicomponent, and multiscale reactive flow and transport processes in porous media. RepoTREND, developed by GRS, is a modularly designed suite of modules for the simulation of near-field, far-field, and biosphere domains, specifically designed to model processes in a deep geologic nuclear waste repository.

This summary describes the results of the first portion of the code inter-comparison between PFLOTRAN and RepoTREND, which compares the radionuclide source term used in a typical performance assessment.

# 6 SOURCE TERM COMPARISON SET UP

Common to all geological disposal system models, regardless of the geologic media or repository design, are the waste packages containing nuclear waste. For any geologic disposal system model, proper representation of waste package degradation and waste form dissolution is essential. The first step in the code inter-comparison study was to compare the radionuclide source term, which represents the convolution of the waste-package degradation and waste-form dissolution rates, as well as the solubility of radionuclides in the aqueous phase in contact with the waste form.

The waste packages modeled are assumed to contain spent nuclear fuel. A total of 80 waste packages make up the total inventory for this comparison case. The waste packages are assumed to breach instantly, thus allowing waste form dissolution, and radionuclide release, at the beginning of the simulation. The waste form dissolution rate was set to a fractional rate of $1e^{-7}$ $yr^{-1}$. This means that $1/10000000^{th}$ of the remaining waste form volume dissolves each year. The modeled radionuclide inventory consists of the following decay chain: $^{241}Am$ -> $^{237}Np$ -> $^{233}U$ -> $^{229}Th$ and $^{129}I$. These radionuclides are typically important contributors to potential biosphere dose for waste packages containing PWR spent fuel. The PWR inventory used in this comparison has a burn-up of 60 GW-d/MTHM and is assumed to be 100 yr out of reactor waste. It is emplaced in the repository as 12 PWR assemblies per waste package.

It is noted that PFLOTRAN and RepoTREND treat the waste form radionuclide inventory differently. In PFLOTRAN, each waste form can be explicitly represented, and thus a radionuclide inventory can be defined per waste form in terms of grams-radionuclide per gram-bulk (g/g). However, in RepoTREND, the entire waste inventory is lumped into one value, in terms of g-radionuclide (g). For this reason, radionuclide inventory is given on a waste form basis, as well as a total inventory value representing all 80 modeled waste forms. This 80-package radionuclide inventory is shown in Table 1.

**Table 1 Source term radionuclide inventory**

| | $^{129}$I | $^{241}$Am | $^{237}$Np | $^{233}$U | $^{229}$Th |
|---|---|---|---|---|---|
| **Decay rate [1/s]** | 1.29e-15 | 5.08e-11 | 1.03e-14 | 1.38e-13 | 2.78e-12 |
| **Mass fraction in waste form [g/g]** | 2.17e-4 | 1.01e-3 | 9.72e-4 | 3.01e-8 | 1.03e-11 |
| **Total inventory (g)** | 1.3e5 | 6.07e5 | 5.85e5 | 1.81e1 | 6.19e-3 |

# 7 COMPARISON RESULTS

The radionuclide source term was compared between PFLOTRAN and RepoTREND for a simulation time of 1e$^8$ yr. Both codes calculate the source term as the product of the remaining radionuclide inventory (in grams or moles) and the waste form dissolution rate (yr$^{-1}$) at each time step of the simulation as it runs. For the results presented here, the PFLOTRAN results were extracted from the simulation after a careful time stepping scheme was chosen, but the RepoTREND results were generated separately (not as part of the RepoTREND simulation) using a constant, and small timestep size because extracting the source term value from the output of RepoTREND was too difficult at the time. The value of the timestep size used is unknown at the time of this writing.

Additional differences between the two codes include the algorithm used to solve the partial differential equations that govern radionuclide decay and ingrowth. In PFLOTRAN, the system of equations can be solved for any number of generations iteratively and implicitly in time using Newton's method and LU decomposition. However, for simple decay chains that involve three radionuclide generations or less, and zero initial daughter concentration, PFLOTRAN can use an analytical solution, which is exact. For the results presented here, the analytical solution approach was chosen for the PFLOTRAN source term calculations. At time of this writing, the method that RepoTREND solves the system of equations is unknown.

