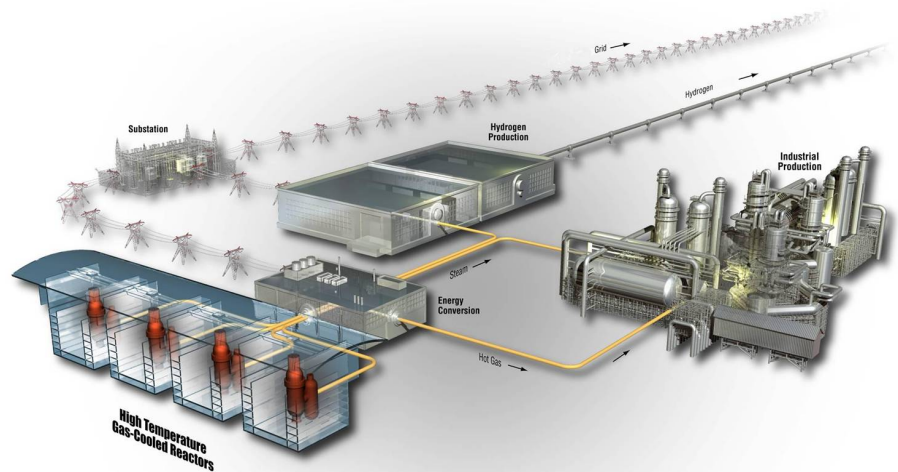


Generation IV Benchmarking of TRISO Fuel Performance Models under Accident Conditions – Modeling Input Data

Blaise P. Collin

September 2016

The INL is a
U.S. Department of Energy
National Laboratory
operated by
Battelle Energy Alliance



DISCLAIMER

This information was prepared as an account of work sponsored by an agency of the U.S. Government. Neither the U.S. Government nor any agency thereof, nor any of their employees, makes any warranty, expressed or implied, or assumes any legal liability or responsibility for the accuracy, completeness, or usefulness, of any information, apparatus, product, or process disclosed, or represents that its use would not infringe privately owned rights. References herein to any specific commercial product, process, or service by trade name, trade mark, manufacturer, or otherwise, does not necessarily constitute or imply its endorsement, recommendation, or favoring by the U.S. Government or any agency thereof. The views and opinions of authors expressed herein do not necessarily state or reflect those of the U.S. Government or any agency thereof.

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

Blaise P. Collin

September 2016

**Idaho National Laboratory
INL ART Program
Idaho Falls, Idaho 83415**

<http://www.inl.gov>

**Prepared for the
U.S. Department of Energy
Office of Nuclear Energy
Under DOE Idaho Operations Office
Contract DE-AC07-05ID14517**

INL ART Program

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

INL/EXT-14-33117
Revision 1

September 2016

Prepared by:

Blaise P. Collin 9/26/16
Blaise P. Collin Date

Approved by:

John T. Maki 9-26-16
John T. Maki Date
Technical Lead, Fuel Performance Modeling

Paul A. Demkowicz 9/27/16
Paul A. Demkowicz Date
Director/Lead, TRISO Fuel Program

Michelle T. Sharp 9/26/16
Michelle T. Sharp Date
INL Quality Engineer

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 Coordinated Research Program on coated particle fuel technology (CRP-6). The coordination effort for this benchmark is led by Idaho National Laboratory.

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 and second experiments of the Advanced Gas Reactor program (AGR-1 and AGR-2) and the High Flux Reactor EU1bis experiment.

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 Idaho National Laboratory.

CONTENTS

ABSTRACT.....	v
ACRONYMS.....	ix
1. INTRODUCTION.....	1
2. GUIDELINES.....	2
3. RECOMMENDATIONS.....	2
3.1 Numerical Calculation Case.....	3
3.2 AGR-1.....	5
3.3 AGR-2.....	7
3.4 IAEA Diffusion Coefficients.....	11
4. REFERENCES.....	13

TABLES

Table 1. Benchmark cases.....	3
Table 2. NCC irradiation characteristics.....	3
Table 3. NCC irradiation temperatures.....	4
Table 4. NCC fuel modeling parameters.....	4
Table 5. NCC safety test heating plan.....	5
Table 6. AGR-1 compact selection and irradiation characteristics.....	5
Table 7. AGR-1 fuel modeling parameters.....	6
Table 8. AGR-1 safety test heating plans.....	7
Table 9. AGR-2 compact selection and irradiation characteristics.....	7
Table 10. AGR-2 fuel modeling parameters.....	8
Table 11. AGR-2 safety test heating plans.....	9
Table 12. HFR-EU1bis sphere selection and irradiation characteristics.....	9
Table 13. HFR-EU1bis irradiation temperatures.....	9
Table 14. HFR-EU1bis fuel modeling parameters.....	10
Table 15. HFR-EU1bis safety test heating plans.....	11
Table 16. Recommended IAEA diffusion coefficients.....	12

ACRONYMS

AGR	Advanced Gas Reactor
CO	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 carbide
ST	safety testing
TRISO	tristructural isotropic
UCO	uranium oxycarbide
UO ₂	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), AGR-2 (Collin 2011), and HFR-EU1bis (Fütterer 2004) experiments.

