Sensitivity Analysis of Probabilistic Dose Results in SKB's License Application

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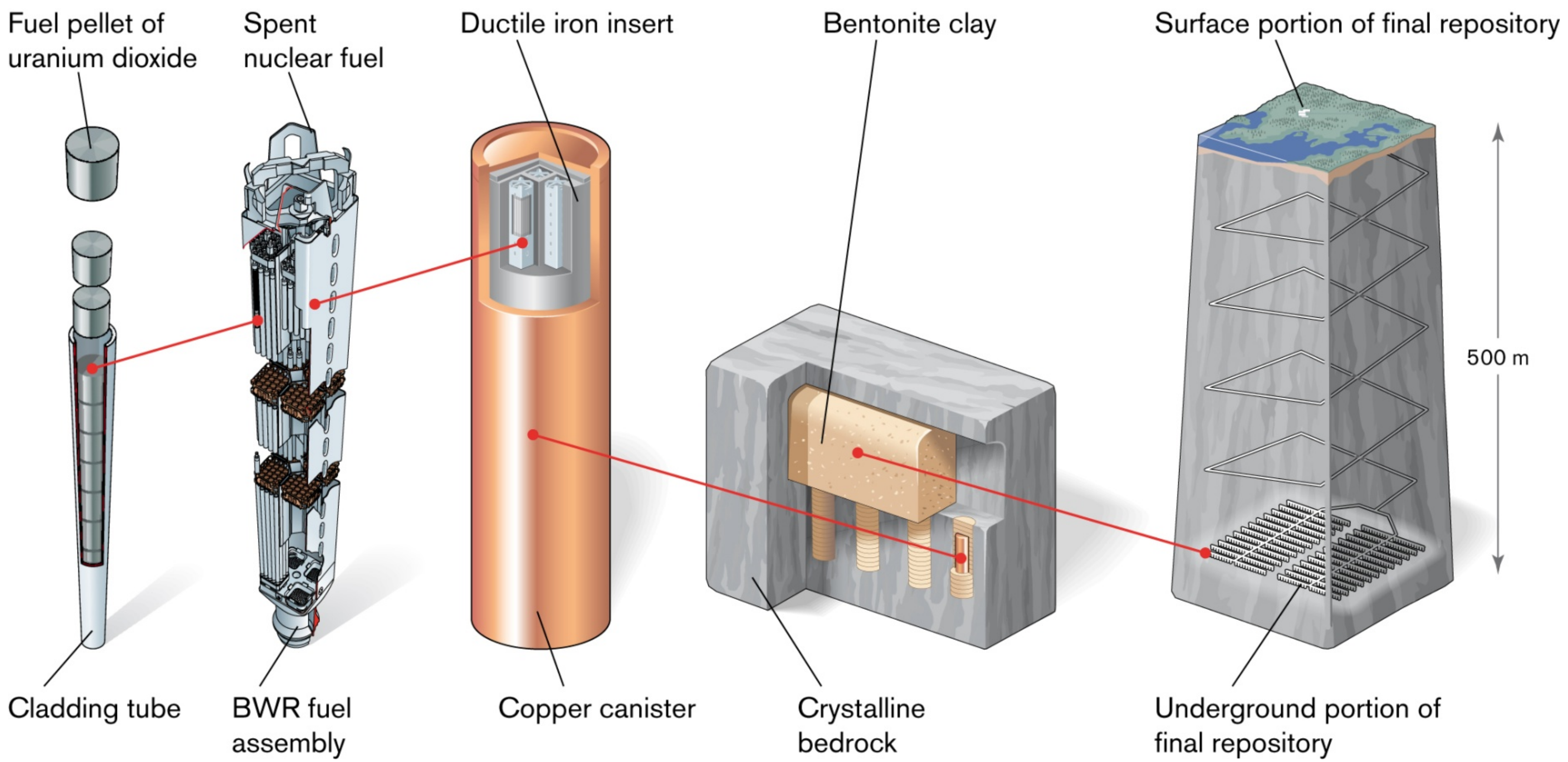
Background

- On March 16, 2011 SKB applied for licences
  - to construct and operate an encapsulation plant for spent nuclear fuel in the municipality of Oskarshamn
  - to construct and operate a KBS-3 repository for final disposal of spent nuclear fuel at the Forsmark site in the municipality of Östhammar
- The safety assessment SR-Site is a key component in the safety case for the final repository
- The safety case is currently under review by the Swedish Radiation Safety Authority, SSM
- This presentation concerns sensitivity analyses of probabilistic dose results in SR-Site
  - Some results are included in the assessment, some were obtained later

