# **Cadini Francesco**

**Avram Diana**  *Politecnico di Milano – Dipartimento di Energia, Milan, Italy* 

**Zio Enrico**  *Politecnico di Milano – Dipartimento di Energia, Milan, Italy Ecole Centrale Paris* – *Supelec, Paris, France* 

**Luce Alfredo** 

**Taglioni Alberto**  *ENEA CR Saluggia, Saluggia (VC), Italy* 

# **Monte Carlo simulation-based reliability model for the PSA of a radioactive waste repository**

## **Keywords**

radioactive waste repository, probabilistic safety assessment, reliability-based model, Monte Carlo simulation

## **Abstract**

Disposal facilities for radioactive wastes comprise a series of engineered barriers whose purpose is to contain the radionuclides until their radiation hazard has decreased to acceptable levels. In this regard, it is required that the long-term functionality of the system of barriers be evaluated by a quantitative risk analysis procedure, also called performance assessment. In this paper, a Monte Carlo simulation-based reliability model is propounded for the preliminary analysis of the safety performance of a radioactive waste repository, accounting also for barrier degradation processes. The model strengths are: simplicity, which allows ease of computation, and flexibility, which allows modification to account for various physical aspects and inter-comparison of their effects. An application to a case study of literature is presented to validate the approach and demonstrate its flexibility.

### **1. Introduction**

The objective of the engineered and natural barriers of a radioactive waste repository is to prevent the release of radionuclides and retard their migration to the groundwater, and eventually to 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 successive intake by humans  $[1]$ ,  $[2]$ ,  $[3]$ ,  $[4]$ . Eventually, what is required is the estimation of the expected dose to some defined critical groups, with the associated aleatory (stochasticity of the future system behavior) and epistemic (lack of knowledge of the model parameter values) uncertainty [3], [5], [6]. In this context, by critical group is intended a homogeneous group of individuals who might live in the area near a repository, whose water would be obtained from a nearby groundwater aquifer and would receive the highest radiation dose. Because the actual doses in the entire population will constitute a distribution for which the critical group represents the extreme, this definition is intended to ensure that no individual doses are unacceptably high [7]. To this aim, a performance assessment of the radioactive waste disposal facility is carried out; this entails: i) the identification of the scenarios that influence the repository integrity behavior; ii) the estimation of their probabilities of occurrence; iii) the estimation of the consequences associated to the release of radionuclides provoked by them,

typically in terms of the expected radiation dose; iv) the evaluation of the uncertainties associated to the aforementioned estimates.

In this framework of assessment, the quantitative analysis of the processes of radionuclide migration across the barriers of the repository to the main intake paths, plays a fundamental role. Since the available information does not allow a clear understanding of the radionuclide release mechanisms out of the waste forms and/or of the geohydrological and geochemical features of the repository site governing the radionuclide transport in the geosphere, a Probabilistic Safety Assessment approach is necessary for a proper modelization of the barriers failure behavior and the associated uncertainties [8], [9], [10], [11], [12], [13].

The complexity of the failure mechanisms and of the occurring processes does not allow for an analytic treatment of the problem, so that resorting to numerical schemes becomes mandatory.

In this paper, a Monte Carlo simulation-based modeling approach is proposed for addressing the problem of estimating the repository barriers failure time distribution and the associated doses to the critical individual, within a Probabilistic Safety Assessment framework. The aim is that of providing a lean modeling framework for performing preliminary evaluations of the barriers performance within a simplified scheme of calculations which allows a quick and relatively light analysis, while offering the flexibility for maintaining the necessary realism in the description of the failure and transport processes. To offer clarity, a reliability-based modelling is embraced; to offer flexibility in the description of the stochastic failure and transport processes, Monte Carlo simulation is used for the solution of the model.

For simplicity, but with no loss of generality, the approach taken here is presented with reference to a normal evolution scenario which accounts for the degradation of the barriers in the disposal and postclosure phases of the repository lifetime [8], [14]; consideration is given to the fact that the failure behavior of the engineered barriers may be affected by phenomena of water infiltration and degradation, but also of cracking due to settling of the structure under gravity forces or temperatureinduced volume changes [15].

The paper is organized as follows. In Section 2, the reliability model for the multi-barrier system of the repository is introduced, with reference to a simplified case of a near-surface disposal facility of literature [8] related to this, the Monte Carlo simulation approach to dose estimation is presented. In Section 3, the Monte Carlo method is

validated against the analytic results of the case study of literature and then extended to include some realistic features of the barriers degradation dynamics. Finally, some conclusions are provided in Section 4.

