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AN INTEGRATED SIMULATION MODEL FOR THE PERFORMANCE ASSESSMENT OF A RADIOACTIVE WASTE REPOSITORY

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Summary. Disposal facilities for radioactive wastes comprise a series of engineered and natural (geologic) barriers to contain the radionuclides until their radiation hazard has decreased to acceptable levels. It is required that the long-term functionality of the containment barriers be evaluated by a quantitative risk analysis, also termed performance assessment. This entails the implementation of a Probabilistic Safety Assessment model of the stochastic failure behavior of the repository barriers and the release and transport of radionuclides into the groundwater bodies, to estimate the doses which can be transferred to humans from subsequent ingestion of water and other intake paths. Here, we propose an integrated model for the analysis of the safety performance of a radioactive waste repository, accounting for barrier degradation processes and groundwater transport processes. The model combines a Monte Carlo simulation-based reliability module for the estimation of radionuclide release from the repository (due to failures in the engineered barriers) and a numerical solution of flow and transport processes in the aquifer (performed by MODFLOW and MT3DMS codes). The model strengths are: 1) modularity of modeling of (a) failure of the engineered barriers and (b) groundwater contaminant transport and intake processes: this allows zooming in and out at different levels of detail while keeping the computational efforts manageable; 2) simplicity and flexibility of the Monte Carlo simulation module which can account for various physical aspects. The model can be used for screening analyses aimed at identifying the need for further detailed studies on relevant phenomena. An application to a case study of literature is presented to validate the approach and demonstrate its merits.

1 INTRODUCTION

The objective of the multiple engineered and natural barriers of a radioactive waste repository is to prevent the release of radionuclides and delay their migration to the groundwater and/or the biosphere[1]. The assessment of the resistance of these barriers is necessary for evaluating the harm caused by the potential release of radioactive wastes from the repository and intake by humans[2],[3],[4]. This leads to the estimation of the expected dose to some defined critical groups, with the associated aleatory and epistemic uncertainty[3],[5]. To this aim, a performance assessment of the radioactive waste repository typically entails: (*i*) identification of the scenarios that challenge the integrity of the repository barriers; (*ii*) estimation of their probabilities of occurrence; (*iii*) the estimation of the consequences associated with the release of radionuclides, typically in terms of the expected dose received by a pre-defined critical target group; and (*iv*) the evaluation of the uncertainties associated with the aforementioned estimates[3]. In this framework, a fundamental role is played by the quantitative analysis of the processes of radionuclide migration across the barriers of the repository to the main intake paths. The information content which is usually available does not allow a clear understanding of the mechanisms governing the release of radionuclides from the waste forms and the transport processes across the engineered barriers. A Probabilistic Safety Assessment approach is then needed for properly modeling the associated uncertainties[6]. This must be interfaced with a model of the evolution of the released radionuclides within the groundwater system.

Here, we present a modeling approach which couples a Monte Carlo-based estimate of the repository barriers failure time distribution and associated release rates with a groundwater flow and transport model. For simplicity, the latter is based on the widely documented packages MODFLOW and MT3DMS[7],[8]. We aim at providing a lean and modular modeling framework for performing tailored evaluations of the performance of engineered and/or natural barriers within a simplified scheme of calculations. This should allow a quick and relatively light analysis, while maintaining the necessary realism in the description of the failure and transport processes. For ease of illustration, and without loss of generality, the modeling scheme is presented with reference to a typical evolution scenario. The latter accounts for the degradation of the engineered barriers in the disposal and post-closure phases of the repository lifetime[6]. The failure behavior of the engineered barriers may be affected by phenomena of water infiltration and degradation[9].

The paper is organized as follows. In Section 2, the reliability-based modeling scheme for the multi-barrier system of the repository is introduced, with reference to a simplified case of a near-surface disposal facility [6]; within this scheme, a Monte Carlo simulation approach to estimate the release is presented. In Section 3, the repository and groundwater flow-transport modules are effectively coupled with reference to a case study; finally, the flexibility of the methodology is exploited to include some complex features of the engineered barriers degradation dynamics.

