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Generation IV Benchmarking of TRISO Fuel Performance Models under Accident Conditions – Modeling Input Data

Blaise P. Collin

September 2014



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VHTR Program

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ABSTRACT

This document presents the benchmark plan for particle fuel performance calculations of safety tests that are representative of accident transients.

The benchmark is developed in the frame of Generation IV, as a follow-on of a previous benchmark performed as part of the International Atomic Energy Agency (IAEA) Coordinated Research Program on coated particle fuel technology (CRP-6). The coordination effort for this benchmark is led by Idaho National Laboratory (INL).

The benchmark is dedicated to the modeling of fission product release under accident conditions by fuel performance codes from around the world, and the subsequent comparison to experimental data from the modeled safety tests. Safety tests chosen for modeling include the first experiment of the Advanced Gas Reactor program (AGR-1) and the High Flux Reactor (HFR) EU1bis experiment. Other experiments, such as AGR-2, may be added to the benchmark in the future.

Modeling of fission product release during these safety test experiments will be performed by the benchmark participants, and subsequent results will then be collected and compared to experimental data by INL.

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ACRONYMS

AGR	Advanced Gas Reactor
СО	Carbon monoxide
CRP	Coordinated Research Program
EFPD	Effective Full-Power Days
FIMA	Fissions per Initial Metal Atom
FRG	Federal Republic of Germany
HFR	High Flux Reactor
IAEA	International Atomic Energy Agency
INL	Idaho National Laboratory
IPyC	Inner Pyrocarbon
NCC	Numerical Calculation Case
OPyC	Outer Pyrocarbon
PARFUME	PARticle FUel ModEl
SiC	Silicon Sarbide
ST	Safety Testing
TRISO	TRistructural ISOtropic
UCO	Uranium Oxycarbide

UO₂ Uranium Dioxide

Generation IV Benchmarking of TRISO Fuel Performance Models under Accident Conditions Modeling Input Data

1. INTRODUCTION

This document presents the benchmark plan for particle fuel performance calculations of safety tests that are representative of accident transients.

The benchmark is developed in the frame of Generation IV, as a follow-on of a previous benchmark performed as part of the International Atomic Energy Agency (IAEA) Coordinated Research Program on coated particle fuel technology (CRP-6). The coordination effort for this benchmark is led by Idaho National Laboratory (INL).

The benchmark is dedicated to the modeling of fission product release under accident conditions by fuel performance codes from around the world, and the subsequent comparison to experimental data from the modeled safety tests. Safety tests chosen for modeling include the AGR-1 (Maki 2009) and HFR-EU1bis (Fütterer 2004) experiments. Other experiments, such as AGR-2, may be added to the benchmark in the future. At this point, the Safety Testing Plan for AGR-2 has not yet been finalized, so no guidelines or recommendations are provided for this experiment. The following guidelines and recommendations apply to the AGR-1 and HFR-EU1bis experiments only.

Modeling of fission product release during these safety test experiments will be performed by the benchmark participants, and subsequent results will then be collected and compared to available experimental data by INL. The accident benchmark is divided into three parts:

- The modeling of a simplified benchmark problem to assess potential numerical calculation issues at low levels of fission product release.
- The modeling of fission product release during the AGR-1 and HFR-EU1bis safety testing (ST) experiments.
- The comparison of all the AGR-1 and HFR-EU1bis modeling results with experimental data.

The simplified benchmark case, thereafter named NCC (Numerical Calculation Case), is derived from Case 5 of the IAEA CRP on coated particle fuel technology (IAEA 2012). It is included so participants can evaluate their codes at low levels of fission product release. Case 5 of the IAEA CRP-6 showed large code-to-code discrepancies in the release of fission products, which were attributed to the "effects of the numerical calculation method rather than the physical model" (IAEA 2012). The NCC is therefore intended to check if these numerical effects subsist.