### **2. The Monte Carlo-based reliability model of the repository**

In the following, reference is made to a typical design of an engineered near-surface disposal facility for low and intermediate level radioactive wastes [6], [8], [14], [16]. After proper conditioning, the radioactive wastes are encapsulated within concrete matrices (waste forms) enclosed in special steel drums (waste containers); the waste drums are disposed 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 water. Eventually, the final release of radionuclides into the groundwater stream below the repository is retarded by the unsaturated (vadose) zone. Thus, the repository structures and its site 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 person.

The reliability model of the repository considers its barriers as binary components in series (*Figure 1*), characterized by two states: "working", if the barriers are effective in preventing radionuclide migration and "failed", if the barriers properties are degraded so that they cannot perform their containment functions [8]. The containment function 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 transports the radioduclides through the pores/fractures of the repository and site media into the groundwater stream.



*Figure 1*. Schematic illustration of the engineered and natural barriers of the repository.

The estimation of the radionuclide release to the groundwater is then based on considering the sequential failure of the series of barriers:

- top cover (barrier a): due to rainfall water infiltration and degradation;
- waste containers (barrier b): the water reaches the container resulting in corroding the mild steel;
- solidified waste forms (barrier c): as the corrosion of the container proceeds, the water starts interacting with the waste form, eventually leaching the radionuclides out of the concrete matrices;
- backfill (barrier d): the leached radionuclides are then transported by water through the backfill;
- bottom cover (barrier e): due to water infiltration and degradation, allows the radionuclides to exit the repository;
- the unsaturated zone (barrier f): before contaminating the groundwater, the radionuclides are transported by water through the last natural barrier.

In  $[8]$ , the failure of the  $i<sup>th</sup>$  barrier is modeled as a stochastic event whose time of occurrence is distributed according to an exponential distribution of constant rate  $\lambda_i$  [17]:

$$
f_i(t) = \lambda_i e^{-\lambda_i t}, t > 0, i = a, b, ..., f, \lambda_i > 0 \quad (1)
$$

The repository probabilistic model can then be interpreted as a reliability model of 6 components (the barriers) in cold stand-by [17], i.e. each component is demanded to provide its containment function at the time of failure of the preceding component in the physical sequence above illustrated. In this setting, the repository failure time distribution, i.e. the distribution of the time of release of the radionuclides into the groundwater stream, can be determined analytically as [8], [17]:

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

Under the hypothesis 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 into groundwater during the disposal period is [8]:

$$
R_d(t) = S_d(t) \cdot f_s(t) \tag{3}
$$

where  $S_d(t) = (Q/\lambda_r) \cdot (1 - e^{-\lambda_r t})$  (Bq) is the inventory of a radionuclide at a time *t* after the beginning of the disposal operations (the index *d* stands to indicate "disposal"), *Q* is the radionuclide disposal rate (Bq/y) and  $\lambda_r$  is the radioactive decay constant of the radionuclide under consideration. On the other hand, the release rate  $R_p$  (Bq/y) of a radionuclide into the groundwater after closure of the repository at time *T* is:

$$
R_p(t) = S_p(t) \cdot f_s(t+T)
$$
\n(4)

where  $S_p(t) = S_d(T) \cdot e^{-\lambda_r t}$  (Bq) is the inventory of the radionuclide after a time *t* from closure of the disposal facility (the index p stands to indicate post-closure).

In the hypotheses that *i*) the prevalent advective component in the groundwater flow allows representation in one dimension and *ii*) the repository release is dimensionless, the timedependent concentrations  $(Bq/m^3)$ ) of the radionuclide in the groundwater before the closure of the repository can be evaluated as the convolution integral [8]:

$$
C_d(x,t) = \int_0^t R_d(t-\tau)C_g(x,\tau)d\tau
$$
 (5)

where *t* is the time elapsed since the beginning of the disposal operations and  $x$  is the longitudinal distance in the flow direction; similarly, the concentrations after the closure of the repository can be evaluated as [8]:

$$
C_p(x,t) = \int_0^T R_d (T - \tau) C_g(x, t + \tau) d\tau + \int_0^t R_p(t - \tau) C_g(x, \tau) d\tau
$$
\n(6)

where *t* is the time elapsed from the termination of the disposal operations. In both equations,  $C_g(x, t)$ is the solution of the one-dimensional advectiondispersion equation with instantaneous point source [18]:

$$
C_g(x,t) = \frac{e^{-\lambda_r t} e^{-(x-U_{x}^1)^2/(4D_{x}^1)}}{2\pi AR\theta \sqrt{D_x^1 t}}
$$
(7)

where  $U_x^1 = U_x / R$  is the retarded groundwater velocity (m/y),  $D_x^1 = D_x / R$  is the retarded longitudinal dispersion coefficient  $(m^2/y)$ , *A* is the aquifer cross sectional area  $(m^2)$ ,  $R$  is the retardation factor defined as  $1 + K_d \cdot \rho_b / \theta$ , where  $K_d$  is the distribution coefficient (ml/g),  $\rho_b$  is the bulk density and  $\theta$  is the effective porosity.

Finally, considering a scenario leading to drinkingwater intake, the dose  $D(x,t)$  (mSv/y) to the critical individual can be estimated as:

$$
D(x,t) = C_{d,p}(x,t) \cdot \gamma \cdot \delta \tag{8}
$$

where  $C_{d,p}$  is the concentration before and after the closure of the repository,  $\gamma$  (l/day) is the average quantity of drinking water consumed per year and  $\delta$  (mSv/Bq) is the dose conversion factor for ingestion [8], [19].

Other degradation mechanisms affecting the repository barriers may need to be taken into account in the estimation of the radionuclide release into the groundwater and the consequent dose to the critical individual; this may entail the relaxation of the assumptions of cold stand-by barriers and/or exponential failure time distributions. In this regard, one may take into consideration more realistic assumptions related to the reliability model (i.e., hot stand-by configuration of the barriers) or more comprehensive failure time distributions (i.e., which account for aging degradation behavior), making analytic solutions of the dose and the repository failure time distribution very cumbersome if not impossible.

To overcome the problems associated to finding an analytic solution to the repository probabilistic model, a Monte Carlo simulation approach is here proposed. The time horizon during which the repository is expected to maintain the integrity and perform its containment function, *Tmiss* (mission time), is discretized in channels of width ∆*t* and a fault state counter is associated to each channel  $j =$ 1,2,…, $T<sub>miss</sub>/\Delta t$ ; a large number *N* of repository evolutions are then simulated by sampling the failure times of each barrier from the related distributions; in each simulation, the counter  $C_i$ associated to the time channel *j* within which the failure time of the disposal facility occurs is increased by one. At the end of the *N* simulations,

the repository failure time probability density function (pdf)  $f<sub>s</sub>(t)$  can be estimated as:

$$
f_s(t) \approx \frac{C_j}{N \cdot \Delta t} \qquad j \cdot \Delta t \le t < (j+1) \cdot \Delta t \qquad (9)
$$

Estimation of the dose before and after closure of the disposal facility can then be numerically performed resorting to equations (5), (6) and (8): at each time step *j* the concentrations are given by the cumulated summations up to time  $t = j \cdot \Delta t$  of the products of the estimated release rates,  $R_d$  or  $R_p$ , by the function  $C_g$ , evaluated at the proper time instants.

#### **3. Results**

For validation purposes, the Monte Carlo simulation approach proposed in the previous Section is first applied to the base case of [8] and compared to the analytic results therein, with reference to the migration of a single species of radionuclide i.e., <sup>239</sup>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 activity concentration in a near-surface repository be kept below the limits prescribed by the IAEA safety requirements [20], [21].

A Monte Carlo simulation of  $N = 30 \cdot 10^6$  repository histories has been performed over a time horizon  $T_{miss} = 10^7$  y, divided in  $N_t = 10^6$  time channels of width  $\Delta t = 10$  y. The failure times of the repository barriers are sampled from exponential distributions with parameters as shown in Table 1 [8]. *Table 2* and *Table 3* summarize the physical parameters used in the simulation.

*Table 1*. Stochastic failure parameters of the repository engineered and natural barriers [8].

<b>Type</b>	<b>Barrier</b>	Failure rate $\lambda_i$ (1/y)	
a	Top cover	0.04	
b	Waste container	0.08	
$\mathbf{C}$	Waste form	0.0034	
d	<b>Backfill</b>	0.034	
e	Bottom cover	0.067	
f	Unsaturated	$1/RT_r$	
	zone		

*R* is the retardation factor and  $T_r = z/U_z$  (Table 3) is the travel time

*Table 2*. Radionuclide dependent parameters [8].

