Testing and Intercomparison of Model Predictions of Radionuclide Migration from a Hypothetical Area Source

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Abstract. This work was carried out as part of the International Atomic Energy Agency’s EMRAS program. One aim of the work was to develop scenarios for testing computer models designed for simulating radionuclide migration in the environment, and to use these scenarios for testing the models and comparing predictions from different models. This paper presents the results of the development and testing of a hypothetical area source of NORM waste/residue using three complex computer models. There are significant differences in the methods used to model groundwater flow between the models. The hypothetical source was used because of its relative simplicity and because of difficulties encountered in finding comprehensive, well-validated data sets for real sites. The source consisted of a simple repository of uniform thickness, with 1 Bq g⁻¹ of uranium-238 (²³⁸U) (in secular equilibrium with its decay products) distributed uniformly throughout the waste. This approximates real situations,
such as engineered repositories, waste rock piles, tailings piles and landfills. Specification of the site also included the physical layout, vertical stratigraphic details, soil type for each layer of material, precipitation and runoff details, groundwater flow parameters, and meteorological data. Calculations were carried out with and without a cover layer of clean soil above the waste, for people working and living at different locations relative to the waste. The predictions of the models showed several differences which need more detailed examination. The scenario is available for testing by other modellers. It can also be used as a planning tool for remediation work or for repository design, by changing the scenario parameters and running the models for a range of different inputs. Further development will include applying models to real scenarios and integrating environmental impact assessment methods with the safety assessment tools currently being developed by the IAEA.

KEYWORDS: NORM, area source, scenario development, model testing, model intercomparison

1. Introduction
The Environmental Modelling for radiation Safety (EMRAS) project was set up by the IAEA in 2003 to continue and expand upon the work carried out in earlier programs such as BIOMOVS, BIOMASS and VAMP. A working group on materials containing naturally occurring radionuclides (NORM) was set up to look at modelling of the movement of naturally occurring radionuclides in the environment. The aims of this group included looking at legacy sites, existing sites, and planning for future operations, with particular emphasis on the assessment or prediction of health and environmental impacts of NORM. These materials can include waste, residues, and products, with a very wide range of volumes and radionuclide concentrations. The large number of naturally occurring radionuclides and the wide range of chemical and physical properties of these radionuclides have to be taken into account in the models.

Further aims of the work were to evaluate existing models, develop scenarios for testing and verifying models, and develop new models. Very few models, and no well-documented scenarios for model testing, were available at the start of the program. Therefore a suite of hypothetical scenarios (a point source, an area source, and an area source plus river) was developed for validating and comparing models. This work describes the use of the hypothetical area source scenario for model testing and presents some of the results of the testing and model intercomparisons.

Potential applications of this work include the evaluation of legacy sites, assessment of remediation strategies for legacy sites and existing operations, and prediction of potential impacts of future operations (in particular, assessment of different management strategies).

2. The area source scenario
The main physical features of the site are shown in Figure 1. A detailed description of the scenario, including the modelling input data, can be found in [1]. The radionuclides are assumed to be uniformly distributed throughout the waste. Modellers were also asked to calculate doses to people working in each of the three fields and living in the house within that field. The modellers were asked to carry out the calculations for both covered and uncovered waste, and to consider the effect of rotating the wind rose through all four quadrants.
3. Models used in this work

The models used were PRESTO-CPG ver.4.2, RESRAD-OFFSITE, and DOSDIM + HYDRUS.

PRESTO (Prediction of Radiological Effects Due to Shallow Trench Operations) [2] is a computer package for the maximum annual effective dose to a critical population group from contaminated soil layers, for scenarios involving near surface waste disposal, soil cleanup, agricultural land application, and land reclamation. The package is designed to calculate the maximum annual effective dose to a critical population group for a range of scenarios, and includes models which simulate the transport of radionuclides in air, surface water, and groundwater pathways, and evaluate exposures through ingestion, inhalation, immersion and external exposure pathways. The models used for groundwater dynamics (infiltration, leaching, flow and extraction) are sufficiently detailed to avoid unnecessarily conservative results. The radionuclide migration model assumes the same partition coefficient ($K_d$) values for parent and daughter radionuclides in decay chains. The model also assumes that the waste is separated from the aquifer by one unsaturated soil layer. Simulation time is limited to 10,000 years.

RESRAD-OFFSITE [3-4] is designed to handle the assessment of both on-site and off-site impacts for situations such as buried waste and landfill (uncovered waste). The package allows for an optional cover layer, up to five partially saturated layers below the waste, and an aquifer (saturated layer). Allowance is also made for the effects of surface water bodies such as ponds, lakes and rivers, and for variations in land use near the disposal site. The models used in the package are complex and require considerable input data, but provide considerable
flexibility when carrying out assessments. The package has been designed to be user friendly and is well documented. The user can select a range of exposure pathways appropriate to the scenario being considered. The ability to carry out both deterministic and probabilistic is also provided. Only deterministic calculations were used for the work described here.