The first two steps imply the involvement of the benchmark participants with a modeling effort following the guidelines and recommendations provided by this document. The third step involves the collection of the modeling results by INL and the comparison of these results with the available experimental data.

The objective of this document is to provide all necessary input data to model the benchmark cases, and to give some methodology guidelines and recommendations in order to make all results suitable for comparison with each other.

The participants should read this document thoroughly to make sure all the data needed for their calculations is provided in the document. Missing data will be added to a revision of the document if necessary.

2. GUIDELINES

The modeling focuses on radiologically significant fission products. The key nuclides relevant to reactor safety and modeled in this benchmark are silver (Ag), cesium (Cs), strontium (Sr), and krypton (Kr). Other nuclides can have an impact on safety but they are encompassed with the above-mentioned fission products by lack of specific knowledge about their own diffusivities in TRISO particles. This is the case of europium whose diffusivity is assumed to be similar to that of strontium, or iodine and xenon which are assumed to be similar to krypton.

The AGR-1 and HFR-EU1bis experiments are to be modeled based on their respective specific experimental irradiation characteristics and fuel properties. On the other hand, NCC is a study case based on nominal fuel properties and irradiation characteristics suited to match the requirement of low levels of fission product release.

The following section presents the modeling data for the benchmark of NCC and the AGR-1 and HFR-EU1bis safety tests, and the recommended IAEA diffusion coefficients. AGR-1 irradiation temperatures are provided in the Excel document "Temperatures.xlsx". They correspond to predicted daily temperatures averaged over the volume of each compact (Hawkes 2012).

Material properties are not provided in this document, as each participant's code may use its own default correlations and values. In the event that a code does not have some of these material properties, they should be taken from "Case 5" of the IAEA TECDOC-1674 (Tables 9-6 and 9-8 of (IAEA 2012)).

For both the irradiation and the safety testing phases, results to be computed include:

- Failure probability vs. time (broken down by failure mechanism)
- Release fractions of Ag, Cs, Sr, and Kr vs. time (release fractions are relative to total inventory produced during irradiation)
- Centerline temperature of the layers vs. time
- Pressure vs. time
- Fission gas and carbon monoxide (CO) inventories vs. time

3. RECOMMENDATIONS

The participants are asked to provide a short description of their modeling code for inclusion in the final report, similar to that provided to the IAEA TECDOC-1674 (IAEA 2012). In addition, they are encouraged to provide a list of the data they used from Tables 4, 7, and 11 (fuel modeling parameters). This will allow clarification of the input data needs for this benchmark and future benchmark projects. Finally, for the purpose of analysis of the results, participants are asked to provide a list of the material properties they used in their respective codes.

In some codes, fission product transport takes into account the effects of particle failures, which results in a fractional release that weighs the release from intact particles and from particles with failed SiC layers with the corresponding probability of failure of this SiC layer. In an attempt to better match experimental results from AGR-1 and HFR-EU1bis, it is desirable to decouple the effects of failure probability from fission product transport, which amounts to explicitly and separately model the fission product release from intact particles and from particles with both failed inner pyrocarbon (IPyC) and SiC layers. Results will then be combined to be compared to the measured releases. The diffusion of fission products through a failed layer can be simply modeled by setting a high diffusivity (typically 10^{-6} m²/s) in that layer.

In the case of AGR-1, some compacts are known to contain particles that have experienced failure of both their IPyC and SiC layers during safety testing. The selected compacts are listed in Table 6. Post-irradiation examination analysis showed that the AGR-1 compacts selected for safety testing did not contain any particles with failed SiC. Therefore, the modeling of failed coating layers should only be done for the safety testing phase, and failure should be assumed at time zero of the safety tests for these selected compacts.

In the case of HFR-EU1bis, no particle failure was reported during safety testing but the high level of measured cesium release might point to particles with failed SiC during the safety tests. Therefore, both intact particles and particles with failed IPyC and SiC layers should be modeled during safety testing for all four spheres, assuming failure from time zero of the safety tests.