Figure 1 presents the results of the source term comparison between PFLOTRAN and RepoTREND. The RepoTREND results are labeled as CLAYPOS, because that is the name assigned to the module in RepoTREND responsible for calculating the radionuclide source term. The two codes produce identical values for the radionuclide source term as a function of time, and therefore compare exceptionally well, as long as timestep size is similar between the two codes and the analytical solution approach is used in PFLOTRAN.

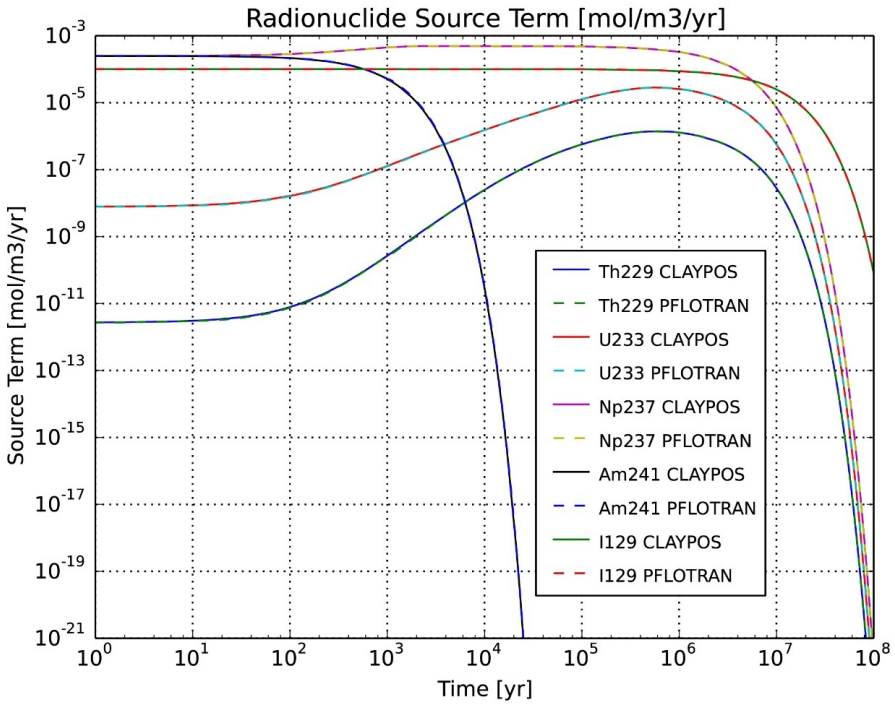


**Figure 1 Radionuclide source term comparison results between PFLOTRAN and RepoTREND (labeled as CLAYPOS). The analytical solution approach is used in PFLOTRAN to solve for decay and ingrowth.**

# 8 TIME STEPPING ISSUES

Initial attempts at the source term comparison showed that the source term calculation is sensitive to the choice of timestep. This is because of two main reasons. The first reason is time truncation error in the iterative numerical algorithm that solves the set of partial differential equations that describe decay and ingrowth (labeled as Type I error). The analytical solution does not suffer from time truncation error, but it is limited to simple decay chains. The second reason is that the source term is a rate which is held constant over the time step. Therefore, taking several small timesteps means the code is updating the source term rate more often than if it took fewer, larger timesteps (labeled as Type II error). This second reason applies to both the implicit, iterative solution method, as well as the analytical solution approach.

As previously noted, the RepoTREND results shown in Figure 1 were generated separately (not as part of the RepoTREND simulation) using a constant, and small timestep size because extracting the source term value from the output of RepoTREND was too difficult at the time. The CLAYPOS results, therefore, minimize the numerical error (both Type I and Type II), but the timestep scheme is not practical for a performance assessment simulation. The PFLOTRAN results in Figure 1, on the other hand, were produced using the following time stepping scheme, which was chosen to minimize Type II error, but still be practical enough for a performance assessment simulation (recall the analytical solution approach has no Type I error). In the following time stepping scheme, note that the timestep size grows gradually.

```
TIME
  FINAL_TIME 1.d08 y
  INITIAL_TIMESTEP_SIZE 1.d-6 y
  MAXIMUM_TIMESTEP_SIZE 1. y at 1. y
  MAXIMUM_TIMESTEP_SIZE 5. y at 10. y
  MAXIMUM_TIMESTEP_SIZE 10. y at 100. y
  MAXIMUM_TIMESTEP_SIZE 50. y at 1000. y
  MAXIMUM_TIMESTEP_SIZE 100. y at 10000. y
  MAXIMUM_TIMESTEP_SIZE 500. y at 100000. y
  MAXIMUM_TIMESTEP_SIZE 1000. y at 500000. y
  MAXIMUM_TIMESTEP_SIZE 2000. y at 700000. y
END
```

