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Studies to Investigate the Relative Significance of Parameter and Model Uncertainty in Calculating the Radiological Risks via Groundwater from a Geological Disposal Facility

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Foreword

The work presented in this report was developed within the Integrated Project PAMINA: **P**erformance **A**ssessment **M**ethodologies **I**N **A**pplication to Guide the Development of the Safety Case. This project is part of the Sixth Framework Programme of the European Commission. It brings together 25 organisations from ten European countries and one EC Joint Research Centre in order to improve and harmonise methodologies and tools for demonstrating the safety of deep geological disposal of long-lived radioactive waste for different waste types, repository designs and geological environments. The results will be of interest to national waste management organisations, regulators and lay stakeholders.

The work is organised in four Research and Technology Development Components (RTDCs) and one additional component dealing with knowledge management and dissemination of knowledge:

- In RTDC 1 the aim is to evaluate the state of the art of methodologies and approaches needed for assessing the safety of deep geological disposal, on the basis of comprehensive review of international practice. This work includes the identification of any deficiencies in methods and tools.
- In RTDC 2 the aim is to establish a framework and methodology for the treatment of uncertainty during PA and safety case development. Guidance on, and examples of, good practice will be provided on the communication and treatment of different types of uncertainty, spatial variability, the development of probabilistic safety assessment tools, and techniques for sensitivity and uncertainty analysis.
- In RTDC 3 the aim is to develop methodologies and tools for integrated PA for various geological disposal concepts. This work includes the development of PA scenarios, of the PA approach to gas migration processes, of the PA approach to radionuclide source term modelling, and of safety and performance indicators.
- In RTDC 4 the aim is to conduct several benchmark exercises on specific processes, in which quantitative comparisons are made between approaches that rely on simplifying assumptions and models, and those that rely on complex models that take into account a more complete process conceptualization in space and time.

The work presented in this report was performed in the scope of RTDC 2.

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PAMINA Task 2.2.B Model Uncertainty
Topic 1: Studies to Investigate the Relative
Significance of Parameter and Model Uncertainty in
Calculating the Radiological Risks via Groundwater
from a Geological Disposal Facility

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Executive Summary

The risk to future populations from a geological repository for radioactive waste is a quantity which is subject to large uncertainties because of the long timescales involved (up to 1 million years). These include data uncertainties, model uncertainties, and uncertainties about future evolution of the system and future human actions. The work reported in this Technical Note had two objectives relating to issues concerning model uncertainty when using probabilistic methods to handle data uncertainty.

- First, to gain an understanding of the relative importance of the complexity of a computer model (and its associated uncertainty), when that model is used probabilistically, compared to the magnitude of the uncertainties and variabilities in the values of the parameters that describe the processes that are significant to safety.
- Secondly, to consider the additional modelling uncertainty that arises because of the probabilistic nature of the calculations when the expectation value of a performance measure such as mean risk is dominated by only a few realisations contributing a high risk because adverse values of several parameters have been sampled at once.

A probabilistic version of the 'insight' model (a simple analytic approximation) for estimating risks from the groundwater pathway for a repository was developed as a very fast static simulation using GoldSim. The results of this model were compared with the results of a full dynamic simulation of radionuclide transport, also using GoldSim.

The insight model was found in most cases to give good agreement with the full dynamic simulation model. The calculation of a mean risk against time curve for the insight model was very coarsely handled. However, provided enough realisations were run, in the region around the peak of this curve, the errors arising from this coarseness were found to cancel each other out as the results from individual realisations were accumulated. This is because parameter uncertainty, rather than model uncertainty, is the main control on the shape of this mean risk curve in this region. This suggests that when carrying out probabilistic calculations to represent parameter uncertainties which are large, the model uncertainty introduced by using a very coarse model such as the insight model, may in fact be rather insignificant. This would need to be assessed on a case-by-case basis, but suggests there may be little benefit in over-complicating a model if it is to be used in a probabilistic calculation with large parameter uncertainty.

It was also shown that in cases where results are poorly converged with a modest number of realisations (e.g. risks from short-lived daughters of long-lived parents such as ^{226}Ra), a more accurate estimate of a quantity such as the peak risk could be obtained from a million realisations of the approximate model than for a thousand realisations of the full dynamic model. It may be, therefore, that convergence problems can be tackled by implementing a very fast, coarse version of a model such as the insight model and running a very large number of realisations.

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1 INTRODUCTION

NDA Radioactive Waste Management Directorate (RWMD) has the responsibility for implementing the governments policy for a deep geological repository for the UK's higher activity radioactive waste¹. The risk to future populations from a geological repository for radioactive waste is calculated subject to large uncertainties because of the long timescales involved (up to 1 million years). As repository systems make use of natural barriers to radionuclide migration, as well as engineered barriers, it is often necessary to manage large uncertainties (and variabilities) in parameters that represent natural processes – and these uncertainties can be several orders of magnitude.

Uncertainties in data can be quantified in terms of 'probability density functions' (PDFs) that give the relative likelihood of different parameter values. With the uncertainty quantified as PDFs, a probabilistic assessment can be carried out using Monte-Carlo methods. In such an assessment, a computer model is run many times (each run is called a *realisation*) with different sets of parameter values. In each realisation, the values of the parameters are chosen at random from the PDFs representing the range of possible values. In the UK, regulatory guidance leads the developer to such a probabilistic approach, to calculate the expectation value (mean value) of risk and compare it with a regulatory target. The work reported in this Technical Note investigates some issues relating to model uncertainty, specifically to the use of a probabilistic approach.

NDA has developed a total system model using the GoldSim software [1] for assessing the risk from the groundwater pathway for a repository system which relies for safety on physical and chemical containment in the engineered system and a long travel time, dilution and dispersion in the geosphere. This model is developed from a similar model (using the MASCOT software [2]) for the Generic post-closure Performance Assessment (GPA) published by Nirex in 2003 [3] which was not a site-specific assessment.

NDA believes there is value in modelling the system at a number of levels of complexity, and has also developed simple analytical ('insight') models that demonstrate a high-level understanding of the key features of the system, and which give approximate agreement with the results of deterministic calculations made with the total system model.

The objective of this task is to use both the models above in a probabilistic context, in order to gain an understanding of the relative importance of the complexity of a computer model (and its associated uncertainty), when that model is used probabilistically, compared to the magnitude of the uncertainties and variabilities in the values of the parameters that describe the processes that are significant to safety.

A secondary objective is to consider the additional modelling uncertainty that arises because of the probabilistic nature of the calculations when the expectation value of a performance measure such as mean risk is dominated by only a few realisations contributing a high risk because adverse values of several parameters have been sampled at once.

Section 2 describes the basics of the insight model, and how it has been implemented in GoldSim. Section 3 presents some results using the probabilistic

¹ NDA RWMD incorporated staff from Nirex from April 2007. Some examples quoted in this note refer to work that Nirex carried out prior to this date.

insight model, comparing them with results from a full dynamic simulation with GoldSim. Conclusions are drawn in Section 4.

2 GOLDSIM IMPLEMENTATION OF THE INSIGHT MODEL

In the Nirex 97 assessment for a potential repository at Sellafield in Cumbria in the UK, a section is presented (Section 8, Volume 3 [4]) in which simple analytic expressions, rather than complex numerical models, are used to provide insight into the results of the complex models, and provide a simple understanding of which parameter values and processes have a key impact on risk. Confidence can be provided in the results of the complex numerical models by showing that similar results may be obtained on the basis of very simple models. The simple analytic model used in Nirex 97 for estimating peak risks from the groundwater pathway have been referred to as the 'insight' model.

The insight model has been used in the past in a deterministic mode to estimate risks from the groundwater pathway (see subsection 2.1 below). Subsection 2.2 describes the implementation of the insight model as a static simulation using GoldSim. The standard insight model calculates *peak* values of performance measures such as risk. Some additional programming was required to accumulate a *time history* of the expectation value (mean value) of such performance measures that can be directly compared with the results of a full dynamic simulation. This was implemented in FORTRAN as a Dynamic Link Library (DLL) that GoldSim calls during each realisation (see subsection 2.3).

