Comparison of Two Numerical Modeling Codes for Hydraulic and Transport Calculations in the Near Field

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Abstract

In past years, the Slovenian PA/SA team has performed many generic PA/SA studies for the future Slovenian LILW repository, most recently a Special Safety Analysis (SSA) for the Krško site. The modeling approach taken was to split the problem into three parts: near-field (detailed model of the repository), far-field (i.e., geosphere) and biosphere. In the SSA, the code used to perform near-field calculations was HYDRUS-2D. Recently, the team has begun to cooperate with CEA/Saclay and, as a result of this cooperation, began investigations into using the Alliances numerical platform for near-field calculations in order to compare the overall approach and calculated results. This article presents the comparison between these two codes for a silo-type repository that was considered in the SSA. We will present the physical layout and characteristics of the repository and develop and implement a hydraulic and transport model of the repository in Alliances. Some analysis of the sensitivity to mesh fineness and to a simulation timestep has been performed and will also be presented. The compared quantity will be the output flux of radionuclides on the boundary of the model. We will compare the results and comment on differences/similarities.

1. Introduction

In the previous years the Slovenian Performance Analysis/Safety Assessment (PA/SA) team has performed many studies for the future low and intermediate level waste repository. The most recent one was a Special Safety Analysis (SSA) (Petkovšek et al., 2006) for three proposed preliminary designs, including a silo-type subsurface repository.

In the SSA, the code used to perform near-field calculations was HYDRUS-2D (HYDRUS, 2013). However, the team investigated the possibility of using Alliances (Montarnal et al., 2006) - a numerical platform co-developed by CEA, ANDRA and EDF for the numerical simulation of nuclear waste disposal - to perform near-field transport and other calculations. In the decision process one of the tasks was to repeat the near-field calculations for the silo-type repository with Alliances and compare results with those obtained with HYDRUS.

2. System Description

The silo-type subsurface repository is buried in a silty soil. It is a cylindrical concrete structure with a 12.8 m inner radius, 0.9 m thick walls and an inner height of 33 m after closure. The space inside the repository is filled with layers of 70 waste-containing concrete blocks with external
dimensions 2.45m × 2.45m × 3.2m. Any remaining space between the blocks and silo walls is filled with drainage gravel. The whole of the repository lies underneath the water table so the hydraulic conditions in the soil and in the repository are saturated. There is a general horizontal hydraulic gradient of 0.00118 in the aquifer.

Since the hydraulic flow is driven by an external horizontal gradient and the repository is completely below the water table, the end effects of top and bottom of the silo can be neglected and the model simplifies to horizontal flow in 2D. The red rectangle in figure 1 marks the boundary of the 40 m × 20 m modeled domain. The other three red lines mark the boundaries between different regions of the repository; from the center outwards: the boundary between waste containing blocks and drainage gravel, the boundary between drainage gravel and a silo wall, and the boundary between a silo wall and silt. The direction of the gradient was chosen so that the water flows from left to right.

3. Hydraulic Calculations

The hydraulic conditions are saturated, so the only parameters needed are the saturated hydraulic conductivities of materials, listed in Table 1.

Barrier degradation was simulated by artificially changing the hydraulic conductivities of materials at specified times. Up to 10,000 years, there is no degradation. It is assumed that between 10,000 and 100,000 years, the silo wall degrades. This is simulated by increasing the hydraulic conductivity of the silo wall to that of the silt. After 100,000 years, the containers also degrade so that their hydraulic conductivity increases to that of the silt.
Table 1. Saturated hydraulic conductivities of materials.

<table>
<thead>
<tr>
<th>Material</th>
<th>$K_s$ [m/s]</th>
</tr>
</thead>
<tbody>
<tr>
<td>Silt</td>
<td>$10^{-7}$</td>
</tr>
<tr>
<td>Concrete (silo and containers)</td>
<td>$10^{-10}$</td>
</tr>
<tr>
<td>Drainage Gravel</td>
<td>$10^{-3}$</td>
</tr>
</tbody>
</table>

Figure 2 shows the Darcy velocity field in the un-degraded state. The velocity field looks right, but when the Darcy velocities in the middle of the repository were compared, there were large discrepancies between the Alliances and HYDRUS results, as can be seen in Table 2.

Table 2. Darcy velocities (in m/s) in the middle of the repository.