If in PFLOTRAN, the iterative, implicit solution approach is used instead of the analytical solution approach, then the comparison is slightly worst due to the introduction of Type I error. Figure 2 presents the source term comparison between PFLOTRAN and RepoTREND using the same time stepping scheme as shown above, but using the iterative, implicit solution approach. Note that the $^{241}$Am source term is slightly larger in PFLOTRAN than the RepoTREND results.

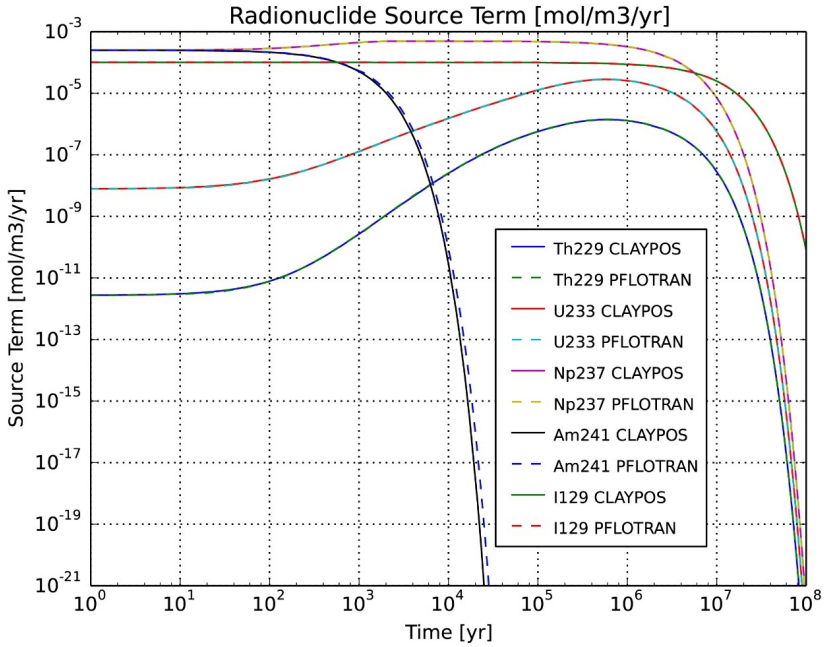


**Figure 2 Radionuclide source term comparison results between PFLOTRAN and RepoTREND (labeled CLAYPOS). The implicit, iterative solution approach is used in PFLOTRAN to solve for decay and ingrowth, with slowly growing timestep size.**

As a final example, Type II error is introduced if the timestep is allowed to grow too large, too fast, and too suddenly. Using the following time stepping in PFLOTRAN demonstrates this rapid timestep growth, and the results are shown in Figure 3.

```
TIME
  FINAL_TIME 1.d08 y
  INITIAL_TIMESTEP_SIZE 1.d-6 y
  MAXIMUM_TIMESTEP_SIZE 1. y at 1. y
  MAXIMUM_TIMESTEP_SIZE 10. y at 10. y
  MAXIMUM_TIMESTEP_SIZE 100. y at 100. y
  MAXIMUM_TIMESTEP_SIZE 1000. y at 1000. y
  MAXIMUM_TIMESTEP_SIZE 5000. y at 10000. y
END
```

