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Source Term Modelling Parameters for Project-90

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Contents

List of Tables

1 Overview

This document summarises the input parameters for the source term modelling within Project-90. In the first place, the parameters relate to the CALIBRE near-field code [1, 2] which was developed for the Swedish Nuclear Power Inspectorate's (SKI) Project-90 reference repository safety assessment exercise [3]. An attempt has been made to give best estimate values and, where appropriate, a range which is related to variations around base cases. It should be noted that the data sets contain amendments to those considered by KBS-3 [4]. In particular, a completely new set of inventory data has been incorporated.

The information given here does not constitute a complete set of parameter values for all parts of the CALIBRE code. Rather, it gives the key parameter values which are used in the constituent models within CALIBRE and the associated studies. For example, the inventory data acts as an input to the calculation of the oxidant production rates, which influences the generation of a redox front. The same data is also an initial value data set for the radionuclide migration component of CALIBRE. Similarly, the geometrical parameters of the near-field are common to both sub-models. The principal common parameters are gathered here for ease of reference and avoidance of unnecessary duplication and transcription errors.

1.1 Radionuclide Inventory

Table 1 gives the radionuclide inventories, and associated half-lives for the nuclides included in the Project-90 calculations. Preliminary calculations used inventory data based on several sources [5, 6, 7, 8, 9]. For the final calculations, completely new data based on the central values of table 20 of [10] have been used. These calculations by Liljenzin give the inventory at the year 2100 based on a detailed analysis of the Swedish fuel concept.

1.2 Solubility Limits

Table 2 lists data for solubility limits in oxidising and reducing conditions [11]. The selection of data has focussed on deriving ranges of solubilities. In many cases the broad ranges given reflect the great uncertainty in these parameters that must be considered, until an acceptable procedure is chosen for discarding old or non-relevant data from further discussion.

1.3 Sorption Data

Tables 3 and 4 give the values of distribution coefficients for many of the relevant elements in granite and bentonite, as found in a literature survey [11]. Concerning sorption in granite it must be determined whether the process in question relates to sorption in micro-pores following matrix diffusion, on the joint or fracture surfaces, or in fracture in-fill which may be weathered and unlike the bulk granite material. A number of references provide values for sorption on hard rock materials but there is little discussion in the above context. However the various sources do provide starting points for discussion.

Although information about sorption on bentonite does not appear to be as extensive as might be hoped, non-equilibrium data for U, Np, Pu and Am under air saturated conditions [12] have been examined, and estimates based on these data have been incorporated in table 4. These have not altered from the preliminary estimates supplied in earlier versions of this document.

1.4 General Parameter Values

General, element and nuclide-independent parameters are listed in tables 5 and 6. It should be noted that the number of canisters is listed as 4400, rather than the 5000 specified in Project-90 and KBS-3. This error results in a total of 1.55 tonnes of spent fuel per canister, compared with 1.4 for 5000 canisters. The difference is only of the order of 10 % however, and so it is not considered to be an error which would significantly affect the results of the CALIBRE calculations.

Nuclide	Inventory g/T	Inventory (Bq/T)	Half-life (years)
Se-79	5.928×10^{0}	1.528×10^{10}	6.50×10^{4}
Sr-90	5.985×10^{1}	3.053×10^{14}	2.91×10^{1}
Zr-93	8.675×10^{2}	8.063×10^{10}	1.53×10^{6}
Tc-99	9.627×10^{2}	6.011×10^{11}	2.13×10^{5}
Pd-107	1.990×10^{2}	3.786×10^{9}	6.5×10^{6}
Sn-126	1.314×10^{1}	1.380×10^{10}	1.0×10^{5}
I-129	2.425×10^{2}	1.554×10^{9}	1.57×10^{7}
Cs-135	3.331×10^{2}	1.088×10^{10}	2.3×10^{6}
Cs-137	1.360×10^{2}	4.352×10^{14}	3.02×10^{1}
Ra-226	2.659×10^{-5}	9.731×10^{5}	1.60×10^{3}
Th-229	1.773×10^{-5}	1.403×10^{5}	7.34×10^{3}
Th-230	6.794×10^{-2}	4.884×10^{7}	7.70×10^{4}
Th-232	1.034×10^{-2}	4.181×10^{1}	1.41×10^{10}
Pa-231	1.905×10^{-3}	3.326×10^{6}	3.28×10^{4}
U-233	2.385×10^{-2}	8.504×10^{6}	1.59×10^{5}
U-234	3.218×10^{2}	7.426×10^{10}	2.45×10^{5}
U-235	2.486×10^{3}	1.989×10^{8}	7.04×10^{8}
U-236	2.986×10^{3}	7.148×10^{9}	2.34×10^{7}
U-238	9.446×10^{5}	1.175×10^{10}	4.47×10^{9}
Np-237	7.929×10^{2}	2.068×10^{10}	2.14×10^{6}
Pu-239	4.832×10^{3}	1.108×10^{13}	2.41×10^{4}
Pu-240	1.978×10	1.659×10^{13}	6.54×10^{3}
Pu-242	6.888×10^{2}	1.001×10^{11}	3.76×10^{5}
Am-243	2.267×10^{2}	1.675×10^{12}	7.38×10^{3}