On the other hand, NCC is aimed at checking for potential numerical issues with the calculation of fission product release in a test case designed to have a low SiC failure probability, so the decoupled calculation of the release from intact particles or from particles with failed layers is not requested.

Table 1 summarizes the benchmark cases and the requested ways of modeling fission product release. Depending on their capabilities, codes should model fission product diffusion weighed by the probability of failure of the SiC layer (coupled calculation) on the one hand, and the diffusion from intact particles and from particles with failed IPyC and SiC decoupled from any failure probability modeling intact particles and particles with failed SiC implies two combination cases. Indeed, intact particles during irradiation can either stay intact during safety testing or fail their IPyC and SiC layers. Consequently, there are two "Irradiation/ST" combinations for AGR-1 and HFR-EU1bis: "Intact/Intact" and "Intact/Failed".

Table 1. Benchmark cases.

		Decoupled failure and diffusion					
Case	Coupled failure and diffusion	Intact part	icles	Particles with both failed IPyC and SiC			
		Irradiation	ST	Irradiation	ST		
NCC	Yes	-	-	-	-		
AGR-1	Yes	Yes	Yes	No	Yes		
HFR-EU1bis	Yes	Yes	Yes	No	Yes		

3.1 Numerical Calculation Case

Table 2 provides the irradiation characteristics of the Numerical Calculation Case intended to check for potential numerical effects (IAEA 2012).

Table 2. NCC irradiation characteristics.

Case	Burnup (%FIMA)	Fast Fluence (10 ²⁵ n/m ² E > 0.18 MeV)	Irradiation Length (EFPD)
NCC	10	2	1000

NB: Burnup and fast fluence assumed to follow linear evolution throughout irradiation. Fast Fluence (E > 0.18 MeV) = $0.91 \times$ Fast Fluence (E > 0.1 MeV) Table 3 contains the irradiation temperatures for NCC (IAEA 2012). It consists of ten successive linear ramps from 600 to 1000°C during an irradiation length of 100 EFPD each.

Cycle Number	Cycle EFPD	Surface Temperature (°C)
1	100	Ramp $600 \rightarrow 1000$
2	100	Ramp $600 \rightarrow 1000$
3	100	Ramp $600 \rightarrow 1000$
4	100	Ramp $600 \rightarrow 1000$
5	100	Ramp $600 \rightarrow 1000$
6	100	Ramp $600 \rightarrow 1000$
7	100	Ramp $600 \rightarrow 1000$
8	100	Ramp $600 \rightarrow 1000$
9	100	Ramp $600 \rightarrow 1000$
10	100	Ramp $600 \rightarrow 1000$

Table 3. NCC irradiation temperatures.

Table 4 contains the fuel modeling parameters for NCC (IAEA 2012).

Table 4.	NCC fu	el modeling	g parameters.
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Category	Parameter	Mean Value ± Standard Deviation
	U-235 enrichment (wt%)	10
Fuel properties	Oxygen/uranium (atomic ratio)	2
ruei properties	Carbon/uranium (atomic ratio)	0
	Uranium contamination fraction	0
	Kernel diameter (µm)	350
	Buffer thickness (µm)	100
	IPyC thickness (µm)	40
	SiC thickness (µm)	35
	OPyC thickness (µm)	40
	Kernel density (g/cm ³)	10.8
	Kernel theoretical density (g/cm ³)	10.96
Particle properties	Buffer density (g/cm ³)	0.95
	Buffer theoretical density (g/cm ³)	2.25
	IPyC density (g/cm ³)	1.9
	SiC density (g/cm ³)	3.20
	OPyC density (g/cm ³)	1.9
	IPyC anisotropy (BAF)	1.03
	OPyC anisotropy (BAF)	1.03
	Particle asphericity (SiC level)	1.0
Boundary conditions	Ambient pressure (MPa)	0.1

Table 5 shows the heating plan for NCC (IAEA 2012). It consists of a temperature step from the final irradiation temperature of 1000°C to the safety test temperature of 1600°C, where the temperature stays constant for 200 hours.