Radionuclides are removed from the waste by leaching, surface runoff, erosion, resuspension (dust) and exhalation (radon). A Gaussian Plume model is used to calculate airborne radionuclide activity concentrations at downwind locations and allows for both wet and dry deposition. The groundwater transport model is also a Gaussian dispersion model, which takes both horizontal and vertical dispersion into account when calculating radionuclide concentrations at off-site locations. This model also considers the decay of the parent radionuclide, the ingrowth of progeny radionuclide(s), and their respective retardation due to sorption/desorption in the solid phase. Drinking water is drawn from a well and the effects of irrigation using water from the well or a surface water body can be estimated using a food chain model.

DOSDIM (+ HYDRUS) calculations involved the use of two modelling packages. DOSDIM (DOSe DIstribution Model) is a compartmental type of model of the biosphere, partly dynamic, depending on the time frame and on the exposure pathways considered. It includes a module, based on a multi-source Gaussian dispersion model, which calculates radon concentrations in the air from point and area sources [5]. The DOSDIM package has been used in the BIOMOVS [6], VAMP [7-8] and BIOMASS [9] model validation and verification studies.

The radon dispersion was calculated by subdividing the area of the repository (1 km x 1 km) into of 100m × 100m cells. At the point of interest (e.g. house 2 in Figure 1), the contribution from each cell was calculated, and the individual contributions were then summed to give the total radon concentration [1]. For the covered waste scenario a radon exhalation rate of 0.02 Bq m⁻² s⁻¹ was used, while a value of 1 Bq m⁻² s⁻¹ was used for the uncovered waste scenario. For the uncovered waste situation the exhalation of radon from the waste directly into the house was included. The effects of erosion on the thickness of the cover were also allowed for in the calculations.

HYDRUS 1D and HYDRUS 2D were used for modelling the transport of the radionuclides in the variably saturated medium under the waste. Both models use finite element methods to simulate water and solute movement in unsaturated, partially saturated, or fully saturated porous media. For this work the one-dimensional version HYDRUS 1D was used to model the transport of the radionuclides through the vadose (unsaturated) zone under the waste into the aquifer (saturated zone). The concentrations of the radionuclides in the aquifer at the location of the exposure point (a well at the house) were then calculated with HYDRUS 2D using the output values from HYDRUS 1D as input.

4. Results
A number of exposure pathways were considered, including external exposure, inhalation of radon and contaminated dust, and ingestion of contaminated water and food. The effects of erosion on covering material were also considered, and the RESRAD-OFFSITE package gave the modellers the option of considering the effects of different types of land use following the deposition of the waste material.

The important factors which can influence the impact of surface and near-surface disposal of waste include future land use, the diet and general life-style of the inhabitants of the area, rainfall, groundwater transport, surface water transport, radon exhalation, the presence or absence of covering material above the waste, and erosion. The models should be able to simulate each of these processes.
Future land use can both influence and depend on the outcome of an assessment of the potential impact of a proposed waste repository, and can also affect doses once the waste is emplaced.

There are a large number of exposure pathways to be considered for scenarios of the type discussed here. However, in general, the exposure pathways can be put into groups; these groups are external exposure, exposure to airborne radionuclides (dust, radon, and thoron), food chain pathways, surface water transport pathways and groundwater transport pathways.

The effects of surface water transport were not considered in this scenario. Covering the waste should significantly reduce the contributions of airborne radionuclides, and external exposure, provided the cover remains intact. However, for long-term predictions the effect of erosion can be expected to be important. Erosion of the cover should increase the dose contributions from the airborne radionuclides and from external exposure, while erosion of the waste material itself should decrease the contributions from all exposure pathways. In addition, because groundwater transport is much slower than airborne transport, there should be significant delays in the effects of the groundwater pathways relative to the placement of the waste and the removal of the cover and waste by erosion. These considerations helped to guide the modellers in both developing the models used in this study, and in interpreting the results of the scenario testing.

The detailed results are presented in the main report [1] of the NORM working group (to be published). Some of these results are presented in the following sections. Total dose predictions are discussed in Section 4.1, dose contributions from individual exposure pathways are discussed in Section 4.2, and $^{238}$U concentrations in well water are discussed in Section 4.3.

Most of the results presented in the following sections were generated by the RESRAD-OFFSITE and DOSDIM (+HYDRUS) models.

4.1 Total doses

Total doses were calculated in all models by summing the contributions from all exposure pathways included in the model. The results for house 1 and house 2 are shown in Figure 2.
Figure 2: Total doses for houses 1 and 2, as calculated by the models PRESTO, DOSDIM and RESRAD-OFFSITE.

In Figure 2 the labels (D), (P) and (R) refer to the models DOSDIM (+ HYDRUS), PRESTO and RESRAD-OFFSITE respectively. DOSIM results are presented as black lines, while PRESTO results are represented by red lines and RESRAD-OFFSITE results are represented by blue lines. This allows comparison of the prediction of different models by comparing curves of the same line type but with different colours. The solid lines refer to the doses for a resident of house 1 for uncovered waste. The dashed lines (– – –) refer to house 2 for uncovered waste. The dotted lines (·····) refer to house 1 for covered waste. The broken dashed lines (– - – -–) refer to house 2 for covered waste.