The KBS-3 concept



Primary safety function: Complete containment

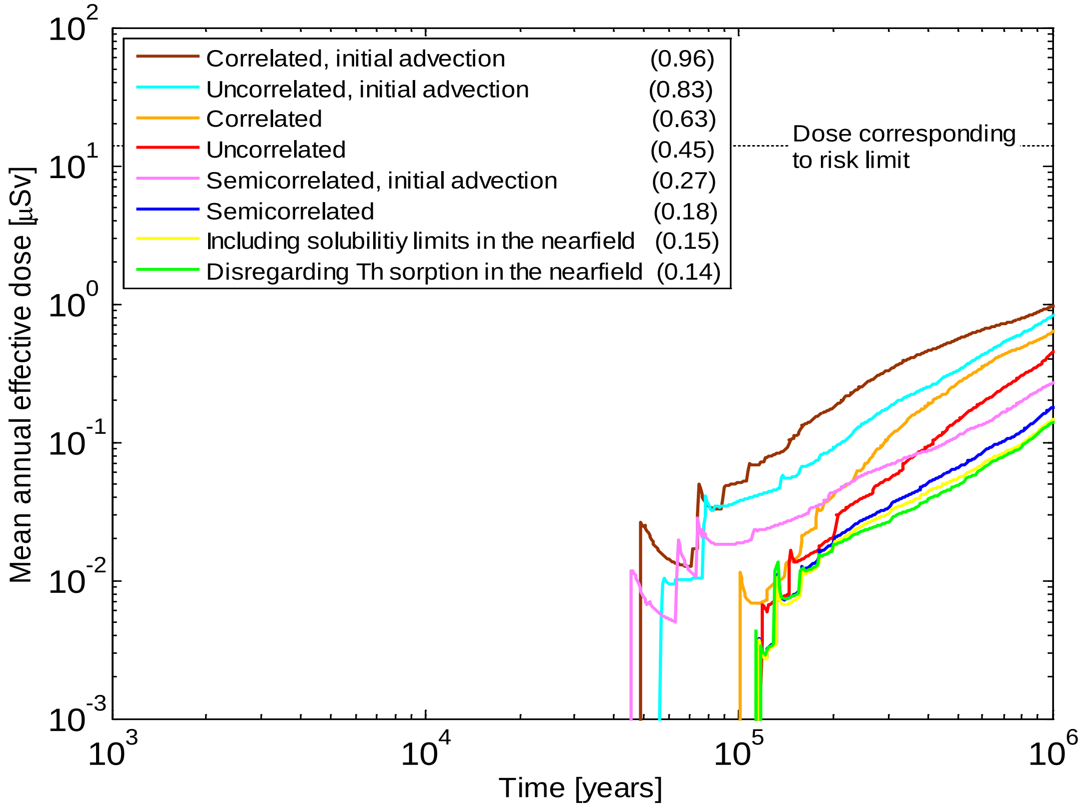
Secondary safety function: Retardation

Dose results

- All 6,000 canisters are expected to be tight at deposition.
- Two failure modes of the canister could not be ruled out in the safety assessment and hence contribute to risk
  - Canister failure due to **earthquake** induced secondary shear movements in rock fractures intersecting a canister position
  - **Canister** failure due to enhanced **corrosion** following loss of the protecting clay buffer as a result of **buffer erosion**
- The latter dominates, and is addressed in the following

Probabilistically calculated doses; erosion/corrosion scenario

- A number of probabilistic cases to explore impact of uncertainties related to erosion, corrosion, transport
  - Mean dose as a function of time shown for each case in figure
  - No failure is also possible!
- All cases dominated by Ra-226 @ 1MYr
- Case with highest consequences used to demonstrate compliance



Sensitivity analysis methods, overview

- Of interest to determine

  A. input parameters that correlate most strongly with dose over entire dose range; Global sensitivity analysis; methods:

     1. *standardized rank regression coefficients (SRRC) – not further discussed*
     2. variance based sensitivity indices

  B. input parameter values that are related to high and low doses; methods:

     1. *conditional mean values – not further discussed*
     2. cobweb plots

- Will also show tailored regression model
  - demonstrates how the variability in the output can be explained with analytic expressions derived from the conceptual understanding of the transport processes

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A. Global sensitivity analysis
2) Variance based method (Sobol' indices)

- Variance of output decomposed into terms attributable to single inputs and to combinations of inputs
- Yields good understanding of sensitivites but computationally costly
  - Dose calculations in SR-Site done with comparatively fast numerical models; ~one minute per realization.
  - Also: key results can be reproduced with simple analytical expressions; ~1/10 second per realization
  - Further, considerable reduction if only <u>peak dose</u> of <u>dominating</u> nuclide calculated
  - Thus good potential for these simplified models to be efficiently used in the determination of variance based sensitivity indices.
- The number of realizations required for variance based sensitivity analysis reduced by sampling scheme utilizing quasi random numbers (QMC sampling)
  - Much more efficient than random numbers (MC) or Latin Hypercube Sampling (LHS).

Computing Sobol indices for SR-Site dose results

- Used simplified analytical expressions to calculate peak dose over time

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

- Sampled five uncertain input variables…
  - K_d for Ra (sorption coefficient in rock matrix)
  - D_e for cations (effective diffusivity in rock matrix)
  - D_{Fuel} (dissolution rate of the spent fuel)
  - F (flow related transport resistance parameter in rock)
  - $t_{Failure}$ (time of canister failure)
- …according to Quasi Monte Carlo scheme, QMC
  - Software for QMC scheme from www.broda.co.uk

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Computing Sobol indices…

- 5 input variables means $2^5-1 = 31$ first and higher order Sobol' indices to be calculated
- One million model realisations for each of the 2^5-1 indices,
  - i.e. in total about 30 million realisations.
  - Required only a couple of minutes of calculation time due to extremely fast model

Sobol sensitivity indices for the Ra-226 dose at 10^6 years. Uncertain input parameters:

1 = K_d for Ra, 2 = D_e for cations, 3 = D_{Fuel}, 4 = F, 5 = $t_{Failure}$

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

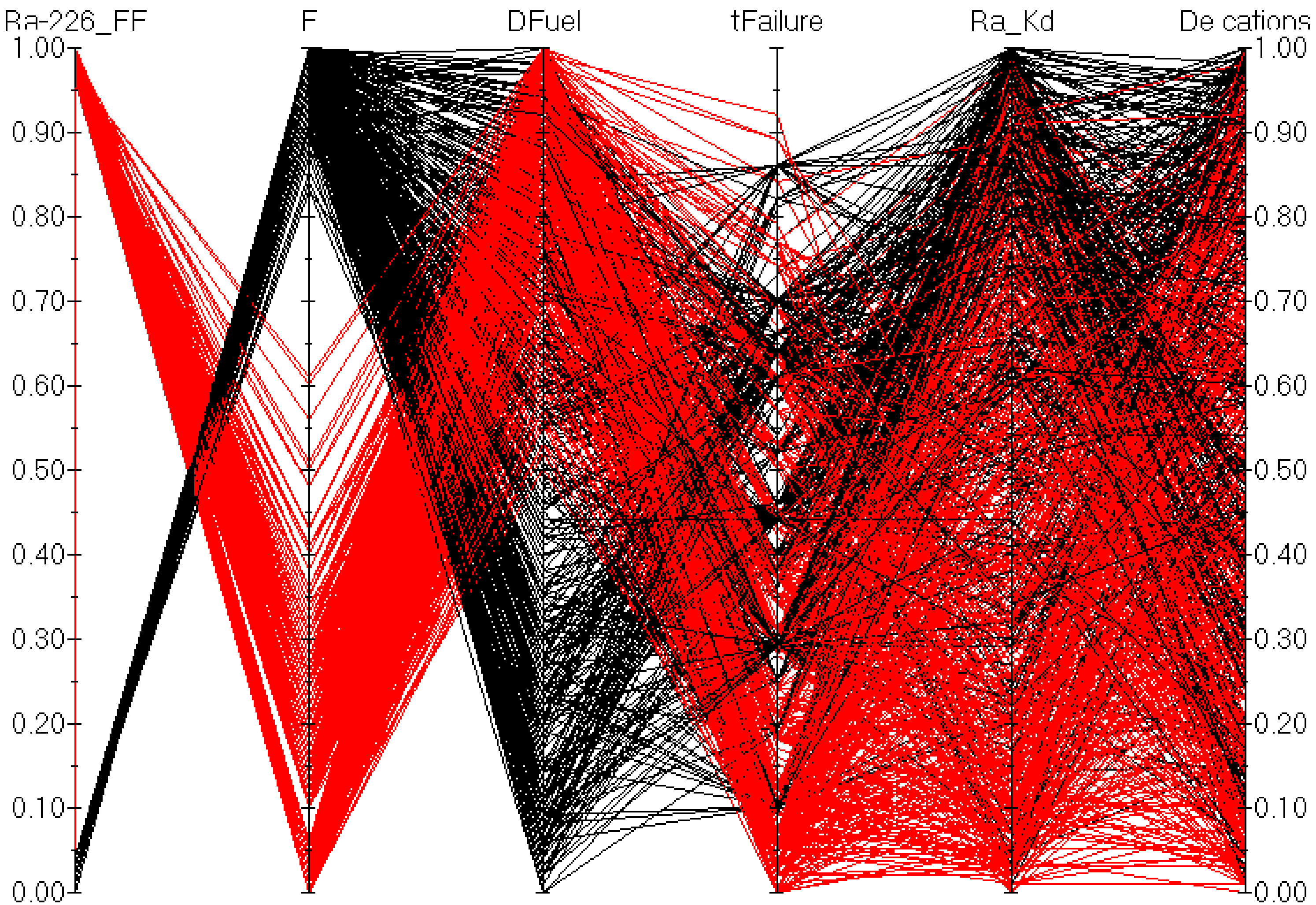
Comments on results

- Example to demonstrate feasibility
- Sobol indices did not really yield new information about uncertainties in this particular case
- Unrealistic to calculate full set of Sobol indices in most cases
- Has been demonstrated that first order indices, together with so called total order indices sometimes yield useful sensitivity results at a reasonable computational cost
  - Still, computational costs to determine Sobol indices are prohibitive in many cases

B. Variables correlated with extreme doses
2) Cobweb plots

- Straightforward method to visualize relationships between input and output data for probabilistic modeling results
- Freeware available at http://risk2.ewi.tudelft.nl/oursoftware/3-unicorn