2 THE INTEGRATED SIMULATION MODEL

We consider a typical design of an engineered near-surface disposal facility for low and intermediate level radioactive wastes[6]. After proper conditioning, the radioactive wastes are encapsulated within concrete matrices (waste forms) enclosed in steel drums (waste containers). The waste drums are placed over a concrete floor and backfilled with proper material, *i.e.*, grout or soil mixed with clay, which guarantees structural stability and enhances the isolation capabilities. A top concrete cover ensures long term protection against infiltrations from rainfall. The release of radionuclides into the groundwater system below the repository should also be retarded by the effect of the partially saturated zone. Thus, the repository site and structural elements act as a sequence of both engineered and natural barriers aimed at preventing the contamination of the groundwater from radioactive waste and the subsequent release of a dose to a properly defined critical group.

The reliability model of the repository considers its engineered barriers as binary components in series, characterized by the two states “working” or “failed”, depending on whether the barriers are effective or not in preventing radionuclide migration and fulfill their containment role[6]. Containment failure of a barrier is mainly due to the action of water which infiltrates into the facility through precipitation, accelerates the degradation of the barriers and conveys radioduclides through the pores/fractures of the repository and site media to reach the groundwater system. The estimation of the radionuclide release to the groundwater is based on considering the sequential failure of the series of barriers. The failure of the top cover (barrier A) is due to rainfall water infiltration and degradation; this leads to the water reaching the waste containers (barrier B) and corroding the mild steel; as the corrosion proceeds, the water starts interacting with the solidified waste forms (barrier C), eventually leaching the radionuclides out of the concrete matrices; the radionuclides are then transported by water through the backfill (barrier D), thus reaching the bottom cover (barrier E), whose failure finally allows the radionuclides to exit the repository; before contaminating the groundwater, the radionuclides are transported through the last natural barrier, *i.e.* the partially saturated zone (barrier F). The failure of the *i-th* engineered barrier is modeled[7] as a stochastic event whose time of occurrence is assumed to be described by an exponential distribution with rate λ_i[10]:

$$f_i(t) = \lambda_i e^{-\lambda_i t} \qquad i = A, B, \ldots, F \tag{1}$$

The repository probabilistic model can then be interpreted as a reliability model of six components (the engineered barriers) in cold stand-by[10]. The distribution of the time of release of the radionuclides into the groundwater system can be determined as[6,10]:

$$f_s(t) = \left(\prod_{i=A,\ldots,F} \lambda_i \right) \left(\sum_{i=A,\ldots,F} \frac{e^{-\lambda_i t}}{\prod_{j \neq i} \left(\lambda_j - \lambda_i \right)} \right) \tag{2}$$

Under the assumption of a constant rate of waste placement in the repository for a period T [y] until the closure of the facility and neglecting for simplicity the radionuclides that are generated by the decay chains of other radioactive elements contained in the repository, the release rate R_d [Bq/y] of a radionuclide during the disposal period is[6]:

$$R_d(t) = S_d(t) \cdot f_s(t); \qquad S_d(t) = Q/\lambda_r \cdot \left(1 - e^{-\lambda_r t}\right) \tag{3}$$

Here, $S_d(t)$[Bq] is the inventory of a radionuclide at a time t after the beginning of the disposal operations, Q[Bq/y] is the radionuclide disposal rate and λ_r [1/y] is the radioactive decay constant of the radionuclide considered. The release rate of a radionuclide into the groundwater after closure of the repository at time T is

$$R_p(t) = S_p(t) \cdot f_s(t+T); \qquad S_p(t) = S_d(T) \cdot e^{-\lambda_r t} \tag{4}$$

where $S_d(t)$[Bq] is the inventory of the radionuclide after a time t from closure of the disposal facility.

