Sensitivity analyses of a fast analytical radionuclide transport and dose model

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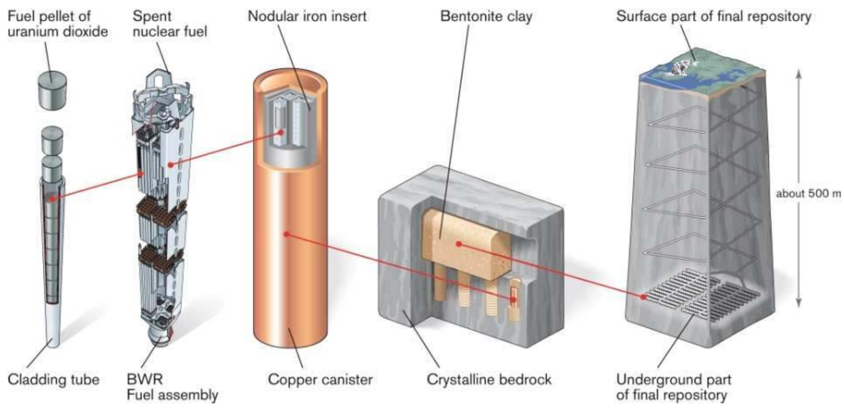
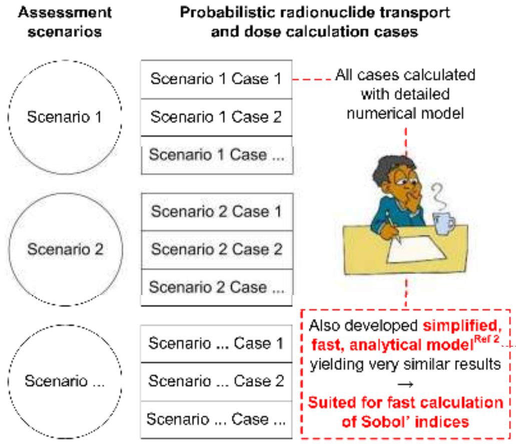
1. Final repository for spent nuclear fuel



2. Assessment of long-term safety[Ref. 1]



3. Method for calculation of higher order Sobol' indices for simple analytical model

3a. Starting point: best practices for 1st order indices in Saltelli et al (2010)[Ref 3]

$$V_{X_i}\left(E_{X_{\sim i}}(Y|X_i)\right)=\frac{1}{N}\sum_{R=1}^{N} f(\mathbf{B})_R\left(f\left(\mathbf{A}_{\mathbf{B}}^{(i)}\right)_R - f(\mathbf{A})_R\right)$$

Index $i = 1$ to k denotes variables; Index $R = 1$ to N denotes model realisations

Highly improved convergence with QMC sampling

3b. Extended this to higher order indices

$$V_{X_{i,j}}\left(E_{X_{\sim i,j}}(Y|X_{i,j})\right)=\frac{1}{N}\sum_{R=1}^{N} f(\mathbf{B})_R\left(f\left(\mathbf{A}_{\mathbf{B}}^{(i,j)}\right)_R - f(\mathbf{A})_R\right)$$

$$V_{X_{i,j,k}}\left(E_{X_{\sim i,j,k}}(Y|X_{i,j,k})\right)=\frac{1}{N}\sum_{R=1}^{N} f(\mathbf{B})_R\left(f\left(\mathbf{A}_{\mathbf{B}}^{(i,j,k)}\right)_R - f(\mathbf{A})_R\right)$$

Etc.; Highest order indices obtained as 1 – sum of all other

Note: With this approach total indices T_i are obtained directly from all S containing index i.

3c. Testing the method for higher order indices

Test case: Sobol' G-function of order 5: $G=\prod_{i=1}^{5}\frac{|4X_i-2|+a_i}{1+a_i}$ and $a_i = 0,\ \forall i$

$V = 3.21$; $S_i = 0.104\ \forall i$; $S_{ij} = 0.0346\ \forall i, j$; $S_{ijk} = 0.0115\ \forall i, j, k$;