This implementation has the following advantages:

- It can be run probabilistically, so that the uncertainty in parameter values can be taken into account.
- It is extremely quick to run (a few seconds for a 1000 realisations) compared to carrying out the full dynamic simulation with GoldSim or MASCOT. It is therefore possible to carry out probabilistic calculations with many more realisations (e.g. 1 million) than is feasible for the full dynamic simulation. This is useful for investigating cases where the calculation is poorly converged with a modest number of realisations (see Section 3.3).
- The parameters in the insight model can be linked to data already present in a GoldSim model e.g. the current implementation directly makes use of the data for the GoldSim implementation of the GPA reference case [3] without modification.
- The model can be readily altered to carry out very quick initial scoping calculations e.g. for analysis of alternative options, or alternative geologies.

2.1 The Insight Model

The insight model is a method for estimating the peak value, time of peak and spread, given a simple distribution of a performance measure such as risk in time, based on the moments of that distribution [4].

The amount of repository-derived radionuclides received in the biosphere depends upon the initial inventory, I (Bq) of radionuclide in the repository. However, not all this initial inventory will reach the biosphere because of the barriers in the disposal system. The longer it takes a particular radionuclide to pass through a barrier, the more time it has to decay, and hence the smaller the amount released to the next

barrier. Therefore each barrier will transmit only a certain fraction of the amount of radionuclide that reaches it.

This means the total amount of a radionuclide leaving the engineered system would be $I \times N$ where N is the (dimensionless) source-term release fraction, determined by the radionuclide solubility, the degree to which it is sorbed onto repository materials, the groundwater flux through the repository and radioactive decay in the engineered system.

The total amount transmitted through the geosphere and therefore entering the biosphere is $I \times N \times G$ where G is the (dimensionless) release fraction from the geosphere, determined by the path length, the groundwater travel time, the retardation factor, the dispersion length and radioactive decay in the geosphere.

However, this amount of radionuclide will not all enter the biosphere at once, it will be spread over time as a result of both source-term spreading and geosphere spreading.

The maximum flux of radionuclide, F_p , into the biosphere is therefore given by the proportionality:

$$F_p \propto \frac{ING}{\sigma} \quad (1)$$

where σ (years) is the spreading time.

The spreading time, σ , has two components, source-term spreading, σ_s (years), and geosphere spreading, σ_g (years). The source-term and geosphere spreading times combine in such a way that the overall spreading time is given by the square root of the sum of the squares of the spreading times:

$$\sigma = \sqrt{\sigma_s^2 + \sigma_g^2} \quad (2)$$

To calculate the potential peak annual individual risk, R_p , arising from this radionuclide flux, it is necessary to multiply by a flux-dose conversion factor, known as a biosphere factor, B_t (Sv Bq^{-1}) which can be calculated for each radionuclide, and the dose-risk conversion factor, r , which is a constant (0.06 Sv^{-1}) for all radionuclides. A constant of proportionality, S , is also required – a good approximation is provided using a value of about 0.4. Therefore:

$$R_p \approx \frac{SrB_tING}{\sqrt{\sigma_s^2 + \sigma_g^2}} \quad (3)$$

This approximation for estimating the peak risk (the ‘insight’ model) is discussed in more detail in Section 8 of Volume 3 of Nirex 97 [4]. Equations that relate the quantities described here to specific physical and chemical properties are given in [4] and are not repeated here.

2.2 GoldSim Implementation

The GoldSim implementation of the insight model is structured to take the probabilistic data from a full time-dependent GoldSim model. The current implementation is based on the data from the GPA reference case [3], and contains the following containers directly from the GoldSim version of the GPA model:

Materials – defines the species and the properties of the groundwater. In addition, a vector is defined which is the decay constants for the radionuclides.

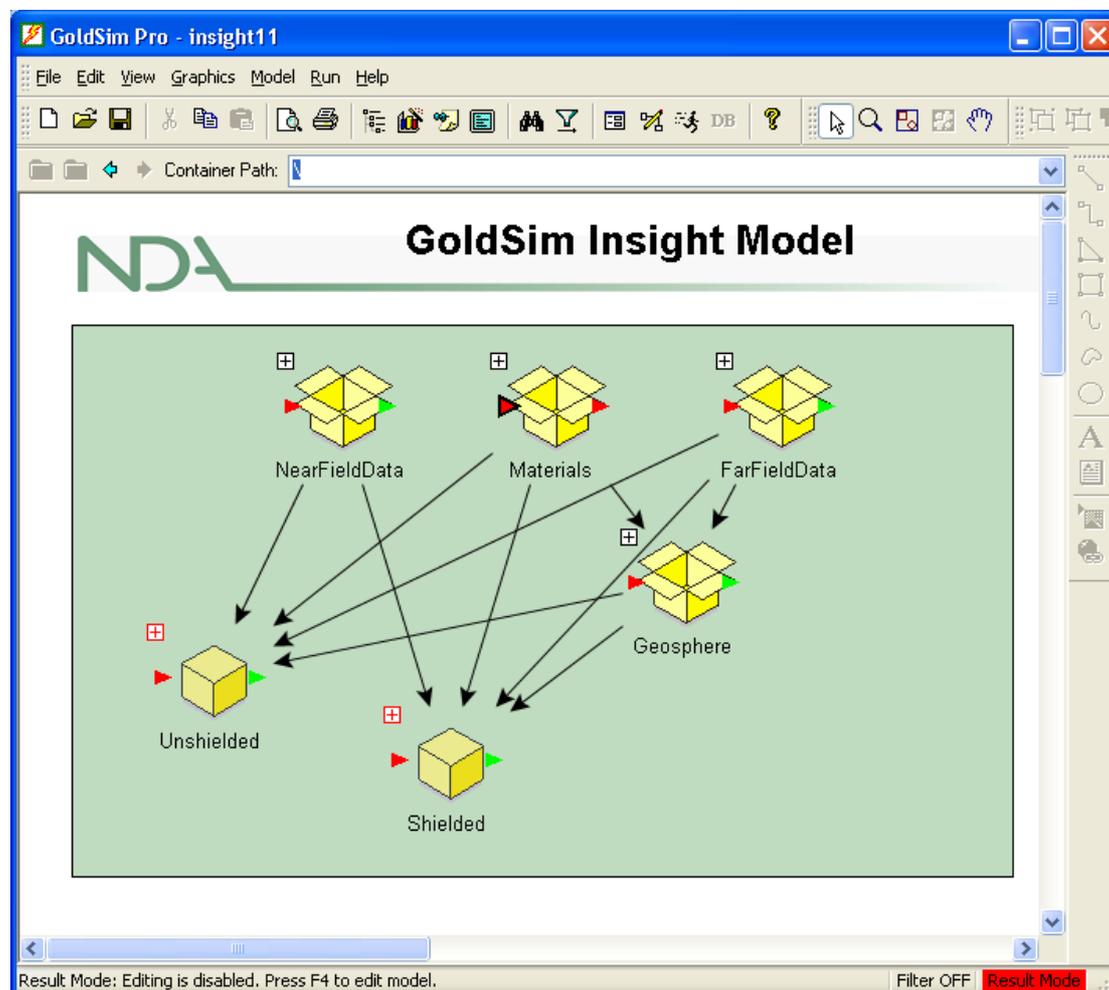
NearFieldData – PDFs and other data for the near field from the GPA model.

FarFieldData – PDFs and other data for the far field from the GPA model.

The fact that the probabilistic data are *identical* to those for the full dynamic GoldSim model means that the same sequence of random numbers leads to identical realisations for the insight model and the dynamic model, thus aiding their comparison.

The insight model structured as shown in Figure 1 below.

Figure 1 Structure of the insight model



There are individual models for the two source terms for the GPA reference case, representing the Unshielded ILW and the Shielded ILW and LLW vaults. Up to four geosphere layers have been included – for the GPA example, just two are used, representing the reducing and oxidising layers (see [3] for more information about the GPA reference case which has been used throughout this task as an example).