Figure 2 shows a number of interesting features. In general, the RESRAD-OFFSITE predictions are higher than those from PRESTO and DOSIM (+ HYDRUS). In particular, the RESRAD-OFFSITE results appear to be a factor of approximately 100 higher than the DOSIM (+ HYDRUS) results. The ratio between the waste with no cover case and the waste with cover case is approximately the same for times greater than 5,000 years, but is greater for RESRAD-OFFSITE than for DOSIM(+ HYDRUS) for times less than 5,000 years. The reason(s) for these differences are not understood at this time.

In RESRAD-OFFSITE the erosion rate was calculated from the rainfall, infiltration and run-off data. For this scenario the erosion rate was estimated as 0.99 millimetres per year.
(approximately 1 metre per 1,000 years). The erosion of the cover could explain the increase in dose over the first 2,000 years for the covered waste.

To examine the reasons for the reasons for this increase in dose, it is necessary to look at the contributions to the total dose from individual pathways.

4.2 Dose contributions from individual pathways

The predicted dose contributions for the important exposure pathways are presented in Figure 3.

Figure 3: Dose contribution from individual pathways, calculated by RESRAD-OFFSITE

In Figure 3 there are several points to note. RESRAD-OFFSITE predicts significantly higher radon doses than DOSDIM (+ HYDRUS). The reason for this difference is not understood at this time. Leaving aside the possibility of mistakes by the modellers, there are several factors that can influence indoor and outdoor radon concentrations. Outdoor radon concentrations are strongly influenced by atmospheric conditions, and radon concentrations inside a dwelling tend to be dominated by the building materials used in constructing the dwelling, the ventilation rate, the rate at which radon enters the dwelling as a result of exhalation from the soil under the dwelling, and the presence or absence of a basement. Clearly, further work is needed to explain the differences in the model predictions.
Figure 3 indicates that the increase in total dose predicted by RESRAD-OFFSITE during the first 2,000 years is due to the increased exhalation of radon as the cover is removed by erosion. This behaviour is not reproduced by the other two models.

### 4.3 Dose contributions from individual radionuclides

Another useful comparison of model predictions was achieved by examining the predicted radionuclide concentrations in well water. The results of these calculations for RESRAD-OFFSITE and DOSDIM (+HYDRUS) are shown in Figure 4.

Figure 4: $^{238}\text{U}$ concentrations in well water for house 2.

DOSDIM (+HYDRUS) predicted the same concentrations for both the uncovered and covered waste cases. Both models predicted that the $^{238}\text{U}$ will start to appear in the well water after approximately 1,000 years. However, beyond that point the model predictions differed markedly.

If there were no erosion the $^{238}\text{U}$ concentration in well water should be expected to increase with time until most of the $^{238}\text{U}$ has been leached from the waste. However, erosion should remove the waste and hence reduce the source term. Therefore the $^{238}\text{U}$ concentration should increase at first but then start to decrease as the effects of erosion reduce the total amount of $^{238}\text{U}$ (in the waste) available for leaching into the groundwater. The effect of cover material would be expected to delay the expected decrease in $^{238}\text{U}$ concentration in well water because of the extra time needed to erode the cover. The RESRAD-OFFSITE predictions are consistent with this.

### 5. Conclusions

There appear to be significant differences between the predictions of the three models tested in this study. There are many processes which can affect the health and environmental impacts of surface and near-surface disposal of waste. These include erosion (of both cover
material and the waste itself), leaching, ground water transport processes, radon exhalation, rainfall, meteorology, future land use, and the use of (possibly) contaminated water for irrigation and domestic use. These processes are complex, which means that the development of models for simulating the transport of radionuclides in the environment for this type of scenario is not a simple matter. In addition, because of the complexity of the models and the large amount of input data needed by the models, there are many choices to be made by the user when setting up computer packages to model this type of scenario. This was noted by the DOSDIM user, who pointed out several important omissions in the original scenario specifications, and by the RESRAD users, who had difficulty agreeing on the land use specifications for the calculations. The resolution of these difficulties led to several important conclusions:

1. it is not always possible to specify the scenario without going through an iterative process of testing and modification;

2. good communication between modellers is essential, to ensure that all modellers use the same site specifications and the same values for environmental parameters, and produce results that can be directly compared.

3. there appear to be some significant differences between the predictions of different models.

There are significant differences between the PRESTO and RESRAD-OFFSITE results. There also appear to be significant differences between the predictions of the DOSDIM (+ HYDRUS) and RESRAD-OFFSITE, models particularly with respect to the contribution from radon inhalation to the total doses predicted by these models, and the effect of cover above the waste. More work is needed to explain and resolve these differences.

A program to follow-up the EMRAS work has been suggested. Clearly, with respect to NORM there are several issues that still need to be addressed. These include the development of more real scenarios for model testing, further development and testing of the models which are currently available, and the development and testing of models to look at scenarios (such as tailings dams and lakes) which were not looked at in the EMRAS program.

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