Table 5. NCC safety test heating plan.

Time (hh:mn)	Temperature (°C)
00:00	1000
00:01	1600
200:01	1600

3.2 AGR-1

Table 6 provides the list of the AGR-1 compacts to be modeled during the irradiation and safety testing phases (Collin 2012). It includes the irradiation characteristics, the number of particles with failed IPyC and SiC layers to model during safety testing, and the type (variant) of the fuel in the selected compacts, which determines some of the fuel properties (see Table 7). The irradiation temperatures are provided in the Excel document "Temperatures .xlsx".

	Safety Test Temperature (°C)	Compact	Number of particles with failed SiC during ST	Burnup (%FIMA)	Fast Fluence (10 ²⁵ n/m ² E > 0.18 MeV)	Irradiation Length (EFPD)	Variant
	1600	6-4-1	1	13.22	2.43	620.2	Baseline
	1000	4-3-3	0	18.52	4.16	620.2	3
	1700	4-4-3	0	18.83	4.06	620.2	3
	1700	3-3-1	4	19.00	4.23	620.2	Baseline
		5-1-3	7	18.17	3.82	620.2	1
	1900	4-4-1	2	18.84	3.99	620.2	3
	1800	4-3-2	5	16.24	3.68	620.2	3
		3-2-3	11	19.03	4.28	620.2	Baseline
		1-4-2	0	14.83	3.01	620.2	3
	Transient	1-1-3	0	15.21	2.86	620.2	3
		1-1-1	0	15.05	2.81	620.2	3

Table 6. AGR-1 compact selection and irradiation characteristics.

NB: Burnup and fast fluence are assumed to follow linear evolution throughout irradiation. Fast Fluence (E > 0.18 MeV) = $0.91 \times$ Fast Fluence (E > 0.1 MeV) Table 7 provides the fuel modeling parameters for AGR-1 (Maki 2009 / CEGA 1993).

			Fuel type		
Category	Parameter	Mean Value ± Standard Deviation			
		Baseline	Variant 1	Variant 3	
	U235 enrichment (wt%)		19.736 ± 0.047		
E	Oxygen/uranium (atomic ratio)		1.3613 ± 0.0064		
Fuel properties	Carbon/uranium (atomic ratio)		0.3253 ± 0.0028		
	Uranium contamination fraction	3.64×10 ⁻⁷	2.75×10 ⁻⁷	1.26×10 ⁻⁷	
	Kernel diameter (µm)		349.7 ± 9.0		
	Buffer thickness (µm)	103.5 ± 8.2	102.5 ± 7.1	104.2 ± 7.8	
	IPyC thickness (µm)	39.4 ± 2.3	40.5 ± 2.4	38.8 ± 2.1	
	SiC thickness (µm)	35.3 ± 1.3	35.7 ± 1.2	35.9 ± 2.1	
	OPyC thickness (µm)	41.0 ± 2.1	41.1 ± 2.4	39.3 ± 2.1	
	Kernel density (g/cm^3)		10.924 ± 0.015		
	Kernel theoretical density (g/cm^3)	11.64			
	Buffer density (g/cm^3)	1.10 ± 0.04			
	Buffer theoretical density (g/cm ³)	2.25			
Particle properties	IPyC density (g/cm^3)	1.904 ± 0.014	1.853 ± 0.012	1.904 ± 0.013	
	SiC density (g/cm ³)	3.208 ± 0.003	3.206 ± 0.002	3.205 ± 0.001	
	OPyC density (g/cm^3)	1.907 ± 0.008	1.898 ± 0.009	1.911 ± 0.008	
	IPyC anisotropy (BAF)	1.022 ± 0.002	1.014 ± 0.001	1.029 ± 0.002	
	OPyC anisotropy (BAF)	1.019 ± 0.003	1.013 ± 0.002	1.021 ± 0.003	
	IPyC BAF (post compact anneal)	1.033 ± 0.004	1.021 ± 0.002	1.034 ± 0.003	
	OPyC BAF (post compact anneal)	1.033 ± 0.003	1.030 ± 0.003	1.036 ± 0.002	
	Sphericity (aspect ratio)	1.054 ± 0.019 1.056 ± 0.019		1.055 ± 0.018	
	Particle asphericity (SiC level)		1.040		
	Diameter (mm)	12.36 ± 0.01	12.36 ± 0.01	12.34 ± 0.01	
	Length (mm)	25.066 ± 0.080	25.123 ± 0.030	25.227 ± 0.037	
	Compact mass (g)	5.4789	5.3371	5.5930	
Compact properties	Compact density (g/cm ³)	1.822	1.771	1.854	
	Number of particles per compact	4154	4145	4132	
	Volume packing fraction (%)	36.99	37.42	36.04	
	A3-27 matrix density (g/cm ³)	1.297	1.256	1.344	
Boundary conditions	Ambient pressure (MPa)		0.1		