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, AGR-2, and HFR-EU1bis safety testing (ST) experiments.
- The comparison of all the AGR-1, AGR-2, 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, AGR-2, 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, AGR-2, and HFR-EU1bis safety tests, and the recommended IAEA diffusion coefficients. AGR-1 and AGR-2 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, Hawkes 2014).

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, 10, and 14 (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, AGR-2, and HFR-EU1bis, it is desirable to decouple the effects of failure probability from fission product transport, which amounts to explicitly and separately modeling 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 and AGR-2, 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 (AGR-1) and Table 9 (AGR-2). Post-irradiation examination analysis showed that the AGR 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 on the other hand. Because safety testing calculations follow irradiation calculations, separately 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, AGR-2, and HFR-EU1bis: “Intact/Intact” and “Intact/Failed”.

Table 1. Benchmark cases.

Case	Coupled failure and diffusion	Decoupled failure and diffusion			
		Intact particles		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 × 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.

Table 3. NCC irradiation temperatures.

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

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

Table 4. NCC fuel modeling parameters.

Category	Parameter	Mean Value ± Standard Deviation
Fuel properties	U-235 enrichment (wt%)	10
	Oxygen/uranium (atomic ratio)	2
	Carbon/uranium (atomic ratio)	0
	Uranium contamination fraction	0
Particle properties	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
	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. It includes the irradiation characteristics (Collin 2012), the number of particles with failed IPyC and SiC layers to model during safety testing (Demkowicz 2015a), 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”.

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

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
	4-3-3	0	18.52	4.16	620.2	3
1700	4-4-3	0	18.83	4.06	620.2	3
	3-3-1	4	19.00	4.23	620.2	Baseline
1800	5-1-3	7	18.17	3.82	620.2	1
	4-4-1	2	18.84	3.99	620.2	3
	4-3-2	3 ^(*)	16.24	3.68	620.2	3
	3-2-3	11	19.03	4.28	620.2	Baseline
Transient	1-4-2	0	14.83	3.01	620.2	3
	1-1-3	0	15.21	2.86	620.2	3
	1-1-1	0	15.05	2.81	620.2	3

NB: Burnup and fast fluence are assumed to follow linear evolution throughout irradiation.

$$\text{Fast Fluence (E > 0.18 MeV)} = 0.91 \times \text{Fast Fluence (E > 0.1 MeV)}$$

(*) Compact 4-3-2 modeled with 2 particles with exposed kernel and 1 particle with failed IPyC and SiC.

Table 7 provides the fuel modeling parameters for AGR-1 (Maki 2009).

Table 7. AGR-1 fuel modeling parameters.

Category	Parameter	Fuel type		
		Mean Value \pm Standard Deviation		
		Baseline	Variant 1	Variant 3
Fuel properties	U235 enrichment (wt%)	19.736 \pm 0.047		
	Oxygen/uranium (atomic ratio)	1.3613 \pm 0.0064		
	Carbon/uranium (atomic ratio)	0.3253 \pm 0.0028		
	Uranium contamination fraction	3.64 $\times 10^{-7}$	2.75 $\times 10^{-7}$	1.26 $\times 10^{-7}$
Particle properties	Kernel diameter (μm)	349.7 \pm 9.0		
	Buffer thickness (μm)	103.5 \pm 8.2	102.5 \pm 7.1	104.2 \pm 7.8
	IPyC thickness (μm)	39.4 \pm 2.3	40.5 \pm 2.4	38.8 \pm 2.1
	SiC thickness (μm)	35.3 \pm 1.3	35.7 \pm 1.2	35.9 \pm 2.1
	OPyC thickness (μm)	41.0 \pm 2.1	41.1 \pm 2.4	39.3 \pm 2.1
	Kernel density (g/cm^3)	10.924 \pm 0.015		
	Kernel theoretical density (g/cm^3)	11.64		
	Buffer density (g/cm^3)	1.10 \pm 0.04		
	Buffer theoretical density (g/cm^3)	2.25		
	IPyC density (g/cm^3)	1.904 \pm 0.014	1.853 \pm 0.012	1.904 \pm 0.013
	SiC density (g/cm^3)	3.208 \pm 0.003	3.206 \pm 0.002	3.205 \pm 0.001
	OPyC density (g/cm^3)	1.907 \pm 0.008	1.898 \pm 0.009	1.911 \pm 0.008
	IPyC anisotropy (BAF)	1.022 \pm 0.002	1.014 \pm 0.001	1.029 \pm 0.002
	OPyC anisotropy (BAF)	1.019 \pm 0.003	1.013 \pm 0.002	1.021 \pm 0.003
	IPyC BAF (post compact anneal)	1.033 \pm 0.004	1.021 \pm 0.002	1.034 \pm 0.003
	OPyC BAF (post compact anneal)	1.033 \pm 0.003	1.030 \pm 0.003	1.036 \pm 0.002
	Sphericity (aspect ratio)	1.054 \pm 0.019	1.056 \pm 0.019	1.055 \pm 0.018
Particle asphericity (SiC level)	1.040			
Compact properties	Diameter (mm)	12.36 \pm 0.01	12.36 \pm 0.01	12.34 \pm 0.01
	Length (mm)	25.066 \pm 0.080	25.123 \pm 0.030	25.227 \pm 0.037
	Compact mass (g)	5.4789	5.3371	5.5930
	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		