For the source-term models, the following data variables are defined (as far as possible following the notation in Nirex 97):

Cs – solubility limits (vector by species) in mol m^{-3} .

Kd – sorption coefficients (vector by species) in $\text{m}^3 \text{kg}^{-1}$.

Phi – average porosity (scalar).

Rho – average density (scalar) in kg m^{-3} .

Q – groundwater flux (scalar) in $\text{m}^3 \text{yr}^{-1}$.

V – volume (scalar) in m^3 .

M0 – initial inventory (vector by species) in mol.

In the current implementation these are linked to data in the GPA NearFieldData container, and source-term specific data from the GPA (e.g. dimensions of vaults, and treatment of organic complexants) which are located as a sub-container in each source-term model container.

For the geosphere models, the following variables are defined (as far as possible following the notation in Nirex 97 for the porous geosphere):

- R – retardation (vector by species).
- T – groundwater travel time in years.
- aL – longitudinal dispersion length in m.
- L – path length in m.

In the current implementation these are linked to data in the GPA FarFieldData container. The current implementation uses the biosphere model from the GPA for calculating risks.

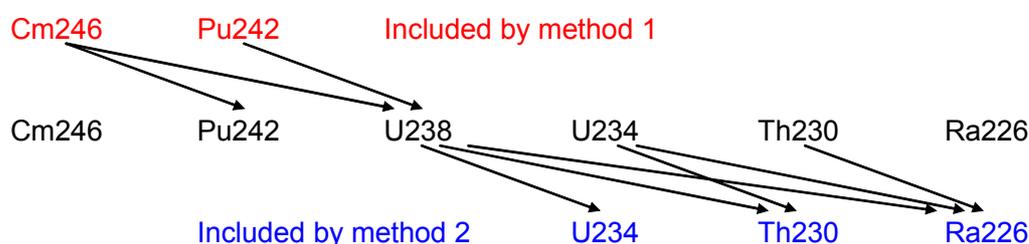
2.2.1 Treatment of decay chains

The insight model for Nirex 97 was developed for single radionuclides and not decay chains. What was required for the GoldSim implementation, was a pragmatic method for including the decay chains, with the aim of achieving a reasonable approximation for as many cases as possible without over-complicating the model.

It was considered that the simplest two alternative methods were:

1. Pre-decay parent to daughter and include inventory for *both* parent and daughter. This is most appropriate for a long-lived daughter of short-lived parent. In this case the long-lived daughter only will give the main contribution to risk for a reasonable groundwater travel time. In the case where the travel time is much shorter than the half life of the short-lived parent, the inventory of the parent will still contribute to *both* the risk from the parent and daughter, giving a double-counting error.
2. Consider daughter to be at, or approaching, secular equilibrium with parent at time that the risk occurs. This is most appropriate for short-lived daughters of long-lived parents, if there is a long travel time. It is assumed that the ingrowth of the daughter occurs in the top layer of the geosphere only. This method is applied, in general, where the half life of the daughter is much shorter than the half-life of the parent.

For each decay chain, a combination of these two methods was used, for example for the Cm-246 chain the following was implemented:



2.2.2 Treatment of shared solubility

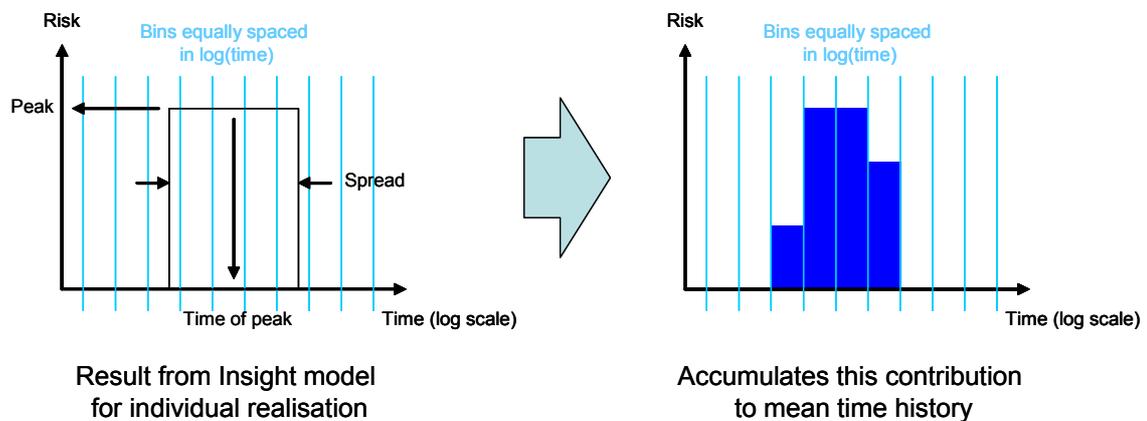
The approach taken for evaluating the solubility limit for elements with more than one isotope was to include the additional inventory of any isotope longer-lived than the isotope in question (and stable isotopes) when testing whether the solubility limit was exceeded.

2.3 Calculation of a Mean Time History

Some additional programming was required to accumulate a *time history* of the expectation value (mean value) of risk or other performance measures that can be directly compared with the results of a full dynamic simulation. This was implemented in FORTRAN as a Dynamic Link Library (DLL) that GoldSim calls during each realisation.

Given a simple distribution of a performance measure such as risk in time, based on the moments of that distribution, the insight model calculates the peak value, time of peak and spread. This information is passed to the DLL by GoldSim at each realisation and used to accumulate a time history by allocating the area under a 'square wave' defined by those parameters to a series of 'bins' logarithmically equally spaced in time as shown in Figure 2. The contribution from each realisation is divided by the number of realisations so as to accumulate the mean risk.

Figure 2 Accumulating the mean time history



3 RESULTS AND DISCUSSION

In this Section, results are presented for two cases:

Case 1: A GoldSim implementation of the GPA reference case [3]. This model calculates risk from the groundwater pathway for a repository system which relies for safety on chemical containment in the engineered system and a long travel time, dilution and dispersion in the geosphere. A log-triangular PDF for the groundwater flux through the repository of $LT(30, 300, 3000) \text{ m}^3 \text{ yr}^{-1}$ and a log-triangular PDF for the groundwater travel time of $LT(10^4, 10^5, 10^6)$ years were used.

Case 2: This case was identical to Case 1 except that a much wider range of uncertainty for the groundwater flux through the repository and travel time were used, so that the performance of the insight model over a wider range of parameter space could be investigated. A log-uniform PDF for the groundwater flux through the repository of $LU(0.1, 10000) \text{ m}^3 \text{ yr}^{-1}$ and a log-uniform PDF for the groundwater travel time of $LU(10^1, 10^6)$ years were used. It is not suggested that this much uncertainty might exist in any real performance assessment for a disposal facility – this case was carried out purely hypothetically to compare the two models.

Both the insight model and the full dynamic model were run for each case. It was found that the insight model ran over a thousand times faster than the dynamic model. 1000 realisations of the insight model took about 3 seconds compared to nearly 2 hours for the equivalent dynamic model.

3.1 PDFs of Fraction Released

As well as performance measures such as risk, the GoldSim insight model calculates the percentage of the inventory that:

1. is released from the source without decaying;
2. reaches the biosphere without decaying.

PDFs for these quantities are shown for Case 1 in Figure 3 for a range of radionuclides. It can be seen that for this case, almost all ^{36}Cl is released from the source and a considerable fraction reaches the biosphere. For ^{99}Tc , although a reasonable fraction is released from the source, only a small fraction is likely to reach the biosphere. For ^{93}Zr , almost all is released from the source but it is unlikely to reach the biosphere before decaying. For ^{238}U , because of its very long half life, almost all is likely to reach the biosphere before decaying.