Table 7. AGR-1 fuel modeling parameters.

Note that AGR-1 fuel is UCO. Due to the lack of published UCO material properties and respective correlations, functional relationships for UCO are assumed to be the same as UO_2 . However, there should be no CO production associated with UCO fuel.

Table 8 shows the heating plans for AGR-1 (Baldwin 2014). The evolution of the temperature between each time step is linear.

Transient		1600°C		1700°C		1800°C	
Time (hh:mn)	T(°C)						
00:00	20	00:00	30	0:00	30	0:00	30
00:30	300	03:05	400	3:05	400	3:05	400
22:30	300	05:05	400	5:05	400	5:05	400
24:00	857	12:10	1250	12:10	1250	12:10	1250
94:00	857	24:10	1250	24:10	1250	24:10	1250
97:48	1300	31:10	1600	31:10	1700	31:10	1800
105:06	1585	331:10	1600	333:10	1700	335:10	1800
109:30	1652	333:47	30	335:57	30	338:07	30
124:00	1695						
136:00	1680						
164:00	1620						
214:00	1508						
294:00	1342						
394:00	1200						
396:00	20						

Table 8. AGR-1 safety test heating plans.

3.3 HFR-EU1bis

Table 9 provides the irradiation characteristics of the HFR-EU1bis spheres to be modeled during the irradiation and safety testing phases (IAEA 2012).

Table 9. HFR-EU1bis sphere selection and irradiation characteristics.

Sphere	Burnup (%FIMA)	Fast Fluence (10 ²⁵ n/m ² E > 0.1 MeV)	Irradiation Length (EFPD)
HFR-EU1bis/1	9.34	2.41	249.55
HFR-EU1bis/3	11.07	2.86	249.55
HFR-EU1bis/4	11.07	2.86	249.55
HFR-EU1bis/5	9.70	2.51	249.55

NB: Burnup and fast fluence are assumed to follow linear evolution throughout irradiation. Fast Fluence $(E > 0.18 \text{ MeV}) = 0.91 \times \text{Fast Fluence} (E > 0.1 \text{ MeV})$ Table 10 provides the irradiation temperatures of the HFR-EU1bis spheres (Fütterer 2004). Temperatures are constant during each cycle.