<b>Nuclide</b>	Half-life $T_{1/2}$ (y)	Waste disposal rate $O$ (Bq/v)	Range of $K_{A}$ value (ml/g)	<b>Reference</b> $K_{\lambda}$ value (ml/g)
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$$
{}^{239}\text{Pu} \quad 2.44 \cdot 10^4 \quad 1.59 \cdot 10^{10} \quad {}^{10^{3}-}_{10^{4}} \quad 2 \cdot 10^{3}
$$

 $K_d$  is the distribution coefficient of radionuclides for clay

*Table 3*. Radionuclide independent parameters [8].

<b>Parameter</b>	<b>Reference</b>	Unit
	value	
Thickness of unsaturated	0.02	m
zone $(z)$		
in Seepage velocity	$1.157 \cdot 10^{-10}$	m/s
unsaturated zone $(U_z)$		
Bulk density $(\rho_b)$	$1.7 \cdot 10^6$	$g/m^3$
Effective porosity $(\theta)$	0.3	
Ground water velocity	$1.157 \cdot 10^{-6}$	m/s
$(U_{r})$		
Aquifer cross sectional	$1.0 \cdot 10^2$	m <sup>2</sup>
area $(A)$		
Dispersivity	1	m
Longitudinal distance of	$1.6 \cdot 10^{3}$	m
well from the repository		
(x)		
End of disposal activities	50	y
(T)		
Yearly drinking water	2.2	l/day
ingestion $(y)$		
Dose conversion factor for	$1.57 \cdot 10^{-5}$	mSv/Bq
ingestion $(\delta)$		

At the end of the *N* simulated random walks, the values accumulated in the counters allow estimating the repository failure time pdf  $f_s(t)$  (9). Neglecting for simplicity the radionuclides that are generated by the decay chains of other radioactive elements contained in the repository, its time dependent concentration in the groundwater before and after closure,  $C_d(x,t)$  and  $C_p(x,t)$  (Bq/m<sup>3</sup>) respectively, and the associated dose from drinking water ingestion  $D(x,t)$  (mSv/y) can then be estimated resorting to equations (5), (6) and (8). The comparison between the Monte Carlo estimates of the <sup>239</sup>Pu release rate, and related dose from ingestion of drinking water at a well 1.6 km downstream from the disposal site, with the semianalytic solutions, obtained by coupling equation (2) with equations  $(5)$ ,  $(6)$  and  $(8)$ , shows a satisfactory agreement (*Figure 2 (a)* and *Figure 2(b)*, respectively).

In a realistic setting, the failure behavior of the engineered barriers may be affected by phenomena additional to water infiltration and degradation. For example, a concrete structure may show a tendency to cracking due to settling of the structure under gravity forces or temperature-induced volume changes [15]. In such cases, when a concrete barrier of the repository is reached by the infiltrating water, its containment functionality

may already be compromised and the water, possibly transporting the radionuclides, could cross the barrier in a relatively short period of time: from the viewpoint of reliability modelling, the barrier can be considered in a "hot stand-by" configuration, i.e. it may fail before being called to operation [17]. This behavior renders an analytic solution approach impractical; on the contrary, the Monte Carlo simulation approach does not suffer of this.

*Figures 3* (a) and (b) show the results of a Monte Carlo simulation of  $N = 30 \cdot 10^6$  repository histories with the barrier e (i.e., the bottom concrete cover) in a hot stand-by: during stand-by, the failure times of this barrier are distributed according to an exponential distribution with parameter  $\lambda_e^H = 1.34$  $1/y$ ; in operation (i.e. when called to perform its containment function because of failure of the preceding barrier, *d*), the failure times are exponentially distributed with parameter  $\lambda_e = 0.067$  1/y. As before, the time horizon  $T_{miss} =$  $10^7$  y has been divided in  $N_t = 10^6$  time channels of width  $\Delta t = 10$  y. The Monte Carlo estimate of the <sup>239</sup>Pu release rate (solid line) is slightly larger than that corresponding to the semi-analytic solution of the base case of [8] (dashed line) for approximately the first 300 years and then the two curves basically coincide (*Figure 3 (a)*)*:* this is due to the fact that at larger times, the repository failure behavior is dominated by the last barrier *f*, i.e. the unsaturated zone, which is not affected by the model change. In order to enhance the effects of the hot stand-by failure mode in the first 300 years, the corresponding failure rate has been assumed  $\lambda_e^H = 20 \cdot \lambda_e$  $e_{e}^{H} = 20 \cdot \lambda_{e}$ . The difference in the corresponding doses, plotted in *Figure 3 (b),* is correlated with the Monte Carlo estimated release rate for the first 300 years, as an effect of the hot stand-by assumption for barrier e; at larger times the two curves of the dose (Monte Carlo estimate and analytic solution) overlap (their difference is negligible).