3.2 PDFs of Peak Risk

It is of interest to compare the PDF of peak risk calculated by the insight model with that calculated by the full dynamic model. This comparison can only meaningfully be made for radionuclides that decay before the end of the dynamic simulation at 10^8 years. (The insight model has no time cut-off.)

Figure 4 shows PDFs for the peak risk from ^{36}Cl for Case 1 for both the dynamic and insight models. It can be seen that these look very similar, but they are not identical – recall that exactly the same realisations were run for each model so the differences between the PDFs are a result of the approximations made in the insight model.

Figure 5 shows PDFs for the peak risk from ^{135}Cs for Case 1 for both the dynamic and insight models. For this radionuclide, a large number of realisations give rise to negligible risk due to decay, but the results produced by the two models show good agreement.

The Figures also show the statistics of the distributions calculated by GoldSim and these also show good agreement between the two models.

Figure 3 PDFs showing the percentage of selected radionuclides (^{36}Cl , ^{99}Tc , ^{93}Zr , ^{238}U) leaving the repository (left plot) and reaching the biosphere (right plot)

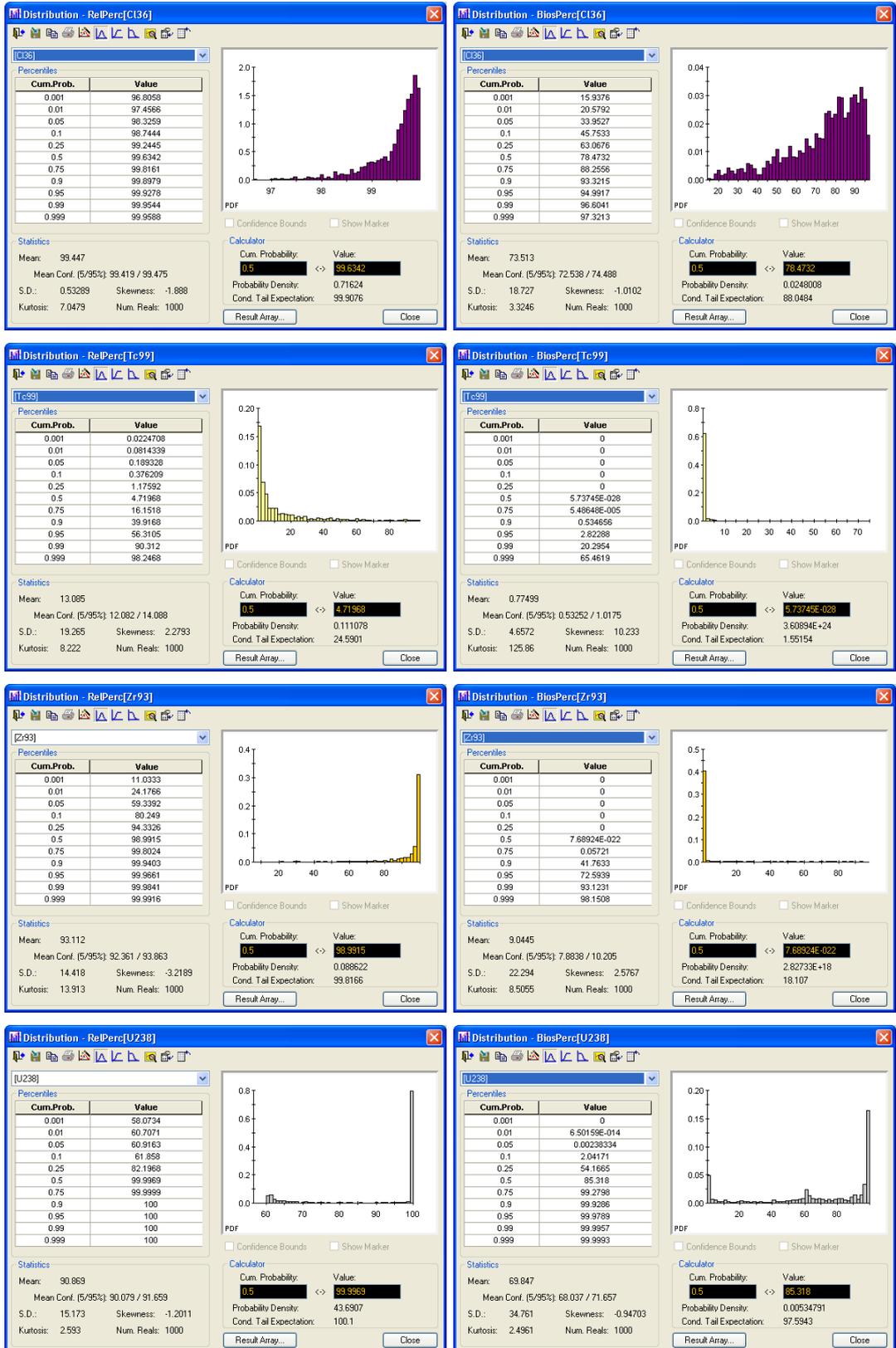


Figure 4 Distribution of the logarithm of peak risk from CI-36 from the dynamic model (left) and the insight model (right).

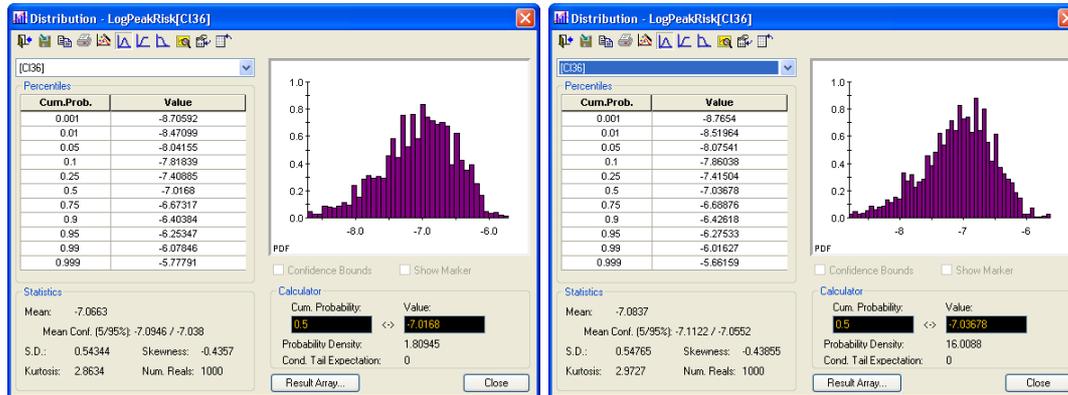
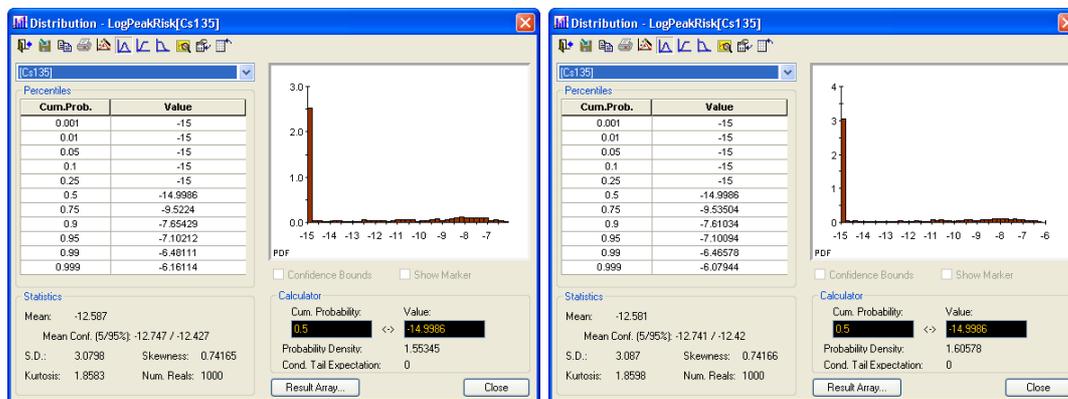


Figure 5 Distribution of the logarithm of peak risk from Cs-135 from the dynamic model (left) and the insight model (right). (Values below -15 are set to -15).