Cuele Number	Cycle Name	Cycle EFPD	Surface Temperature (°C)				Central Temperature (°C)			
Cycle Number			\1	\3	\4	\5	\1	\3	\4	\5
1	04-08	24.97	1014	1009	1015	1006	1216	1250	1247	1227
2	04-09	24.72	1026	1024	1030	1020	1215	1251	1248	1227
3	05-01	25.99	1036	1038	1043	1032	1215	1252	1249	1228
4	05-02	25.67	1042	1047	1052	1040	1211	1249	1246	1224
5	05-03	25.29	1053	1062	1066	1052	1211	1252	1249	1226
6	05-04	25.67	1058	1072	1075	1060	1208	1251	1248	1224
7	05-06	24.26	1065	1082	1086	1069	1207	1252	1249	1224
8	05-07	25.19	1067	1088	1091	1073	1202	1248	1245	1220
9	05-08	22.19	1076	1101	1103	1083	1203	1253	1250	1223
10	05-09	25.60	1079	1108	1109	1088	1199	1252	1248	1220

Table 10. HFR-EU1bis irradiation temperatures.

Table 11 provides the fuel modeling parameters for	HFR-EU1bis (Nabielek 2005 / Pelletier 2003)
Table 11. HFR-EU1bis fuel modeling parameters.	

Category	Parameter	Mean Value ± Standard Deviation				
	U-235 enrichment (wt%)	16.76				
Fuel properties	Oxygen/uranium (atomic ratio) ^(a)	2				
ruei properties	Carbon/uranium (atomic ratio) ^(a)	0				
	Uranium contamination fraction	7.8×10 ⁻⁶				
	Kernel diameter (µm)	502.2 ± 10.6				
	Buffer thickness (µm)	94.3 ± 13.0				
	IPyC thickness (µm)	40.6 ± 3.7				
	SiC thickness (µm)	35.9 ± 2.2				
	OPyC thickness (µm)	39.8 ± 3.3				
	Kernel density (g/cm ³)	10.86				
	Kernel theoretical density (g/cm ³)	10.96				
Particle properties	Buffer density (g/cm ³)	1.012				
	Buffer theoretical density (g/cm ³)	2.2				
	IPyC density (g/cm ³)	1.87				
	SiC density (g/cm ³)	3.20				
	OPyC density (g/cm ³)	1.87				
	IPyC anisotropy (BAF)	1.02				
	OPyC anisotropy (BAF)	1.02				
	Particle asphericity (SiC level)	1.04				
	Sphere diameter (mm) ^(a)	60				
	Fuel zone diameter (mm)	50				
	U-235 content (g/pebble)	1.00 ± 0.01				
Sphere properties	Heavy metal loading (g/pebble)	6.0				
	Number of particles per sphere	9560				
	Volume packing fraction (%)	6.2				
-	A3-3 matrix density (g/cm ³)	1.75				
Boundary conditions	Ambient pressure (MPa)	0.1				

Table 12 shows the heating plans for HFR-EU1bis (Freis 2009 / Verfondern 2013). The evolution of the temperature between each time step is linear.

HFR-EU	J 1bis/1	HFR-EU1bis/3		HFR-EU1bis/4		HFR-EU1bis/5			
Time (hh:mn)	T(°C)	Time (hh:mn)	T(°C)	Time (hh:mn)	T(°C)	Time (hh:mn)	T(°C)	Time (hh:mn)	T(°C)
00:00	20	00:00	20	00:00	20	00:00	300	848:00	300
00:30	300	01:00	20	00:30	300	16:00	300	850:00	1800
06:30	300	01:30	300	03:30	300	23:00	950	852:00	300
09:30	1250	04:30	300	05:30	800	126:00	950	854:00	1800
209:30	1250	06:30	1250	53:30	800	136:00	300	856:00	300
215:30	20	96:00	1250	56:30	1250	157:00	300	858:00	1800
216:30	20	98:00	20	66:30	1250	161:00	950	860:00	300
217:00	300	99:00	20	71:30	1320	185:00	950	862:00	1800
220:00	300	99:30	300	76:30	1390	186:00	1050	864:00	300
222:00	1250	102:30	300	86:30	1500	207:00	1050	866:00	1800
232:00	1250	104:30	1250	91:30	1535	210:00	1250	868:00	300
233:30	1320	114:30	1250	96:30	1570	280:00	1250	870:00	1800
239:30	1600	118:00	1412	106:30	1630	284:00	1500	872:00	300
439:30	1600	122:00	1600	115:30	1666	374:00	1500	874:00	1800
455:00	20	322:00	1600	116:30	1670	378:00	1250	876:00	300
456:00	20	324:00	20	126:30	1695	455:00	1250	878:00	1800
456:30	300			136:30	1710	457:00	300	880:00	300
459:30	300			140:00	1711.5	461:00	300	900:00	300
461:30	1250			160:30	1720	481:00	1250	906:00	1800
471:30	1250			280:30	1720	505:00	1250	980:00	1800
473:00	1321			282:00	20	511:00	1600		
479:00	1605					624:00	1600		
481:00	1700					631:00	1800		
631:00	1700					821:00	1800		
646:00	20					844:00	300		