Cobweb plot

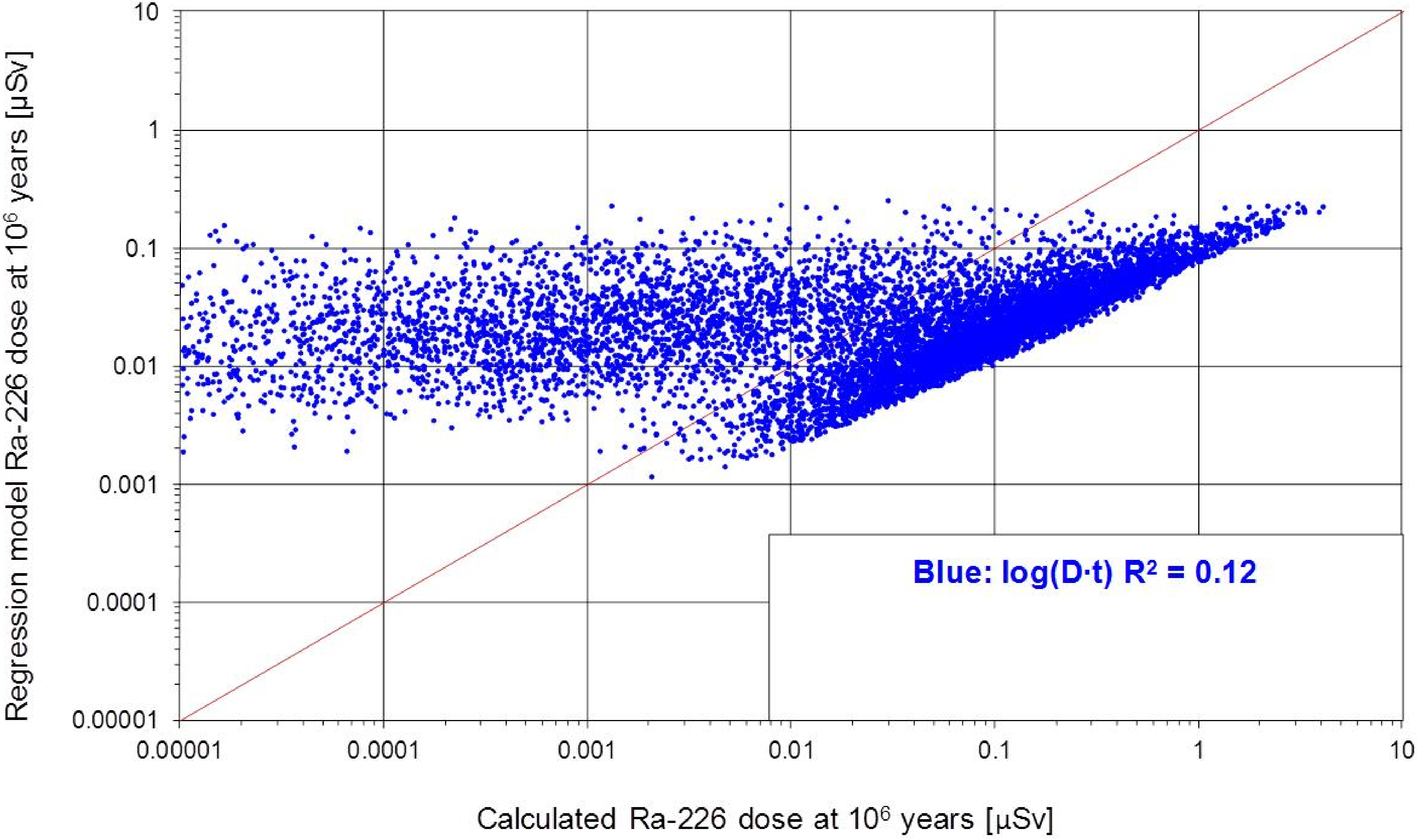

Ra-226_FF
F
DFuel
tFailure
Ra_Kd
De cations
1.00
0.90
0.80
0.70
0.60
0.50
0.40
0.30
0.20
0.10
0.00

Tailored regression model

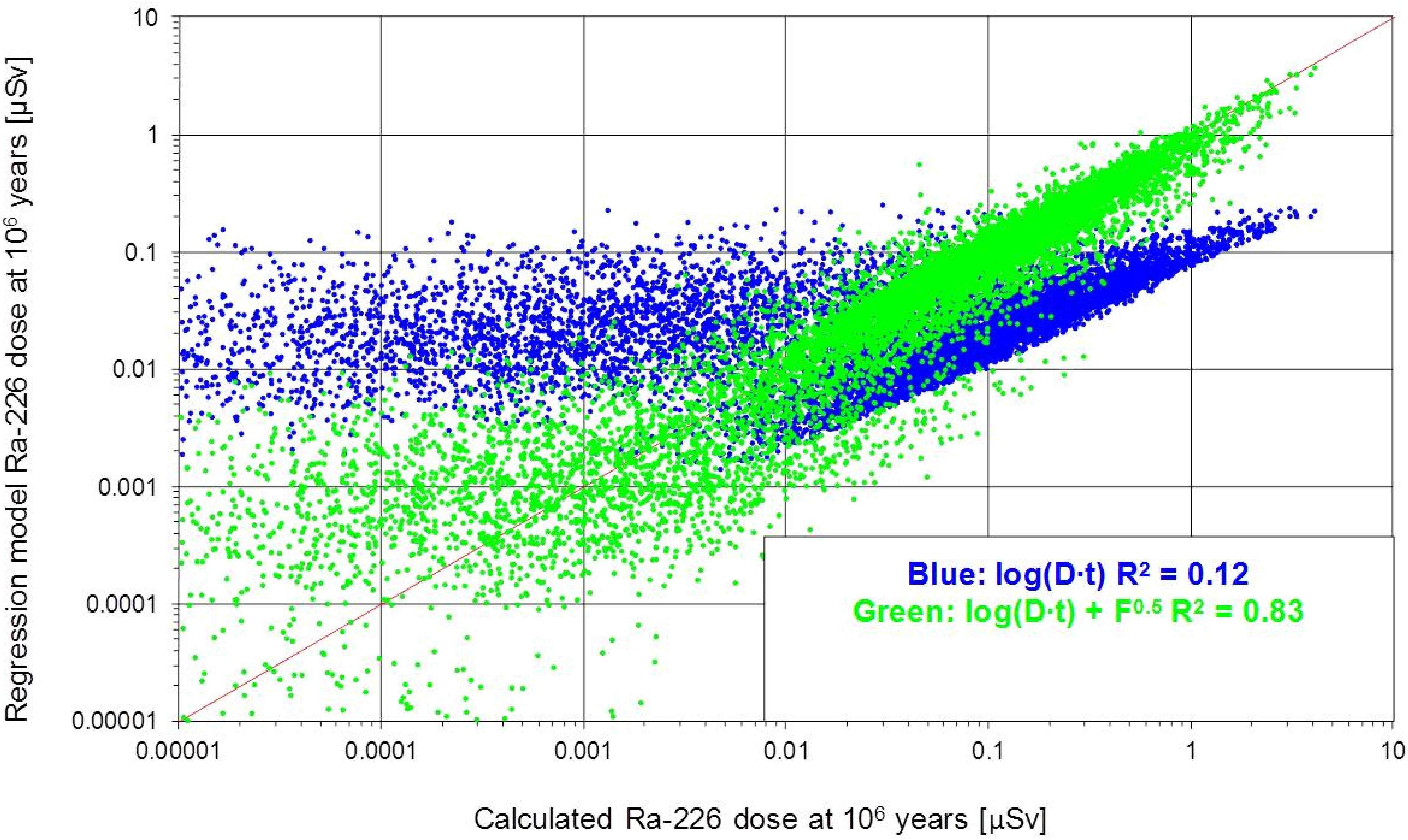
- Simple analytical expressions suggests that the Ra-226 dose varies according to