Other degradation mechanisms affecting the repository barriers may be considered in the estimation of the radionuclide release and migration to the critical group, including the relaxation of the assumption of exponential failure time distributions. This might result in a computationally intensive solution of the doses and repository failure time distribution. To tackle these scenarios, we propose to adopt a Monte Carlo approach to characterize the repository probabilistic model. The time horizon (mission time, T_{miss}) during which the repository is expected to keep its integrity and perform the containment function is discretized into N_t intervals of width Δt and a fault state counter ($Cntr(j)$, j = 1, 2, ..., N_t) is associated with each interval. A large number N of repository evolutions are then simulated as a random walk process by sampling the failure times of each barrier from the related distributions. In each simulation, $Cntr(j)$ associated with the time interval j within which the failure time of the disposal facility occurs is increased by one. At the end of the N simulations, the probability density function (*pdf*) of the repository failure time can be estimated as

$$f_s(t) \approx \frac{Cntr(j)}{N \cdot \Delta t} = \hat{f}_s(t) \qquad j \cdot \Delta t < t < (j+1) \cdot \Delta t \tag{5}$$

whereas the corresponding releases from the repository before and after its closure can be estimated as $\hat{R}_d(t) = S_d(t) \cdot \hat{f}_s(t)$ and $\hat{R}_p(t) = S_p(t) \cdot \hat{f}_s(t+T)$, respectively.

The time-dependent concentrations [Bq/m^3] of the radionuclide, which constitute the input to the groundwater system before ($C_d(x, t)$) and after ($C_p(x, t)$) closure of the repository, can be evaluated by a suitable groundwater flow and transport code. For simplicity, we adopt a MODFLOW-based suite[7,8] in which a one-dimensional groundwater domain is discretized into N_{gw} cells of length l. The Monte Carlo estimation and the groundwater models are then linked by imposing a boundary condition such that for each time step Δt the concentration at the source (*i.e.*, the model element where the repository is located) is

$$C_{source}(x_{source}, t) = \left(\hat{R}_{d,p}(t) \cdot \Delta t\right) / (l \cdot A) \tag{6}$$

where A is the cross-sectional area of the groundwater system.

Finally, considering a scenario leading to drinking-water intake, the dose $D(x, t)$ [mSv/y] to an individual of a critical group can be estimated as

$$D(x,t) = C_{d,p}(x,t) \cdot \gamma \cdot \delta \tag{7}$$

where γ [l/day] is the average quantity of drinking water consumed per year and δ [mSv/Bq] is the dose conversion factor for ingestion[6].

3 RESULTS

The Monte Carlo simulation approach proposed in Section 2 is applied to the study case of literature[6] considering the migration of a single species of radionuclide, *i.e.*, ^{239}Pu. This particular radionuclide has been chosen since it represents a long term threat to the environment for its radioactivity and toxicity. Obviously, it is expected that its concentration in a near-surface repository be kept below the limits prescribed by the IAEA safety requirements[2],[6] characterized the engineered and natural barriers by exponential failure time distributions with the failure rates reported in Table 1, third column.

By a proper choice of the pdfs, structure degradation dynamics occurring in realistic settings may be included in the model, in addition to water infiltration and degradation. For our purposes, the engineered barriers aging degradation behavior is described by Weibull distributions[10]

$$f_i(t) = \alpha_i \beta_i t^{\alpha_i - 1} e^{-\beta_i t^{\alpha_i}} \qquad i = A, B, \ldots, E \tag{8}$$

which renders the semi-analytical approach of Nair and Krishnamoorthy[7] impractical. Table 1 reports also the values of the parameters α_i and β_i of the Weibull distributions adopted in the simulation; the chosen Weibull densities favor smaller failure times than those associated with the exponential distributions of Nair and Krishnamoorthy[7].