3.3 Risk Time Histories

Figure 6 shows a plot of mean risk against time for 1000 realisations of the dynamic model for Case 1. The corresponding plot for the same 1000 realisations of the insight model (produced using the DLL add-in to GoldSim as described in subsection 2.3 above) is shown in Figure 7. Figure 8 shows a plot of mean risk against time for one million realisations of the insight model for Case 1. All radionuclides are shown on each plot. Given the significant approximations in the insight model, results that are within a factor 2 or 3 for the two models should be regarded as reasonable agreement.

It can be seen that for most radionuclides, broadly similar results are obtained from the dynamic and insight models with 1000 realisations. For results that are well-converged (such as those for ^{36}Cl , ^{10}Be and ^{129}I) the curves are a similar shape over the region around the peak, but those for the insight model fall off more steeply at the edges. In the region around the peak, the parameter uncertainty (largely uncertainty in the travel time in this case) is the major control on the shape of the curve. Although the time history information from each realisation is very coarse (see subsection 2.3), in the region around the peak, the errors arising from this coarseness cancel each other out as the contributions from individual realisations are accumulated to give the mean risk curve. At the edges, the shape of the curve is controlled by the physics (dispersion at the early edge, decay at the late edge) for just the few realisations for which extreme values of the key uncertain parameter (the

travel time in this case) have been sampled, and the coarseness of the insight model is noticeable here.

For results that are poorly converged (such as ^{226}Ra , ^{230}Th and ^{210}Pb) it can merely be seen that the insight model results look similarly poorly converged with just 1000 realisations. However, with one million realisations (Figure 8), smooth mean risk curves result for these radionuclides also.

One radionuclide that shows particularly poor agreement between the dynamic simulation and the insight model for Case 1 is ^{233}U . This is a long-lived daughter of ^{237}Np and it is thought that the reason for the poor agreement is that the assumptions about its ingrowth occurring in the top layer of the geosphere only is not valid for all realisations in this case.

Figure 9 shows a plot of mean risk against time for 1000 realisations of the dynamic model for Case 2. The corresponding plot for the same 1000 realisations of the insight model is shown in Figure 10. Figure 11 shows a plot of mean risk against time for one million realisations of the insight model for Case 2.

The PDFs for groundwater flux through the repository and travel time were deliberately chosen to cover a much wider range for Case 2 compared to Case 1, to investigate how the insight model performed over a larger area of the parameter space representing uncertainty. It should be noted therefore that Case 2 is rather artificial. For this case, with 1000 realisations, the results from the insight model are considerably spikier than for the dynamic model, while otherwise still showing reasonable agreement.

Of particular interest for Case 2 are the results from ^{239}Pu which is very strongly sorbed and, for any reasonable groundwater travel time, would be expected to decay in the geosphere. With 1000 realisations, it is clear that very few realisations contribute to the significant calculated mean risk for ^{239}Pu , and imply a peak risk of around 10^{-4} just after 10,000 years (in the dynamic model). However, using the insight model to run one million realisations gives a much more converged result, indicating the peak risk is actually around 10^{-5} , an order of magnitude less.