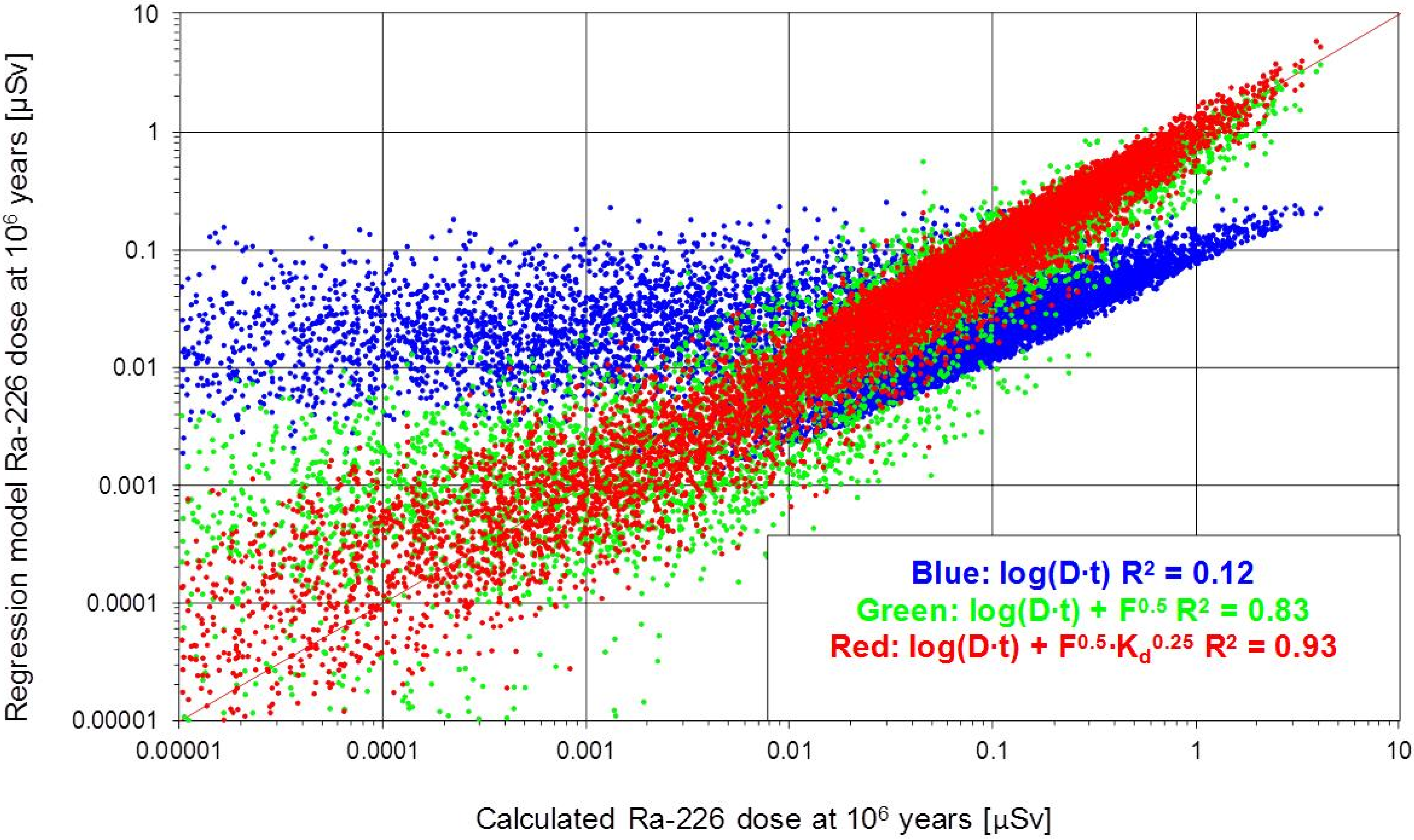
  $\log(Dose_{Ra226}) = Constant + \log(D_{Fuel} \cdot t) - cF^{0.5} \cdot (K_d D_e)^{0.25}$

- Therefore, regress log(DoseRa226) on the transformed variables
  - $D_{Fuel} \cdot t$
  - $D_{Fuel} \cdot t$ and $F^{0.5}$
  - $D_{Fuel} \cdot t$ and $F^{0.5} K_d^{0.25}$
  - $D_{Fuel} \cdot t$ and $F^{0.5} (K_d D_e)^{0.25}$



10
1
0.1
0.01
0.001
0.0001
0.00001
0.00001
0.0001
0.001
0.01
0.1
1
10
Regression model Ra-226 dose at 10^6 years [µSv]
Calculated Ra-226 dose at 10^6 years [µSv]
Blue: log(D·t) R² = 0.12