$S_{ijkl} = 0.00384\ \forall i, j, k, l$; $S_{12345} = 0.00128$

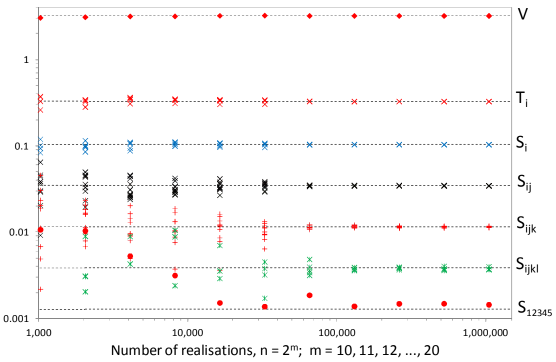
QMC sampling; modified freeware from www.broda.co.uk[Ref 4]

Good convergence

- for variance (V) after ~2^{10} = 1024 realisations
- for total order indices (T_i) after ~2^{12} = 4096 realisations
- for higher order indices (S_i to S_{12345}) after between 2^{13} to 2^{17} (8192 to 131,072) realisations

Total number of model realisations in test: $2^k \times N = 2^5 \times 2^{20}$ = 33,554,432
Total run time: 109 seconds on ordinary laptop and Microsoft Excel VBA

Tested also the triplet **B**, **A** and $\mathbf{B}_{\mathbf{A}}^{(i,\ldots)}$ with similar results.



4. Application to fast analytical radionuclide transport and dose model

Uncertain input parameters

$i = 1$ Sorption coefficient for Radium, K_d^{Ra}
$i = 2$ Effective diffusivity for cations, D_e
$i = 3$ Conversion rate of fuel matrix, D_{Fuel}
$i = 4$ Hyrdological transport resistance in rock, F
$i = 5$ Time of canister failure, $t_{Failure}$

$$Dose^{Ra226} \propto D_{Fuel}\left(t_{Max}-t_{Failure}\right)\exp\left\{\frac{Pe}{2}\left[1-\sqrt{1+\frac{4t_w\lambda^{Ra226}}{Pe}\left(1+\frac{F\sqrt{\left(\varepsilon_p+(1-\varepsilon_p)K_d^{Ra}\rho\right)D_e}}{t_w\sqrt{\lambda^{Ra226}}}\right)}\right]\right\}$$

Result : Calculated sensitivity indices for the Ra-226 dose at 10^6 years

1st order	
S_1	0.0188
S_2	0.0087
S_3	0.1266
S_4	0.2971
S_5	0.0399

2nd order	
S_{12}	0.0005
S_{13}	0.0155
S_{23}	0.0072
S_{14}	0.0152
S_{24}	0.0068
S_{34}	0.2453
S_{15}	0.0049
S_{25}	0.0023
S_{35}	0.0330
S_{45}	0.0774

3rd order	
S_{123}	0.0004
S_{124}	0.0008
S_{134}	0.0126
S_{234}	0.0056
S_{125}	0.0001
S_{135}	0.0040
S_{235}	0.0019
S_{145}	0.0040
S_{245}	0.0018
S_{345}	0.0639

4th order	
S_{1234}	0.0007
S_{1235}	0.0001
S_{1245}	0.0002
S_{1345}	0.0033
S_{2345}	0.0015

5th order	
S_{12345}	0.0002

Total order	
T_1	0.0812
T_2	0.0387
T_3	0.5216
T_4	0.7361
T_5	0.2383

Notes on calculation and results

- Input data distributions transformed to uniform distributions on $0 \le x_i \le 1$
- QMC sampling; modified freeware from www.broda.co.uk[Ref 4]
- Total number of model realisations: 33,554,432 (as in test case)
- Total run time: 540 seconds on ordinary laptop and Microsoft Excel VBA
- S_3 and S_4 dominate 1st and total order, S_{34} dominates 2nd order

5. References

1. Swedish Nuclear Fuel and Waste Management Co., SKB, "Long-term Safety for the Final Repository for Spent Nuclear Fuel at Forsmark. Main Report of the SR-Site Project," SKB Technical report TR-11-01, 2011. Available at www.skb.se
2. A. Hedin, "Integrated analytic radionuclide transport model for a spent nuclear fuel repository in saturated fractured rock", *Nuclear Technology*, **138**, pp 179–205, 2002.
3. A. Saltelli, P. Annoni, I. Azzini, F. Campolongo, M. Ratto and S. Tarantola, "Variance based sensitivity analysis of model output. Design and estimator for the total sensitivity index", *Computer Physics Communications* **181**, pp 259–270, 2010.
4. Freeware for QMC sampling (SobolSeq generator for Microsoft Excel) from www.broda.co.uk