Figure 6 Mean risk vs time for Case 1 (dynamic model) – 1000 realisations

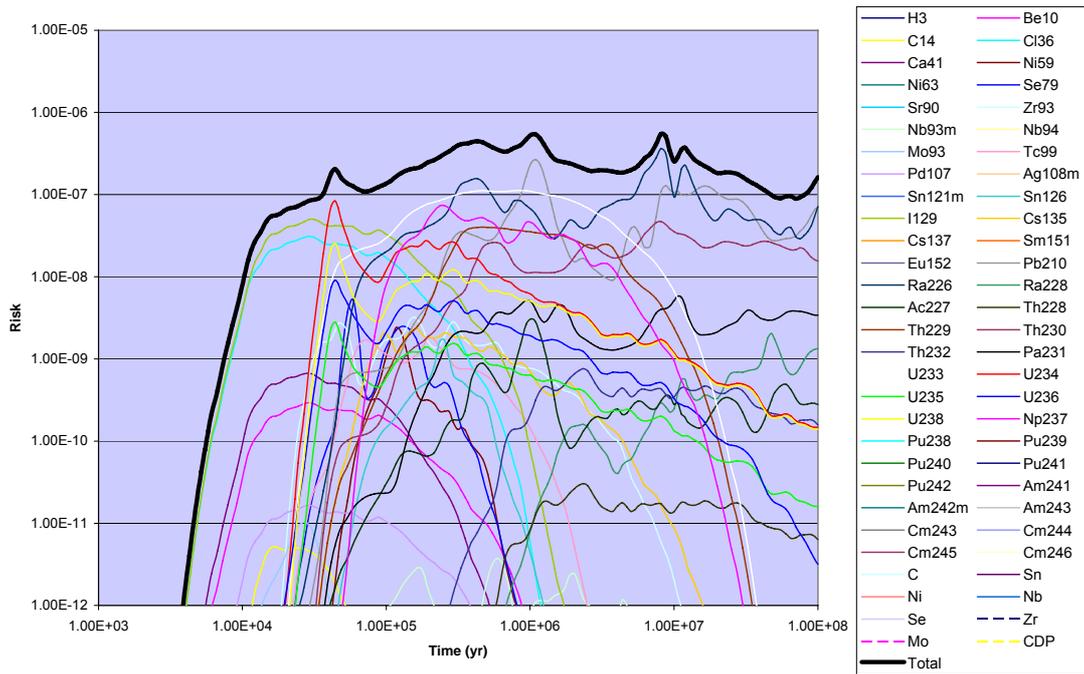


Figure 7 Mean risk vs time for Case 1 (insight model) – 1000 realisations

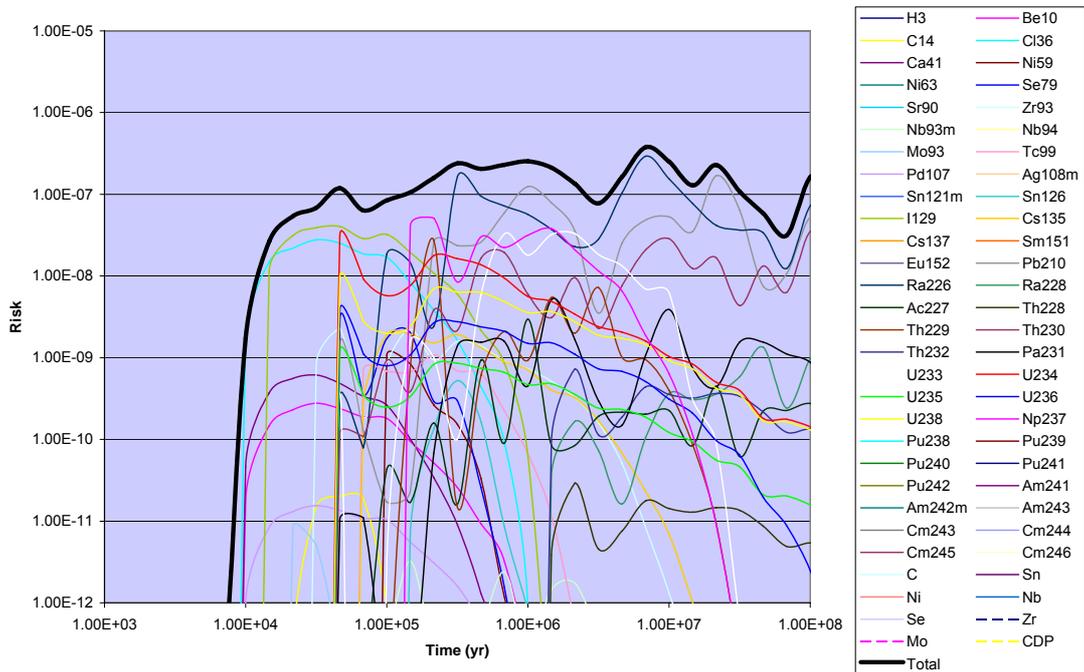


Figure 8 Mean risk vs time for Case 1 (insight model) – million realisations

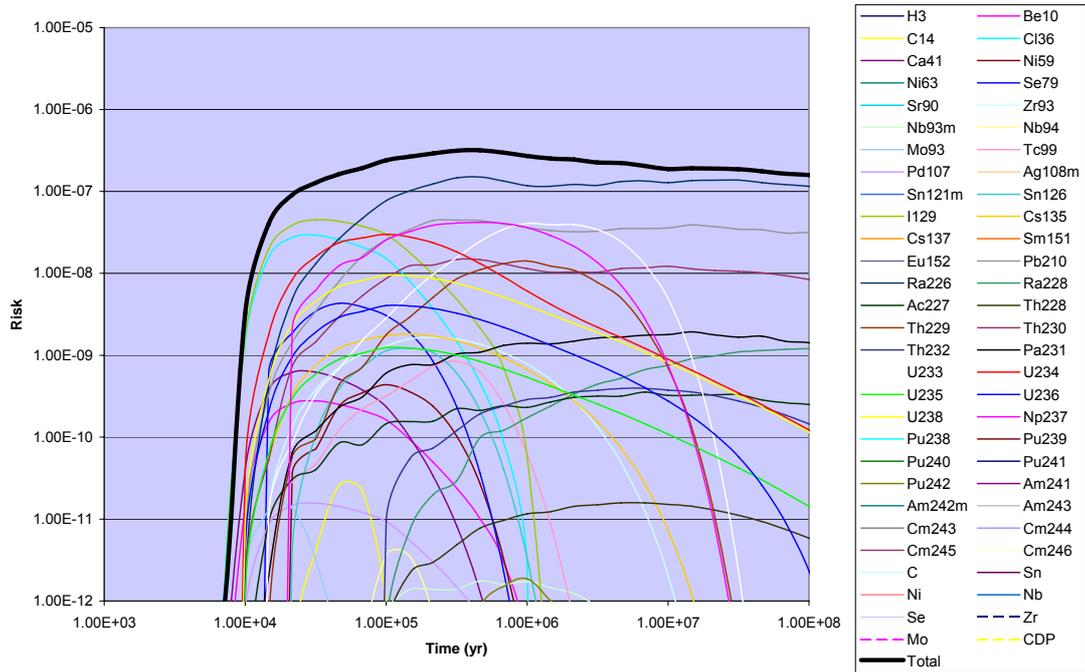


Figure 9 Mean risk vs time for Case 2 (dynamic model) – 1000 realisations

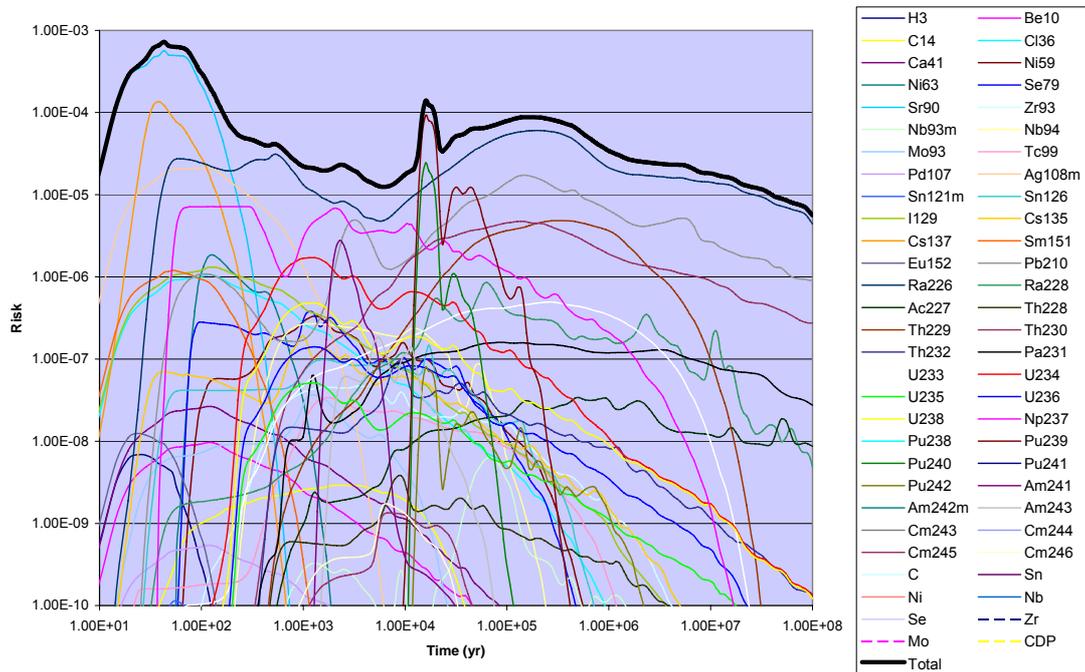


Figure 10 Mean risk vs time for Case 2 (insight model) – 1000 realisations

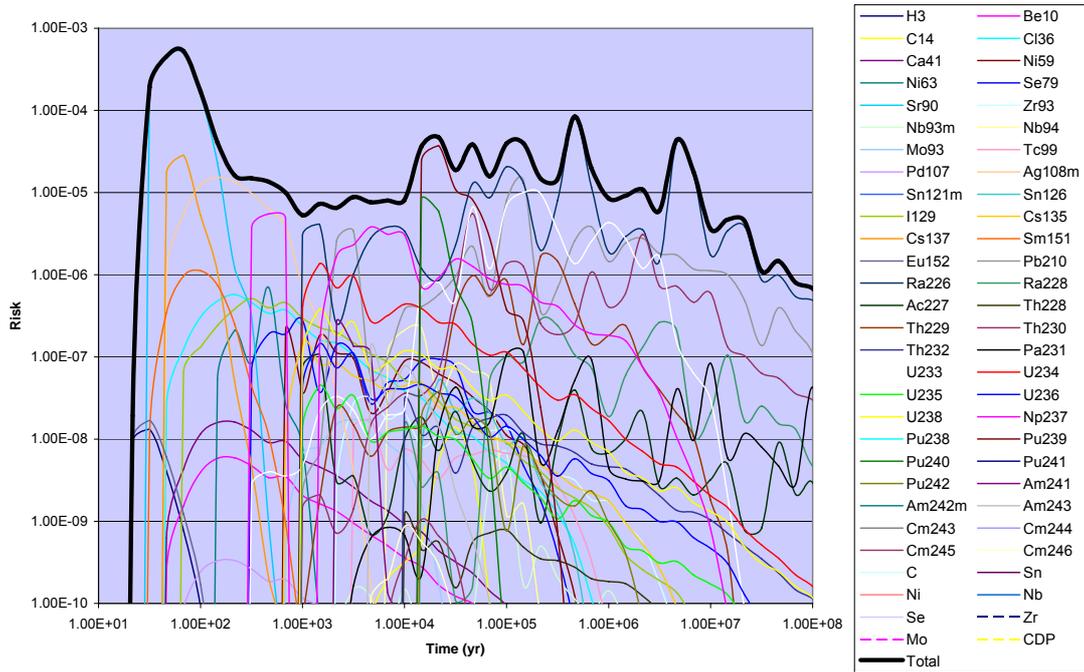


Figure 11 Mean risk vs time for Case 2 (insight model) – million realisations

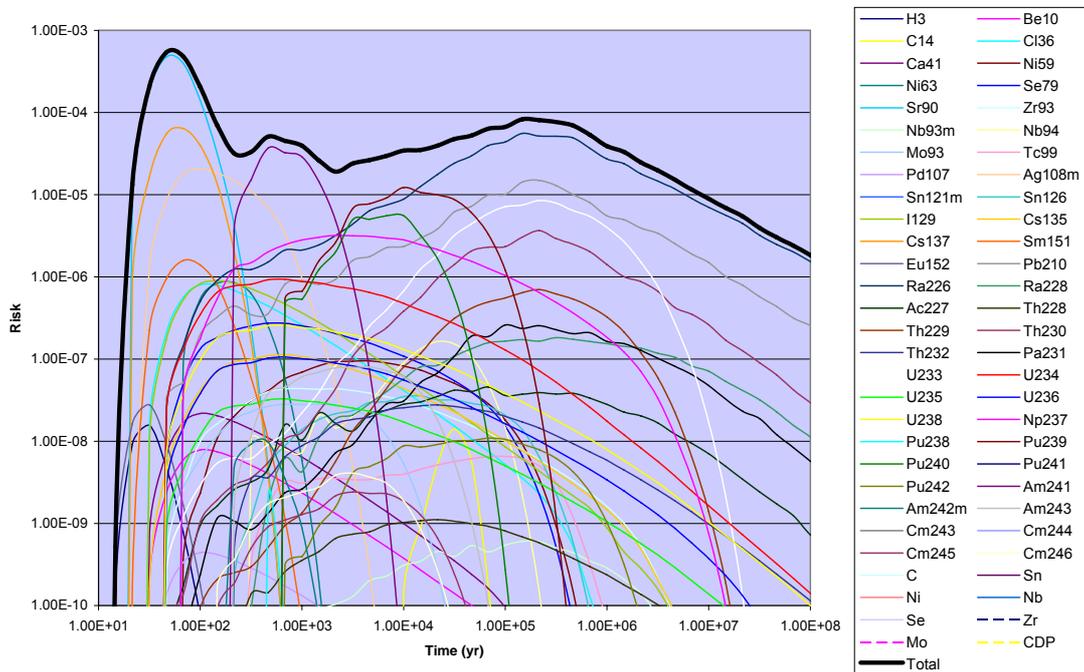


Figure 12 shows mean risk against time curves for selected radionuclides, and a curve for the total risk for Case 1. The results for 1000 realisations of the full dynamic model and for 1 million realisations of the insight model are shown. For some of the radionuclides, particularly short-lived daughters of long-lived parents (such as ^{226}Ra) it can be clearly seen that the results of the dynamic model (with 1000 realisations) are unconverged (see Figure 13 for ^{226}Ra). When compared with the results of the insight model it can be clearly seen that the unconverged solution from the dynamic model would give an over-estimate of the *peak* risk compared to the converged solution from the insight model. The difference in peaks between the red and blue curves on Figure 13 can clearly be seen.

Figure 14 shows mean risk against time curves for selected radionuclides, and a curve for the total risk for Case 2. The results for 1000 realisations of the full dynamic model and for 1 million realisations of the insight model are shown. As noted above, the curve for ^{239}Pu is particularly badly converged for the dynamic model (see Figure 15). At very early times for Case 2, which encompasses a much wider (artificial) range of uncertainty, there appears to be a systematic difference between the results of the insight model and the dynamic model for some radionuclides. This suggests there are some extreme realisations for which the insight model as implemented is less good an approximation.