Regression model Ra-226 dose at 10⁶ years [μSv]
10
1
0.1
0.01
0.001
0.0001
0.00001
0.00001
0.0001
0.001
0.01
0.1
1
10
Blue: log(D·t) R^2 = 0.12
Green: log(D·t) + $F^{0.5}$ R^2 = 0.83
Calculated Ra-226 dose at 10^6 years [μSv]


Regression model Ra-226 dose at 10^6 years [µSv]
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0.1
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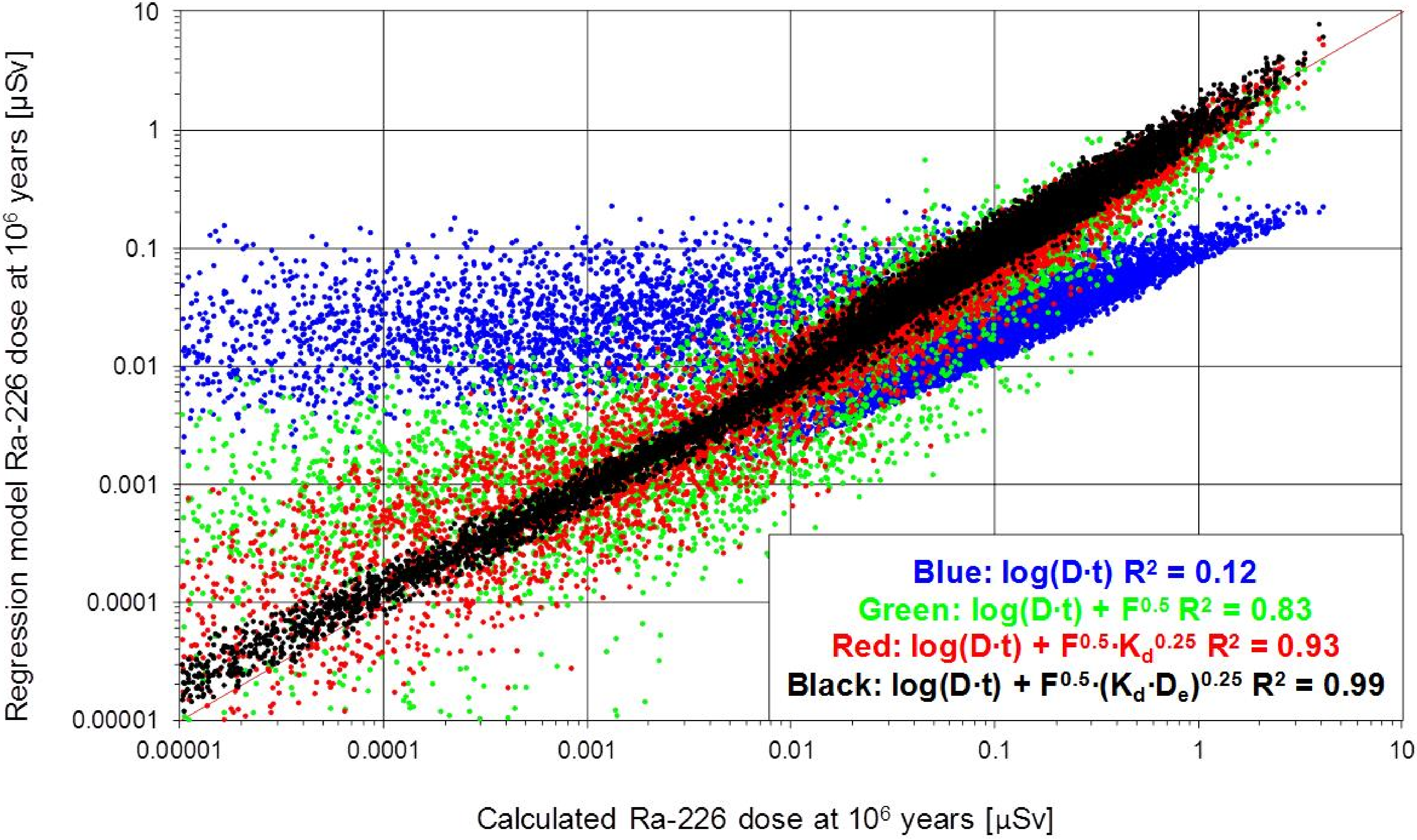
0.00001
0.00001
0.0001
0.001
0.01
0.1
1
10
Blue: log(D·t) R² = 0.12
Green: log(D·t) + F^0.5 R² = 0.83
Red: log(D·t) + F^0.5·K_d^0.25 R² = 0.93


10
1
0.1
0.01
0.001
0.0001
0.00001
0.00001
0.0001
0.001
0.01
0.1
1
10
Regression model Ra-226 dose at 10^6 years [µSv]
Calculated Ra-226 dose at 10^6 years [µSv]
Blue: log(D·t) R^2 = 0.12
Green: log(D·t) + $F^{0.5}$ R^2 = 0.83
Red: log(D·t) + $F^{0.5} \cdot K_d^{0.25}$ R^2 = 0.93
Black: log(D·t) + $F^{0.5} \cdot (K_d \cdot D_e)^{0.25}$ R^2 = 0.99

Summary (1/2)

- Several methods for sensitivity analysis yield similar results regarding
  A. input parameters that correlate most strongly with dose over entire dose range; Global sensitivity analysis; methods:
     1. standardized rank regression coefficients (SRRC)
     2. variance based sensitivity indices (Sobol' indices)
  B. input parameter values that are related to high and low doses; methods:
     1. conditional mean values
     2. cobweb plots
- Tailored regression model demonstrates how output variability is explained with analytic expressions derived from the conceptual understanding of the transport processes
- Mathematical understanding and simplification of transport processes necessary for some of these methods (Sobol' indices, tailored regression model)

Summary (2/2)

- Important uncertain parameters are
  - The fuel degradation rate
  - The rock transport resistance
  - The time of canister failure
- Important uncertain factors not included in this analysis
  - The conceptual understanding of buffer erosion
  - The sulfide concentration in the groundwater
  - Biosphere dose conversion factors

Thank you for your attention!