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, Demkowicz 2015b). The evolution of the temperature between each time step is linear.

Table 8. AGR-1 safety test heating plans.

Transient		1600°C		1700°C		1800°C	
Time (hh:mn)	T(°C)	Time (hh:mn)	T(°C)	Time (hh:mn)	T(°C)	Time (hh:mn)	T(°C)
00:00	30	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	33:10	1700	35:10	1800
104:30	1585	331:10	1600	333:10	1700	335:10	1800
112:00	1670	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						

3.3 AGR-2

Table 9 provides the list of the AGR-2 compacts to be modeled during the irradiation and safety testing phases. It includes the irradiation characteristics (Collin 2014), and the type of the fuel in the selected compacts, which determines some of the fuel properties (see Table 10). The number of particles with failed IPyC and SiC layers to model during safety testing is still to be determined by fuel examination following the safety tests. They will be provided at a later date as they become available. The irradiation temperatures are provided in the Excel document “Temperatures .xlsx”.

Table 9. AGR-2 compact selection and irradiation characteristics.

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)	Fuel Type
1600	5-2-2	TBD	12.34	3.39	559.2	UCO
	3-3-2	TBD	10.54	3.53	559.2	UO ₂
1800	5-4-1	TBD	12.05	3.12	559.2	UCO
	3-4-1	TBD	10.62	3.47	559.2	UO ₂

NB: Burnup and fast fluence are assumed to follow linear evolution throughout irradiation.
Fast Fluence (E > 0.18 MeV) = 0.91 × Fast Fluence (E > 0.1 MeV)

Table 10 provides the fuel modeling parameters for AGR-2 (Collin 2011).

Table 10. AGR-2 fuel modeling parameters.

Category	Parameter	Fuel type	
		Mean Value \pm Standard Deviation	
		UCO	UO ₂
Fuel properties	U235 enrichment (wt%)	14.029 \pm 0.026	9.600 \pm 0.010
	Oxygen/uranium (atomic ratio)	1.428 \pm 0.005	2.003 \pm 0.005
	Carbon/uranium (atomic ratio)	0.392 \pm 0.002	-
	Uranium contamination fraction	1.59 \times 10 ⁻⁶	1.57 \times 10 ⁻⁶
Particle properties	Kernel diameter (μ m)	426.7 \pm 8.8	507.7 \pm 11.9
	Buffer thickness (μ m)	98.9 \pm 8.4	97.7 \pm 9.9
	IPyC thickness (μ m)	40.4 \pm 2.5	41.9 \pm 3.2
	SiC thickness (μ m)	35.2 \pm 1.2	37.5 \pm 1.2
	OPyC thickness (μ m)	43.4 \pm 2.9	45.6 \pm 2.4
	Kernel density (g/cm ³)	10.966 \pm 0.033	10.858 \pm 0.082
	Kernel theoretical density (g/cm ³)	11.37	10.96
	Buffer density (g/cm ³)	1.05	0.99
	Buffer theoretical density (g/cm ³)	2.25	2.25
	IPyC density (g/cm ³)	1.890 \pm 0.011	1.90 \pm 0.05
	SiC density (g/cm ³)	3.197 \pm 0.004	3.199
	OPyC density (g/cm ³)	1.907 \pm 0.007	1.884 \pm 0.004
	IPyC anisotropy (BAF)	1.0349 \pm 0.0012	1.0334 \pm 0.0027
	OPyC anisotropy (BAF)	1.0263 \pm 0.0011	1.0219 \pm 0.0012
	IPyC BAF (post compact anneal)	1.0465 \pm 0.0049	1.0471 \pm 0.0036
	OPyC BAF (post compact anneal)	1.0429 \pm 0.0019	1.0365 \pm 0.0016
	Sphericity (aspect ratio)	1.052	1.052
Particle asphericity (SiC level)	1.037 \pm 0.011	1.034 \pm 0.010	
Compact properties	Diameter (mm)	12.286 \pm 0.005	12.269 \pm 0.007
	Length (mm)	25.141 \pm 0.017	25.135 \pm 0.018
	Compact mass (g)	6.294 \pm 0.011	6.103 \pm 0.015
	Compact density (g/cm ³)	2.11	2.05
	Number of particles per compact	3176	1543
	Volume packing fraction (%)	37	23
	A3-27 matrix density (g/cm ³)	1.589 \pm 0.005	1.680 \pm 0.008
Boundary conditions	Ambient pressure (MPa)	0.1	