Importance sampling can be used to reduce the number of realisations required in a probabilistic calculation by concentrating on regions of parameter space where consequences are potentially large. For the daughters of ^{238}U , this means where the sorption coefficients of the daughters are low. Importance sampling is available in both MASCOT and GoldSim but the implementation has the disadvantage that whilst the convergence of one aspect of the system is improved, the convergence of the rest of the system is degraded.

It may be that such convergence problems are better tackled by implementing a very fast, coarse version of a model such as the insight model and running a very large number of realisations. Comparing 1000 realisations of the insight model with the 1000 realisations of the full dynamic model will give an indication of the error introduced by the use of the simpler model (i.e. the difference between the results shown in Figures 6 and 7 give an indication of how good an approximation the insight model is for each radionuclide). Then, given this understanding, it is possible to get an indication of the error introduced by the lack of convergence of the dynamic model with only 1000 realisations, by comparison with the results for one million realisations of the insight model (i.e. comparison with Figure 8).

Figure 12 Mean risk vs time for selected radionuclides (Case 1) for the dynamic model (1000 realisations) and the insight model (million realisations)

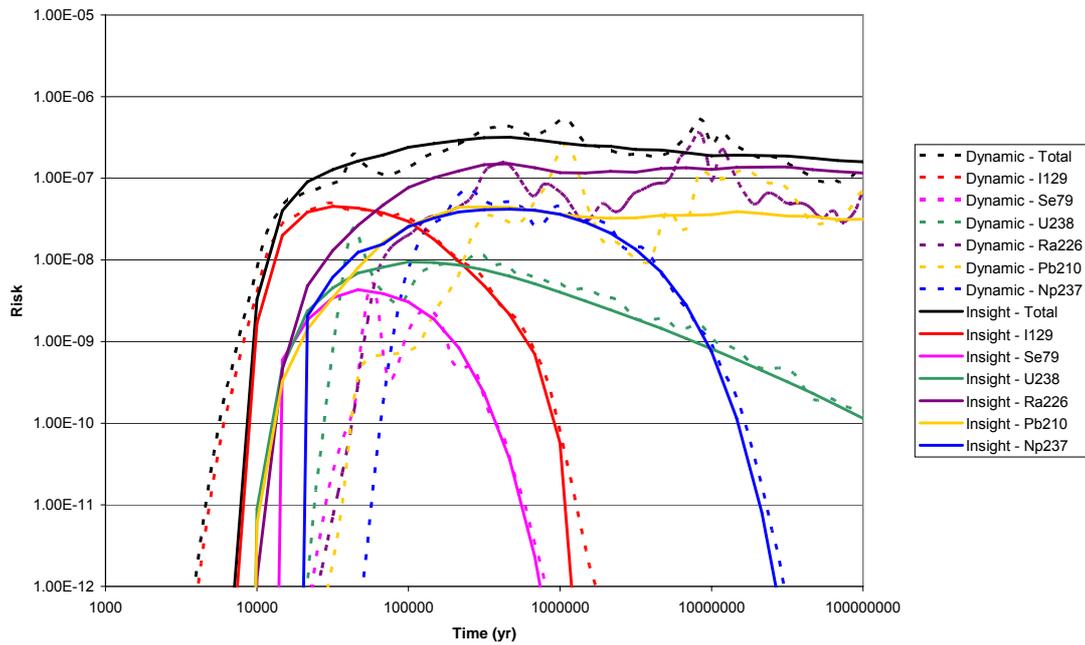


Figure 13 Mean risk vs time for ^{226}Ra for Case 1 for the dynamic model (1000 realisations) and the insight model (million realisations)

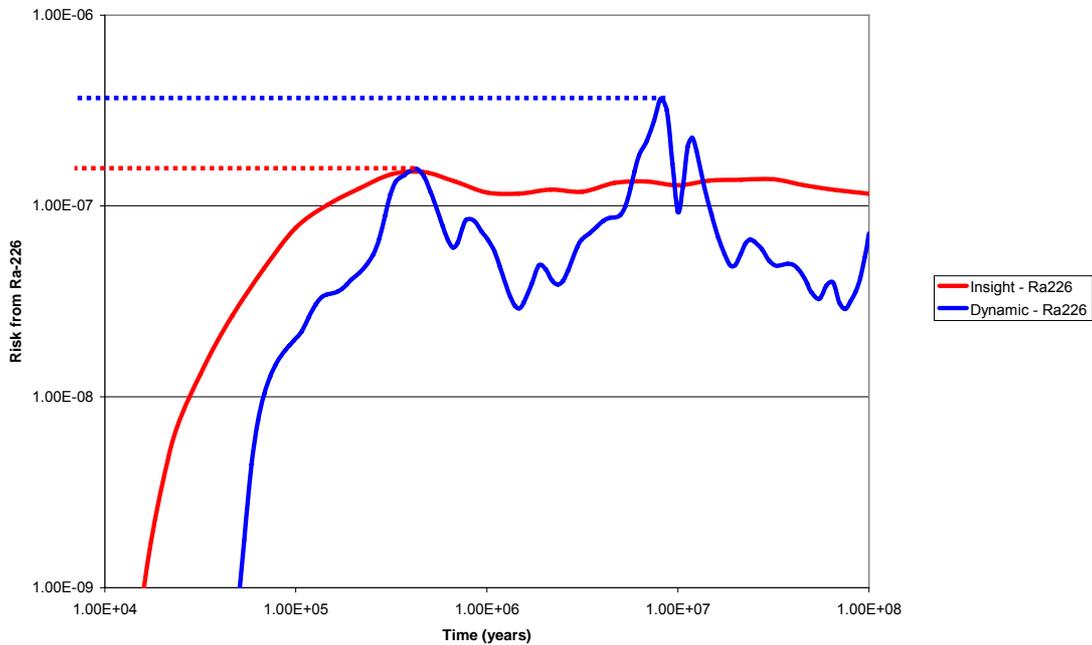


Figure 14 Mean risk vs time for selected radionuclides (Case 2) for the dynamic model (1000 realisations) and the insight model (million realisations)