Type	**Barrier**	**Failure rate λ_i [y^{-1}]**	**α**	**β [y^{-1}]**
A	Top cover	0.04	1.3	0.04
B	Waste container	0.08	1.3	0.08
C	Waste form	0.0034	1.3	0.0034
D	Backfill	0.034	1.3	0.034
E	Bottom cover	0.067	1.3	0.067
F	Partially saturated zone	$1/(R\ T_r)$	1	$1/(R_d\ T_r)$
R and R_d are retardation factors and $T_r = z/U_z$ (Table 3) is travel time				

Table 1: Parameters adopted for the exponential (column 3) and Weibull (columns 4 and 5) stochastic failure models of the repository engineered and natural barriers[6]

A Monte Carlo simulation of $N = 30 \times 10^6$ repository histories has been performed over a time horizon $T_{miss} = 10^7$ [y]. The latter is divided into $N_t = 10^6$ time intervals of uniform width

Δt = 10 [y]. At the end of the N simulated random walks, the values accumulated in the counters allow estimating the repository failure time pdf, $f_s(t)$ and the corresponding releases $R_d(t)$ and $R_p(t)$, as depicted in Figure 1a.

Neglecting for simplicity the ^{239}Pu radionuclides that are generated by the decay chains of other radioactive elements contained in the repository, the concentrations $C_d(x, t)$ and $C_p(x, t)$ are estimated by a one-dimensional simulation of the groundwater transport with boundary conditions given by the releases $R_d(t)$ and $R_p(t)$. To this aim, a 3 Km-long, one-dimensional groundwater domain has been discretized into N_{gw} = 150 cells of uniform length l = 20 m. The repository is considered as a point source[7] and is located 400 m downstream of the domain boundary. Tables 2 and 3 show the physical and geometrical parameters of the simulation.

Nuclide	**Half-life $T_{1/2}$ [y]**	**Radioactive waste disposal rate Q [Bq/y]**	**Range of K_d^* value [ml/g]**	**Reference K_d^* value [ml/g]**
^{239}Pu	$2.44 \cdot 10^4$	$1.59 \cdot 10^{10}$	$10^3 - 10^4$	$2 \cdot 10^3$
$^*K_d$ is the distribution coefficient for clay				

Table 2: Radionuclide dependent parameters[7]

Parameter	**Reference value**	**Unit**
Thickness of unsaturated zone (z)	0.02	m
Seepage velocity in unsaturated zone (U_z)	$1.157 \cdot 10^{-10}$	m/s
Bulk density (ρ_b)	$1.7 \cdot 10^6$	g/m^3
Effective porosity (θ)	0.3	–
Ground water velocity (U_x)	$1.157 \cdot 10^{-6}$	m/s
Aquifer cross sectional area (A)	$1.0 \cdot 10^2$	m^2
Dispersivity	1	m
Distance of well from the repository (x)	$1.6 \cdot 10^3$	m
End of disposal activities (T)	50	y
Yearly drinking water ingestion (γ)	2.2	l/day
Dose conversion factor for ingestion (δ)	$1.57 \cdot 10^{-5}$	mSv/Bq

Table 3: Radionuclide independent parameters[7]

Figure 1b compares the doses, $D(x, t)$ [mSv/y], from ingestion of drinking water from a well located at x = 1.6 Km downstream of the disposal site estimated by coupling our Monte Carlo-based repository model with (a) MODFLOW and MT3DMS (solid line) and (b) the semi-analytical solution of the one-dimensional, point source Advection Dispersion Equation of Nair and Krishnamoorty[7] (dotted line). Figure 2 shows the time evolution of the dose peak in five observation wells located at various distances from the repository estimated by the integrated simulation model proposed. The significant decrease in the peak value is due to the combined ^{239}Pu radioactive decay and diffusion/dispersion effects.