Other considerations of structure degradation dynamics may be included in the model by a proper choice of the pdfs, as derived from actual experiments or detailed analysis at local scales [6], [16], [22].

*Figures 4* (a) and (b) show the results of a Monte Carlo simulation of  $N = 30.10^6$  repository evolutions where the engineered barriers aging degradation behavior is described by Weibull distributions [17]:

$$
f_i(t) = \alpha_i \beta_i t^{\alpha_i - 1} e^{-\beta_i t^{\alpha_i}} \quad i = a, b, \dots e
$$
 (10)

Table 4 reports the values of the parameters  $\alpha_i$ ,  $\beta_i$ used in the simulation. The Monte Carlo estimates of the  $^{239}$ Pu release rate (solid line) are sensibly larger than those obtained by the semi-analytic solution for the base case of [8] (dashed line) for approximately the first 1000 years (*Figure 4 (a)*), due to the fact that the chosen Weibull probability densities favor smaller failure times than the exponential ones in (1); as in the previous case, at larger times the stochastic behavior of the last barrier *f*, i.e. the unsaturated zone, becomes dominant and the two curves overlap. *Figure 4 (b)* shows that the difference in the related doses is correlated with the Monte Carlo-estimated release rate for approximately the first 1000 years, as an effect of the aging degradation behavior of the barriers; at larger times the two curves of the dose (Monte Carlo estimate and analytic solution) overlap (their difference is negligible).

The computational times for the Monte Carlo simulation is approximately 4.5h and for the semianalytic computation of the dose is approximately 1h, on a Pentium 4 CPU 1.73GHz. The memory space allocated is of the order of 10 MB.

*Table 4*. Weibull failure time distribution parameters.

Type	<b>Barrier</b>	$\alpha$	
a	Top cover	1.3	0.04
b	Waste container	1.3	0.08
c	Waste form	1.3	0.0034
d	<b>Backfill</b>	1.3	0.034
e	<b>Bottom</b> cover	1.3	0.067
f	Unsaturated zone		$1/R_aT_r$

 $R_d$  = retardation factor;  $T_r$  = travel time





*Figure 2.* Base case [8]. (a) Estimated <sup>239</sup>Pu release rate and (b) corresponding dose from ingestion of drinking water of a well 1.6 km downstream of the repository area: Monte Carlo simulation (solid line) and semi-analytic solution (dotted line).



*Figure 3*. Barrier *e* in hot stand-by. (a) Estimated  $^{239}$ Pu release rate and (b) difference in the corresponding dose from ingestion (dotted line).





*Figure 4*. Weibull failure time distribution for the engineered barriers. (a) estimated  $^{239}$ Pu release rate and (b) difference in the corresponding dose from ingestion (dotted line).

From the physical point of view, the findings of the analyses performed show that the effects of one barrier in "hot stand-by" configuration and barrier failure times distributed according a Weibull pdf are negligible, ranging from approximately 1% of the peak dose for the former case to approximately 0.01% of the peak dose for the latter case. This is due to the slow migration of the  $^{239}$ Pu radionuclide, which is retarded by its strong adsorption onto the porous transport media (large value of the partition coefficient  $K_d$ ): the early effects on the release rates (up to approximately  $10^3$  years) dilute as the migration process approaches  $10^5 - 10^6$  years.

#### **4. Conclusions**

The main objective of the PSA of a radioactive waste repository is that of verifying the compliance of the expected radiation doses with the legally imposed limits 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 stochasticity of the processes involved and the uncertainties in their 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, to resort to analytical approaches. On the contrary, Monte Carlo simulation offers the potential flexibility needed to realistically describe the occurring phenomena.

In this paper, a Monte Carlo simulation-based reliability model has been developed for the preliminary evaluation of the safety performance of a radioactive waste repository. The simplicity of the model has been demonstrated to allow ease of computation, whereas its flexibility has allowed accounting for various physical aspects and intercomparison of their effects.

The proposed simulation scheme has been first validated on a simple case study of literature; then the flexibility of the stochastic simulation has been exploited to represent realistic phenomena of non– sequential failure of the barriers and ageing.

From the point of view of the physical findings on the case study analyzed, it turns out that the effects of the realistic modelling assumptions introduced are indeed significant on the release rates estimates, but eventually the corresponding doses are not affected very much due to the migration properties of the particular radionuclide analyzed.

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