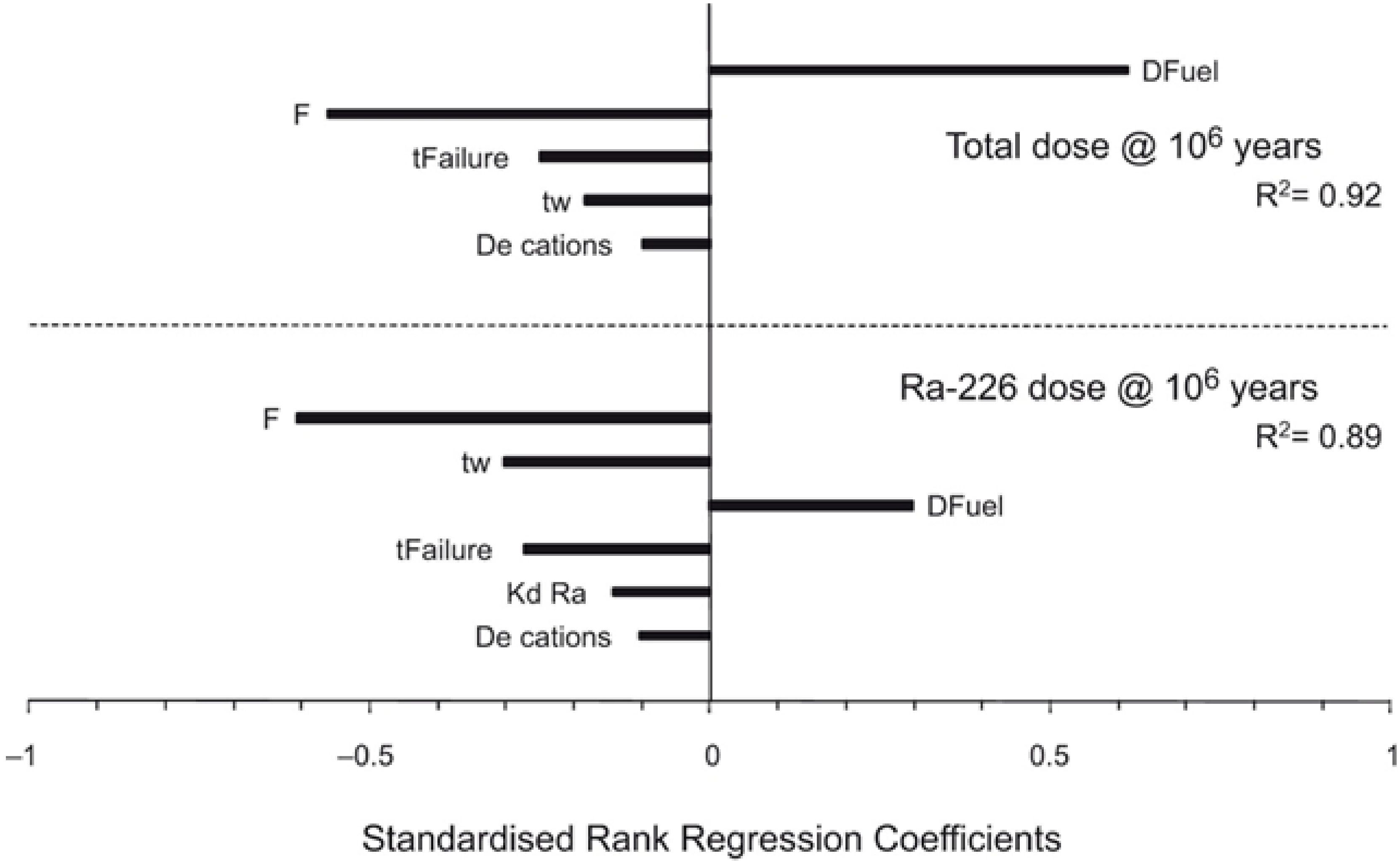
- Kastriot Spahiu & Lena Zetterström Evins, fuel
- Christina Lilja, canister
- Patrik Sellin, buffer, backfill and sealing
- Ignasi Puigdomenech & Birgitta Kalinowski, geochemistry
- Raymond Munier, geology
- Jan-Olof Selroos, ground water flow and transport
- Tobias Lindborg & Ulrik Kautsky, biosphere
- Jens-Ove Näslund, climate
- Fredrik Vahlund, input data, QA modeling
- Martin Löfgren (Niressa AB), input data
- Christina Greis & Maria Lindgren, radionuclide transport
- Kristina Skagius, assistant project manager, FEP data base, intrusion, QA
- Ann-Mari Nisula, administration, QA
- Johan Andersson, co-ordination EBS initial state, rock mechanics issues, BAT issues, design feedback, etc
- Allan Hedin, project manager, methodology, etc