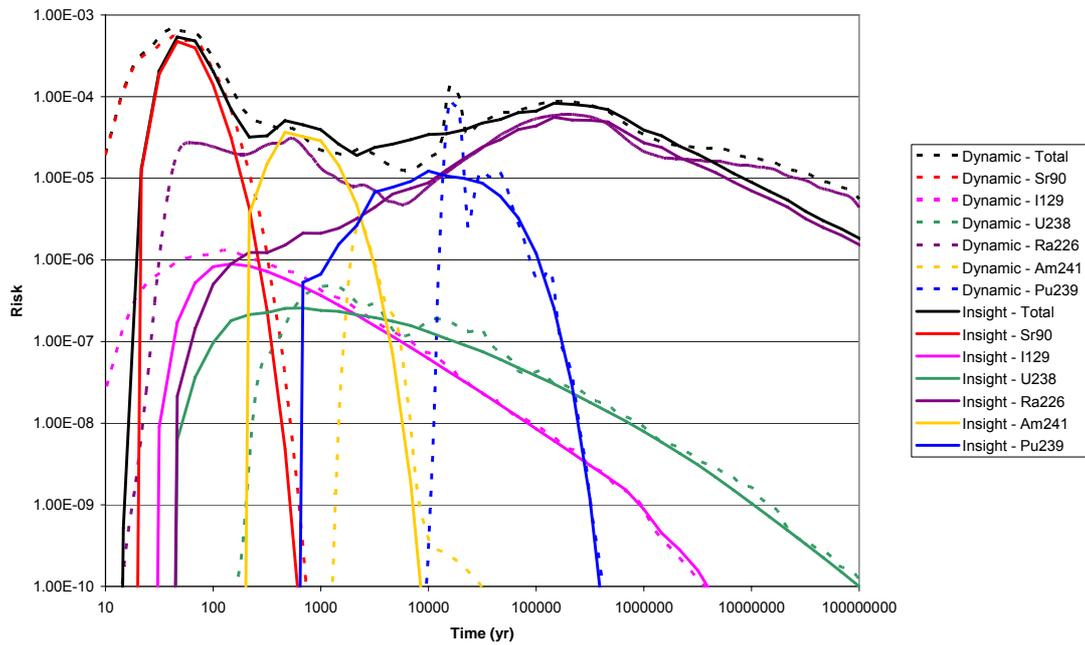
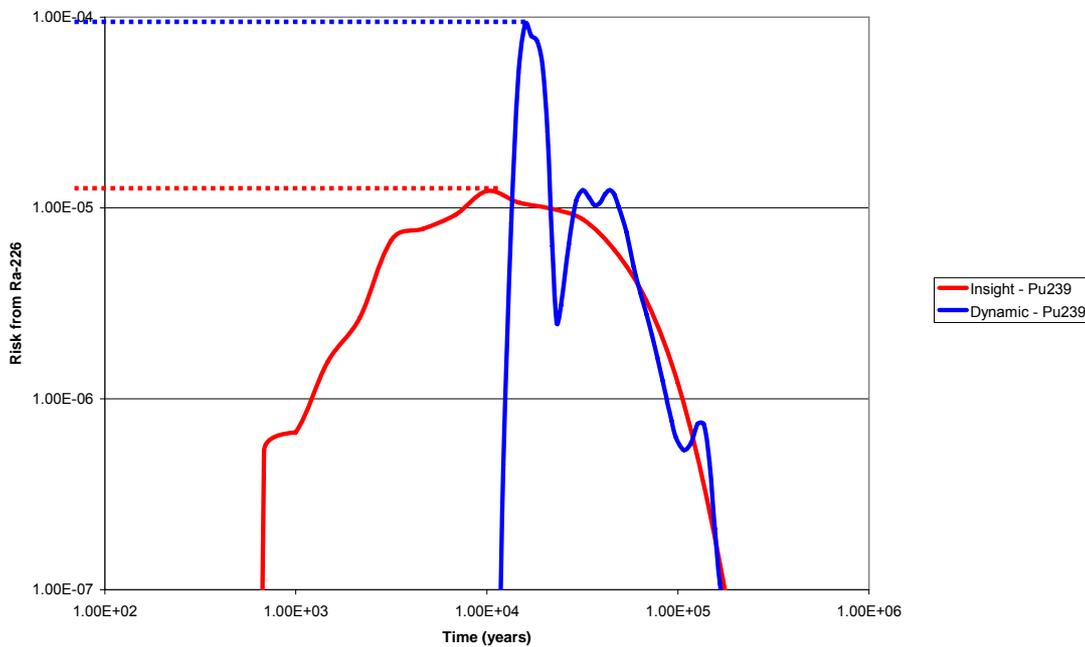


Figure 15 Mean risk vs time for ^{239}Pu for Case 2 for the dynamic model (1000 realisations) and the insight model (million realisations)



4 CONCLUSIONS

A GoldSim implementation of the insight model for estimating peak risks from the groundwater pathway has been developed. The model consists of two source terms and up to four geosphere layers. As it is a static simulation in GoldSim, it is very quick to run which makes it a useful tool for very quick initial scoping calculations (e.g. for analysis of alternative options, or alternative geologies) in cases where it is desirable to investigate the uncertainties in parameter values using a probabilistic approach.

The model can readily be linked to data already present in a full dynamic GoldSim model. The current implementation directly makes use of the data for the GPA without modification. A DLL add-in for GoldSim has been developed that efficiently accumulates a time history for the mean risk (or other performance measure).

The insight model was found in most cases to give good agreement with the same calculation carried out with the full dynamic model in GoldSim. The contribution to the time history for mean risk from each realisation in the insight model is very coarsely handled. However, provided enough realisations are run, in the region around the peak of the mean risk curve, the errors arising from this coarseness cancel each other out as the results from individual realisations are accumulated. This is because parameter uncertainty, rather than model uncertainty, is the main control on the shape of this curve in this region. At the 'edges' of the mean risk curve, well away from the peak, however, the model uncertainty dominates and the errors arising from this coarseness can be clearly seen.

This means that when carrying out probabilistic calculations to represent parameter uncertainties which are large, the model uncertainty introduced by using a very coarse model such as the insight model, may in fact be rather insignificant. This would need to be assessed on a case-by-case basis, but suggests there may be little benefit in over-complicating a model if it is to be used in a probabilistic calculation with large parameter uncertainty.

As the insight model runs over a thousand times faster than the full dynamic model, it is possible to run a very large number of realisations e.g. one million. It has been shown that in cases where results are poorly converged with 1000 realisations (e.g. risks from short-lived daughters of long-lived parents such as ^{226}Ra), a more accurate estimate of a quantity such as the peak risk could be obtained from a million realisations of the approximate insight model than for 1000 realisations of the full dynamic model. It may be, therefore, that convergence problems can be tackled by implementing a very fast, coarse version of a model such as the insight model and running a very large number of realisations.

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