Table 1: Inventory of radionuclides included in the CALIBRE calculations in the spent fuel in the year 2100

Elt.	Oxidising Solubility (moles per m^3)		Reducing Solubility (moles per m^3)	
	Estimate	Range	Estimate	Range
Am	4×10^{-4}	2×10^{-8} - 1	4×10^{-4}	2×10^{-8} -1
Pu	4×10^{-6}	3×10^{-9} - 6×10^{-5}	4×10^{-5}	1×10^{-6} - 3×10^{-2}
Np	1.5	1×10^{-5} - 1.5	4×10^{-6}	1×10^{-9} - 4×10^{-6}
U	0.01	1.5×10^{-4} - 0.01	4×10^{-5}	1×10^{-8} - 1×10^{-2}
Pa	1.6×10^{-5}	10^{-7} - 10^{-2}	1.6×10^{-5}	10^{-7} - 10^{-2}
Th	1.7×10^{-6}	2.6×10^{-7} - 2.2×10^{-5}	1.7×10^{-6}	2.6×10^{-7} - 2.2×10^{-5}
Ra	4×10^{-4}	10^{-5} - 0.1	4×10^{-4}	10^{-5} - 0.1
Cs	3×10^{3}	-	3×10^{3}	-
I	3×10^{3}	-	3×10^{3}	-
Sn	10^{-6}	10^{-8} - 10^{-4}	1×10^{-8}	10^{-10} - 10^{-6}
Pd	10^{-5}	10^{-6} - 10^{-4}	1×10^{-5}	10^{-6} - 10^{-4}
Tc	High	-	2×10^{-6}	10^{-6} - 10^{-3}
Zr	10^{-7}	3×10^{-9} - 10^{-6}	10^{-7}	3×10^{-9} - 10^{-6}
Sr	10^{-1}	10^{-3} - 1	10^{-1}	10^{-3} - 1
Se	10^{2}	10^{1} - 5×10^{2}	3×10^{-5}	10^{-6} - 10^{-4}
Ni	1	10^{-3} - 10^{2}	1	10^{-3} - 10^{2}
C	High	-	High	-

Table 2: Solubility limits of some of the elements with radioactive isotopes in the spent fuel under oxidising and reducing near-field conditions

"High" implies not solubility limited; range then not required

Distribution Coefficients for Elements (granite) (m^3 per kg)				
Element	Oxidising Conditions		Reducing Conditions	
	Estimate	Range	Estimate	Range
Am	5.0	0.5 - 80	5.0	0.5 - 80
Pu	3.0	1 - 80	5.0	0.5 - 80
Np	0.01	0.0001 - 10	5.0	0.1 - 10
U	0.01	0.002 - 1	5.0	0.01 - 10
Pa	0.1	0.01 - 10	0.1	0.01 - 10
Th	5.0	0.01 - 10	5.0	0.01 - 10
Ra	0.01	0.005 - 10	0.1	0.005 - 10
Cs, C	0.05	0.005 - 1	0.05	0.005 - 1
I	0.0	0.0 - 0.004	0.0	0.0 - 0.004
Tc	0.0002	0.0 - 0.05	0.005	0 - 0.25
Zr	4.0	0.1 - 10	4.0	0.1 - 10
Sr	0.004	0.001 -0.1	0.004	0.001 - 0.1
Ni, Sn, Se	0.01	0.001 - 0.5	0.01	0.001 - 0.5