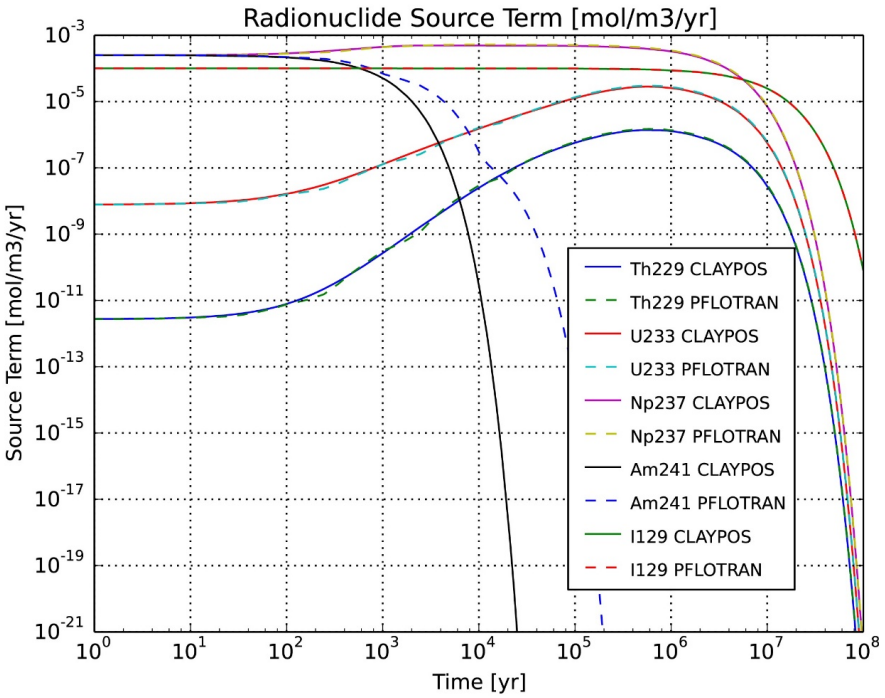


**Figure 3 Radionuclide source term comparison results between PFLOTRAN and RepoTREND (labeled CLAYPOS). The implicit, iterative solution approach is used in PFLOTRAN to solve for decay and ingrowth, with rapid increases in the timestep size.**

Note that the difference in the $^{241}$Am source term is much larger, and each time PFLOTRAN suddenly increases the timestep size, there is a bend, or hump in the curve. The bend is clearly seen for $^{241}$Am, but can also be seen for $^{233}$U and $^{229}$Th at early times. This is not ingrowth. Besides $^{241}$Am, which has a fast decay rate, the Type II error introduced at early times does not seem to affect source term values for later times when the radionuclide decay rate is very slow.

# 9 CONCLUSIONS

This summary describes the results of the first portion of the code inter-comparison between PFLOTRAN and RepoTREND, which compares the radionuclide source term used in a typical performance assessment. The two codes compare exceptionally well when timestep size is small and constant in RepoTREND, and when PFLOTRAN uses slowly increasing timestep size with the analytical solution approach.

However, initial comparison attempts showed that the radionuclide source term is sensitive to timestep size in PFLOTRAN (and probably RepoTREND, although this has not been explicitly shown) due to Type I and Type II error. While the analytical approach to solve the partial differential equations that govern decay and ingrowth in PFLOTRAN can only suffer from Type II error, it is limited to simple decay chains that have three radionuclide generations or less. To model more complex decay chains, the implicit, iterative solution approach must be used, but it additionally suffers from Type I error as well.

In order to minimize both Type I and Type II numerical errors, it is important to carefully choose the time stepping scheme so that timestep size slowly increases over the simulation time. This can be manually controlled in PFLOTRAN by setting the maximum timestep size at pre-determined times in the simulation. However, timestep size cannot be controlled in RepoTREND due to the current automatic timestep algorithm currently implemented in RepoTREND. Without control over the timestep size, the source term will suffer from numerical error. Thus, it is recommended that RepoTREND also implement a timestep control algorithm that can accept user guidance.

Recall that the RepoTREND results shown in all figures were generated separately (not as part of the RepoTREND simulation) using a constant and small timestep size because extracting the source term value from the output of RepoTREND was too difficult at the time. A further study is required where the RepoTREND source term is calculated during the simulation and the results are extracted from the simulation output, with the timestep size reported.

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