Extra

A. Global sensitivity analysis
1) Standardized rank regression, SRRC

- Data in each input and output distribution is replaced by its rank order within that distribution. Hereby, non-linear features of the distributions are "linearized".
- Regress ranked output data on ranked input data, SRRC = regression coefficients
- SRRC measures monotonic change in output vs. monotonic change in input
- Standard method frequently used in similar contexts

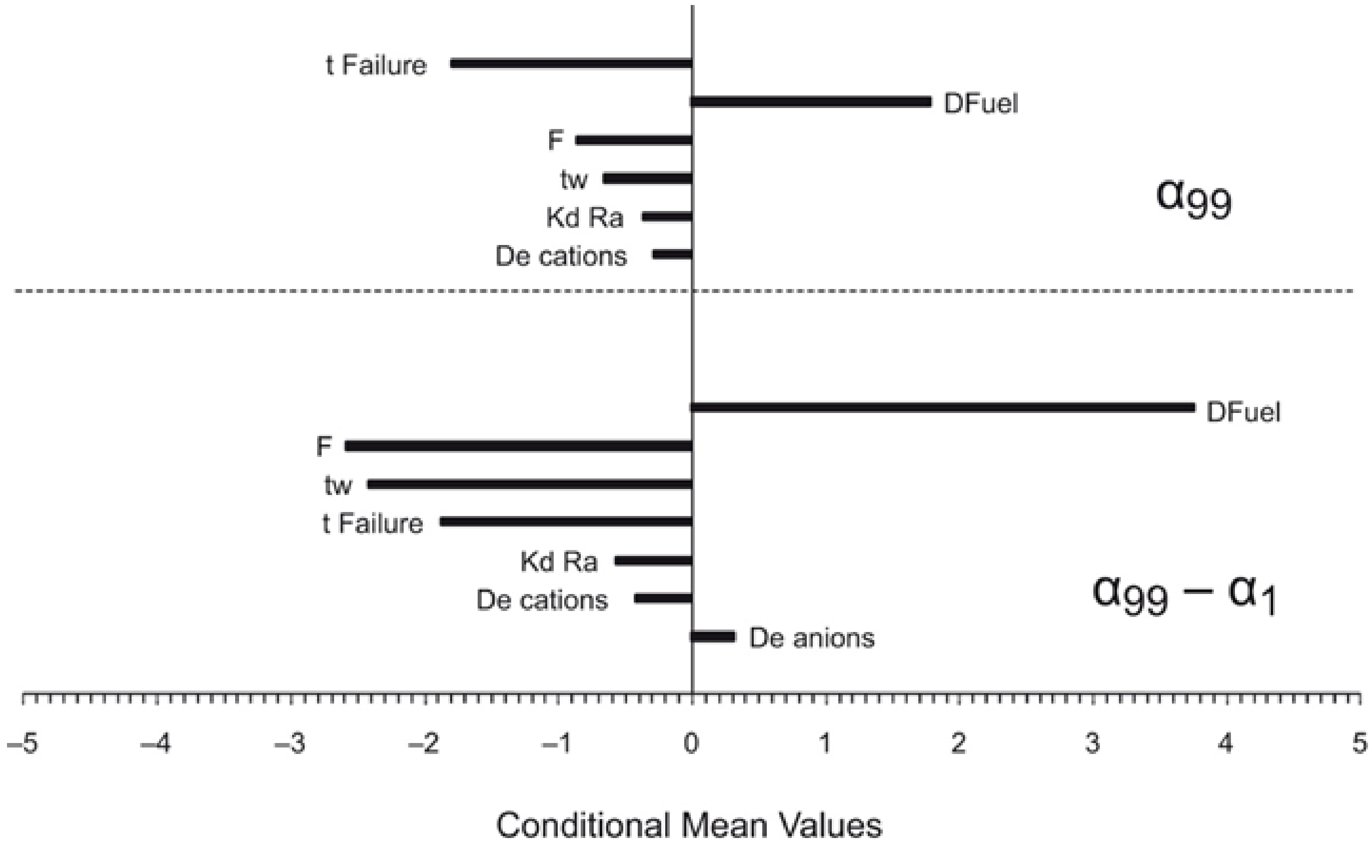
SRRC results for total and Ra-226 dose at 10^6 years



B. Variables correlated with extreme doses
1) Conditional mean values

- Consider top 1% of dose results. For each input variable:
  - Determine mean of input data for top 1%
  - Divide by mean of entire input data distribution
  - Ratio, called α_{99}, informs about correlations of high or low values of input parameter to high dose results
- Similarly, consider bottom 1% of dose results
  - α_1, informs about correlations of high or low values of inpout parameter to high dose results
- May also form $\alpha_{99}-\alpha_1$, to more clearly identify variables for which extreme values relate to extreme inputs

Conditional mean values



Sobol' indices

- Consider model with three uncertain input parameters x_1, x_2 and x_3 with total output variance V.
- It can be shown that, under certain general conditions, V can be decomposed according to
- $V = V_1 + V_2 + V_3 + V_{12} + V_{13} + V_{23} + V_{123}$
  - V_1 = reduction in total output variance V resulting if variable x_1 known, averaged over the distribution of x_1-values.
  - V_1 hence a measure of how much input variable x_1 alone contributes to the total output uncertainty,
  - I.e. a measure of the importance of variable x_1 with respect to output uncertainty
- Higher order terms express variance due to interactions
- Sensitivity indices S defined as quotient of the corresponding variance term and the total variance, $S_1 = V_1/V$, etc
- $\Sigma S = S_1 + S_2 + S_3 + S_{12} + S_{13} + S_{23} + S_{123} = 1$
- S also called Sobol' sensitivity indices after Russian mathematician I.M. Sobol'