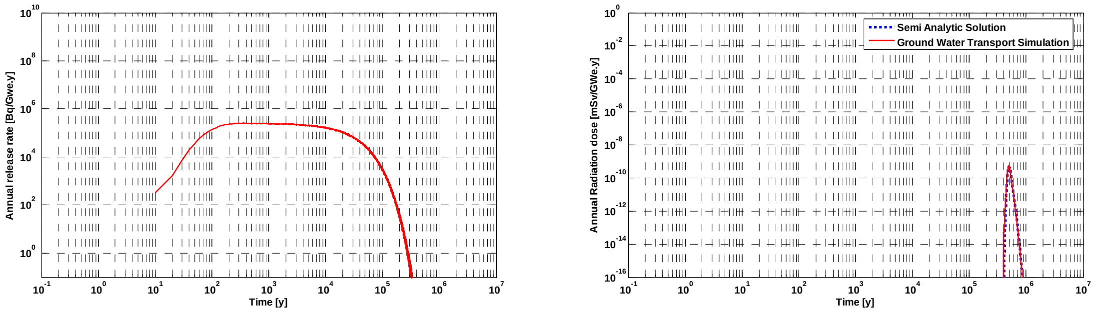

Figure 1: Failure time distribution of the engineered barriers: (a) estimated ^{239}Pu release rate and (b) comparison of the corresponding doses, $D(x, t)$ [mSv/y], from ingestion of drinking water from a well located 1.6 Km downstream of the disposal site estimated by coupling our Monte Carlo-based repository model with (a) MODFLOW and MT3DMS (solid line) and (b) the semi-analytical solution of the one-dimensional, point source Advection Dispersion Equation of Nair and Krishnamoorty[7] (dotted line).

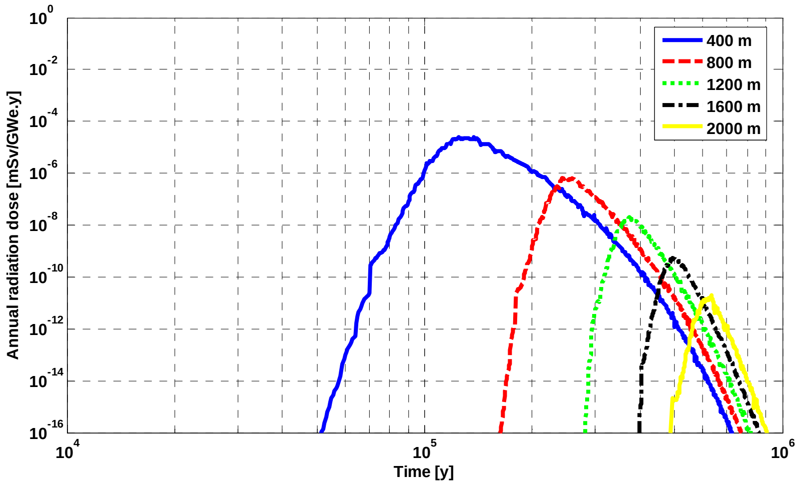

Figure 2: Time evolution of the calculated dose in five wells located at different distances from the repository.

4 CONCLUSIONS

The performance assessment of a radioactive waste repository aims at verifying the compliance of the expected doses to the critical groups, to the limits imposed by law by the various National Regulatory Agencies, taking into account the related uncertainties. To this aim predictive models are used to describe the radionuclide migration through the repository barriers, typically due to water infiltration, leaching of the radionuclide from the waste forms and consequent transport through the groundwater up to the main intake paths. The randomness of the processes involved and the epistemic uncertainties involved in modeling, can be properly captured within a probabilistic framework for the safety function assessment of the engineered and natural barriers of the disposal facility. Under realistic conditions, the complexity of the modeling required renders cumbersome, if not impossible, resorting to analytical approaches. On the contrary, Monte Carlo simulation offers the potential flexibility needed to realistically describe different processes occurring in the system.

Here, we couple a Monte Carlo simulation-based reliability model with the groundwater flow and transport tools MODFLOW and MT3DMS for the preliminary evaluation of the safety performance of a radioactive waste repository. The methodology has a degree of flexibility which allows accounting for complex physical aspects and is conducive to simple and relatively fast computations. The proposed simulation scheme has been applied to a simple case study from the literature which has been properly adjusted to account for realistic ageing phenomena.

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