Table 3: Sorption (distribution) coefficients for some of the elements with radioactive isotopes in the spent fuel, for granite

Distribution Coefficients for Elements (bentonite) (m^3 per kg)				
Element	Oxidising Conditions		Reducing Conditions	
	Estimate	Range	Estimate	Range
Am	2.0	0.25 - 10	2.0	0.25 - 10
Pu	1.0	0.1 - 3.5	1.5	0.1 - 5
Np	0.1	0.05 - 0.12	1	0.1 - 5
U	0.02	0 - 0.1	0.2	0.1 - 1
Pa	0.1	0.02 - 5	1.0	0.02 - 5
Th	1.0	0.002 - 6	1.0	0.002 - 6
Ra	0.02	0.001 - 0.2	0.02	0.001 - 0.2
Cs, C	0.02	0.002 - 2	0.02	0.002 - 2
I	0.001	0 - 0.005	0.001	0 - 0.005
Tc	0.0002	0 - 0.001	0.05	0.01 - 0.25
Zr	0.1	0.02 - 5	0.1	0.02 - 5
Sr	0.005	0.001 - 3	0.005	0.001 - 3
Ni, Sn, Se	0.1	0.01 - 1	0.1	0.001 - 1

Table 4: Sorption (distribution) coefficients for some of the elements with radioactive isotopes in the spent fuel, for bentonite

Symbol	Description	Units	Base Case	Range/Case Variations
A	Cylindrical surface area of canister	m^3	11.3	
b	Half the fracture aperture	m	5×10^{-5}	5×10^{-5}-5×10^{-4}
D_o	Free water diffusivity of oxidants & radionuclides	$m^2\ (ka)^{-1}$	64	32 - 290
D^B	Intrinsic diffusivity of radionuclides in bentonite	$m^2(ka)^{-1}$	1.3	0.6 - 3
D^R	Intrinsic diffusivity of radionuclides in rock	$m^2\ (ka)^{-1}$	1.6×10^{-3}	$0.9 - 3.8 \times 10^{-3}$
D^B_{ox}	Intrinsic diffusivity of oxidants in bentonite	$m^2(ka)^{-1}$	1.26	0.6 - 3
D^R_{ox}	Intrinsic diffusivity of oxidants in rock	$m^2(ka)^{-1}$	1.6×10^{-3}	$(0.9 - 3.8) \times 10^{-3}$
L	Length of canister	m	4.5	
N	Number of canisters		4400	
Q^B	Oxidant which 1 m^3 of bentonite can reduce	$keq.m^{-3}$	0.15	0.05 - 2
Q^C	Oxidant which 1 m^3 of canister can reduce	$keq.m^{-3}$	100	0-150
Q^R	Oxidant which 1 m^3 of rock can reduce	$keq.m^{-3}$	5×10^{-2}	0.01 - 3

1 ka = 1000 years $\sim 3.156 \times 10^{10}$s
no entry indicates no entry required.

Table 5: General parameter values
....Cont/d

Sym.	Description	Units	Base Case Estimate	Range/Case Variations
r_1	Radius of canister	m	0.4	
r_2	Radius of bentonite/rock interface	m	0.74	
T_1	Time to canister failure	a	10^4	$10^3 - 10^6$
V	Volume of canister	m^3	2.26	
Z	Half the inter-fracture space	m	0.5	0.05 - 5.0
ε^B	Porosity of bentonite		0.35	≥ 0.1
ε^C	Degraded canister porosity		0.01	
ε^R	Porosity of rock matrix		10^{-3}	-
p^B	Density of bentonite	$kg.m^{-3}$	2.05×10^3	$(2.0 - 2.1) \times 10^3$

1 ka = 1000 years $\sim 3.156 \times 10^{10}$s
no entry indicates no entry required.

Table 6: General parameter values - cont/d....

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