<table>
<thead>
<tr>
<th>Degradation</th>
<th>Alliances</th>
<th>HYDRUS</th>
</tr>
</thead>
<tbody>
<tr>
<td>0</td>
<td>$4.96\times10^{-18}$</td>
<td>$1.74\times10^{-13}$</td>
</tr>
<tr>
<td>1</td>
<td>$6.32\times10^{-16}$</td>
<td>$5.44\times10^{-13}$</td>
</tr>
<tr>
<td>2</td>
<td>$6.31\times10^{-13}$</td>
<td>$1.19\times10^{-10}$</td>
</tr>
</tbody>
</table>

It turned out that the calculations for the SSA were simplified. In the attempts to calculate the hydraulic field and transport with HYDRUS, the team ran into problems. The difference between hydraulic conductivities of drainage gravel and concrete is 7 orders of magnitude. This caused numerical instabilities on the boundaries between these two materials, especially in the bottom right corner region of the repository. The team worked around this by assigning the hydraulic conductivity of silt to the drainage gravel, effectively substituting the drainage gravel with silt and reducing the difference to 3 orders of magnitude.
The hydraulic field was recalculated with the two hydraulic conductivities that were used for the SSA. As shown in Table 3, the comparison between Darcy velocities in the middle of the repository shows a much better agreement between Alliances and HYDRUS.

Table 3. Darcy velocities (in m/s) in the middle of the repository, 2 hydraulic conductivities.

<table>
<thead>
<tr>
<th>Degradation</th>
<th>Alliances</th>
<th>HYDRUS</th>
<th>Ratio</th>
</tr>
</thead>
<tbody>
<tr>
<td>0</td>
<td>$3.95 \times 10^{-14}$</td>
<td>$1.74 \times 10^{-13}$</td>
<td>4.4</td>
</tr>
<tr>
<td>1</td>
<td>$1.94 \times 10^{-13}$</td>
<td>$5.44 \times 10^{-13}$</td>
<td>2.8</td>
</tr>
<tr>
<td>2</td>
<td>$1.18 \times 10^{-10}$</td>
<td>$1.19 \times 10^{-10}$</td>
<td>1.0</td>
</tr>
</tbody>
</table>

4. Transport Calculations

The processes considered were advection, diffusion, dispersion, sorption and radioactive decay (including chains). The total radionuclide flux through the downstream (right) boundary of the modeled domain was measured, and the height and position of the flux peak compared to the results obtained with HYDRUS.

Of all the radionuclides in the inventory, only those whose half-lives are long enough that they stand a chance of exiting from the repository were considered. The full inventory and transport parameters for the considered radionuclides can be found in (Kalin et al., 2010).

The calculations in SSA stopped at $10^6$ years because that was all that was required for the study and because of the slow calculation speed of HYDRUS. However, since peaks for some radionuclides were not reached, it was decided to run calculations up to $10^{10}$ years. By that time, all the radionuclides have either decayed or have been washed out of the system. It is assumed that the waste is uniformly spread between the containers and within each container and that it is completely dissolved in water at the beginning of the simulation. This is unrealistic, since in reality, the radionuclides would first need to be leeched from solids, but it is conservative. A previous unpublished study determined that all concentrations everywhere are far below solubility limits, so these are reasonable assumptions.

4.1. Mass Balance and Timestep Sensitivity Analysis

All the timesteps were performed using the fully implicit scheme (Press et al., 2007), which is unconditionally stable - one can increase timestep between successive steps (and decrease the real time for simulations) almost arbitrarily. But there’s a trade-off in the loss of accuracy. To determine the optimum balance between computational speed and accuracy, a timestep sensitivity analysis was performed.

A strongly sorbed radionuclide, $^{129}$I, was used to check accuracy. Decay was turned off, which means that at the end of the simulation, the cumulative flux (time integral of flux) exiting the model must match the amount put in the repository at the start of simulation.
Figure 3 shows the results of calculations. The vertical axis is the ratio of cumulative flux to starting amount. One can see that even with relatively large timesteps, the mass balance is off only by 15%. In most other cases the accuracy is better than 3%. For further calculations, such a discretization was chosen that the mass balance for $^{129}$I is accurate to 0.5% (far above what’s needed for the comparison), but still relatively little real time is needed to perform the calculations.

![Figure 3. Timestep sensitivity.](image)

### 4.2. Results and Comparison

First, the mass balances were checked by turning off the decay. All the cumulative fluxes were within 1% of the input activities.

Figure 4 shows the results with decay and Table 4 contains the numerical comparison between results obtained with Alliances and with HYDRUS. The “Ratio” column is the ratio of HYDRUS peak flux height versus Alliances peak flux height.
As noted earlier, the calculations in the SSA were done only for the first $10^6$ years. Considering that the peaks in the case of the $^{238}$U chain occur at $1.25 \times 10^7$ y in Alliances results, these sets of results cannot be compared. Similarly in the case of the $^{241}$Am chain, the peaks in Alliances results occur at $1.13 \times 10^7$ y (except for the $^{241}$Am itself, which rapidly decays into $^{237}$Np), so again the results cannot be compared.