Table 12. HFR-EU1bis safety test heating plans.

3.4 IAEA Diffusion Coefficients

The diffusive transport of fission products is calculated assuming that the fuel materials are homogeneous. Therefore, effective diffusion coefficients are used in code calculations. The set of data to be applied corresponds to the German ("FRG") diffusion coefficients, and Japanese diffusion coefficients for Kr in silicon carbide (SiC), from the IAEA TECDOC-978 (IAEA 1997). Table 13 provides these diffusion coefficients.

	D _{0,i} (m ² /s) Q _{0,i} (kJ/mol)	Kernel	Buffer	РуС	SiC	Matrix graphite	Structural graphite
	D _{0,1}	6.7×10 ⁻⁹	10-8	5.3×10 ⁻⁹	3.6×10 ⁻⁹	1.6	1.6
	Q _{0,1}	165	0	154	215	258	258
Ag	D _{0,2}	_	_	_	_		_
	Q _{0,2}						
	D _{0,1}	5.6×10 ⁻⁸	10 ⁻⁸	6.3×10 ⁻⁸	$5.5 \times 10^{-14} \times e^{\Gamma/4.5 (b)}$	3.6×10 ⁻⁴	1.7×10 ⁻⁶
Cs	Q _{0,1}	209	0	222	125	189	149
	D _{0,2}	5.2×10 ⁻⁴			1.6×10 ⁻²		
	Q _{0,2}	362	-	-	514	-	-
17	D _{0,1}	1.3×10 ⁻¹² / 8.8×10 ⁻¹⁵ (a)	10-8	2.9×10 ⁻⁸	37 / 8.6×10 ^{-10 (c)}	6.0×10 ⁶	6.0×10^{6}
	Q _{0,1}	126 / 54 ^(a)	0	291	657 / 326 ^(c)	0	0
K ſ	D _{0,2}	0 / 6.0×10 ^{-1 (a)}		2.0×10 ⁵			
	Q _{0,2}	$0 \ / \ 480^{\ (a)}$	-	923	-	-	-
Sr	D _{0,1}	2.2×10 ⁻³	10-8	2.3×10 ⁻⁶	1.2×10 ⁻⁹	10-2	1.7×10 ⁻²
	Q _{0,1}	488	0	197	205	303	268
	D _{0,2}			-	1.8×10^{6}		
	Q _{0,2}	-	-		791	-	-

Table 13. Recommended IAEA diffusion coefficients.

a. First values used in irradiation conditions / Second values used in accidental conditions.

b. Γ: fast neutron fluence (10²⁵ n/m², E > 0.18 MeV).
c. First values used above 1626 K / Second values used below 1626 K.

$$D = D_{0,2} e^{-\frac{Q_{0,2}}{RT}} D_{0,1} e^{-\frac{Q_{0,1}}{RT}} + D_{0,2} e^{-\frac{Q_{0,2}}{RT}}$$

 $D_{0,i}$ = pre-exponential factor (m^2/s)

= activation energy (kJ/mol) $Q_{0,i}$

R = gas constant
$$(8.3142 \times 10^{-3} \text{ kJ/mol/K})$$

= temperature (K) Т

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