The fluxes of $^{137}$Cs, $^{90}$Sr, and $^{63}$Ni are so low that they can be neglected; indeed, in the SSA they were not even considered.
The difference in $^{14}$C peak fluxes is over 7 orders of magnitude, but this can be explained by decay. The peak in Alliances results occurs at $7.8 \times 10^5$ y before peak in HYDRUS results, while the half-life of $^{14}$C is $5.7 \times 10^3$ y. The difference in peak times is thus 136 half-lives, and much more $^{14}$C decays in the HYDRUS case.

In any case, the peak fluxes for $^{14}$C are very low - on the order of $10^{-11}$ bq/y for Alliances and $10^{-17}$ bq/y for HYDRUS. At values this low, there’s already a chance of numerical problems, not to mention that values this low are completely undetectable in nature and pose absolutely no problem as far as doses are concerned.

Next are the $^{36}$Cl and $^{94}$Nb, where the HYDRUS results are around an order of magnitude higher. No immediate explanation was found for this.

Values for $^{129}$I, $^{99}$Tc and $^{59}$Ni, however, match very well - within a factor of two. This is very good for the purposes of PA/SA, as $^{129}$I and $^{59}$Ni are exactly the two radionuclides that contribute the most to the total dose.

This leaves us with $^3$H, where the difference is three orders of magnitude. $^3$H is not sorbed, i.e., not retarded. Additionally, it has a short half-life of only 12 y, so a small difference of 5% in peak position (at around 220 y) can alter the peak height by a factor of two. Recalling also that there’s still an appreciable difference in hydraulic conductivities between different regions and that these differences caused problems in HYDRUS, it was decided to investigate the effect of mesh on $^3$H transport.

### 5. Sensitivity to Mesh Density

To check sensitivity to mesh density, the whole calculation (from mesh generation onwards) was repeated with two finer meshes. Figure 5 shows the details of the mesh in the critical region — the bottom right corner of the repository.

![Figure 5. Mesh details.](image)

From left to right the following meshes are depicted: “NetGen2D, very fine mesh” (“NGv”, the mesh used for the calculations so far), “Triangles, fine mesh” (“TRf”) and “Triangles, very fine mesh” (“TRv”). The calculations were run for 1000 years for $^3$H and for $10^{10}$ years for $^{129}$I.
Figure 6 shows the effects of different meshes for $^3$H. Different timestep discretizations were tried, but this did not appreciably affect the results. However, the position and height of the peak are strongly influenced by the mesh details. It seems that the finer the mesh is, the later the peak occurs. In other words, the coarser mesh appears to overestimate the Darcy velocities.
Figure 7 shows the effects of different meshes for $^{129}$I. Note that in this case, only the default timestep discretization was used, as the calculation for the TRv mesh took almost five days on an Intel 2 GHz Core 2 Duo with 800 MHz FSB and 2 GB of memory.

The coarser mesh again has the effect of allowing a contaminant to appear earlier (and to disappear later). The position of the peak does not change (this cannot be verified in the figure, but was checked in the output data). This is understandable, as the majority of the contaminant appears after $10^5$y, when the barriers have all degraded and there is no difference in hydraulic conductivities.

6. Conclusions and Further Work

From the study of mesh sensitivity we can conclude that, especially for the short-lived radionuclides, the mesh details can have a strong influence on the results. For future calculations, the density of the mesh should be increased in the critical areas (around the boundaries between materials) and kept about the same elsewhere. It would be impractical to use the TRv mesh, as the transport calculations for all radionuclides would take around three months.

On the other hand, for the significant radionuclides ($^{59}$Ni and $^{129}$I), the results are very close to the ones obtained by HYDRUS, meaning that in some cases the coarser mesh may be adequate. In any case, the sensitivity to mesh details needs to be investigated further before performing “real” calculations.

It would also be interesting to run transport calculations with the hydraulic fields from three hydraulic conductivities and compare them with results with two hydraulic conductivities. If anything, the mesh details should be even more influential, as the differences between hydraulic conductivities are much bigger.

Last, but not least, Alliances had an enormous advantage in speed for this type of problem, i.e., the calculation of Darcy velocity field and transport in saturated conditions. It took a few days of calculations to produce results for $10^6$ years with HYDRUS and a few hours to produce results for $10^{10}$ years with Alliances - an advantage of $10^5$ in the ratio of real time to simulation time.

At the time when the comparison was performed, HYDRUS did not have any means to automate transitions between degradations - human intervention was necessary to save radionuclide concentration fields produced with one level of degradation, calculate Darcy velocity field for the next level of degradation, and use the saved concentration fields as the initial conditions for concentrations. Since Alliances uses Python (Python, 2013) as the underlying language, it was easy to automate the transitions, thus no human intervention was necessary to obtain final results. This capability was used in an unpublished study and allowed us to perform sensitivity analysis, not only to physical parameters, but also to the mesh, as it is possible to programmatically generate mesh.
References