Note that AGR-2 fuel includes UCO. Due to the lack of published UCO material properties and respective correlations, functional relationships for UCO are assumed to be the same as UO₂. However, there should be no CO production associated with UCO fuel.

Table 11 shows the heating plans for AGR-2. The evolution of the temperature between each time step is linear. The AGR-1 and AGR-2 safety test heating plans are identical. Note that there are no 1700°C safety tests in the AGR-2 test matrix.

Table 11. AGR-2 safety test heating plans.

1600°C		1800°C	
Time (hh:mn)	T(°C)	Time (hh:mn)	T(°C)
00:00	30	0:00	30
03:05	400	3:05	400
05:05	400	5:05	400
12:10	1250	12:10	1250
24:10	1250	24:10	1250
31:10	1600	35:10	1800
331:10	1600	335:10	1800
333:47	30	338:07	30

Table 12 provides the irradiation characteristics of the HFR-EU1bis spheres to be modeled during the irradiation and safety testing phases (IAEA 2012).

Table 12. 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 MeV) = 0.91 × Fast Fluence (E > 0.1 MeV)

Table 13 provides the irradiation temperatures of the HFR-EU1bis spheres (Fütterer 2004). Temperatures are assumed to remain constant during each cycle.

Table 13. HFR-EU1bis irradiation temperatures.

Cycle Number	Cycle Name	Cycle EFPD	Surface Temperature (°C)				Central Temperature (°C)			
			\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 14 provides the fuel modeling parameters for HFR-EU1bis (Nabielek 2005 / Pelletier 2003).

Table 14. HFR-EU1bis fuel modeling parameters.

Category	Parameter	Mean Value ± Standard Deviation
Fuel properties	U-235 enrichment (wt%)	16.76
	Oxygen/uranium (atomic ratio) ^(a)	2
	Carbon/uranium (atomic ratio) ^(a)	0
	Uranium contamination fraction	7.8×10^{-6}
Particle properties	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
	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 properties	Sphere diameter (mm) ^(a)	60
	Fuel zone diameter (mm)	50
	U-235 content (g/pebble)	1.00 ± 0.01
	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 15 shows the heating plans for HFR-EU1bis (Freis 2009/Verfondern 2013). The evolution of the temperature between each time step is linear.

Table 15. HFR-EU1bis safety test heating plans.

HFR-EU1bis/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		

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 16 provides these diffusion coefficients.

Table 16. Recommended IAEA diffusion coefficients.

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

- a. First values used in irradiation conditions / Second values used in accidental conditions.
 b. Γ : fast neutron fluence (10^{25} n/m², $E > 0.18$ MeV).
 c. First values used above 1626 K / Second values used below 1626 K.

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

$D_{0,i}$ = pre-exponential factor (m²/s)
 $Q_{0,i}$ = activation energy (kJ/mol)
 R = gas constant (8.3142×10^{-3} kJ/mol/K)
 T = temperature (K)

4. REFERENCES

- C.A. Baldwin, J.D. Hunn, R.N. Morris, F.C. Montgomery, C.M. Silva, and P.A. Demkowicz, “First elevated-temperature performance testing of coated particle fuel compacts from the AGR-1 irradiation experiment”, *Nuclear Engineering and Design*, 271 (2014) 131-141.
- B.P. Collin, “AGR-2 Irradiation Experiment Test Plan”, PLN-3798, Rev. 1, October 2011.
- B.P. Collin, “AGR-1 Irradiation Test Final As-Run Report”, INL/EXT-10-18097, Rev. 1, June 2012.
- B.P. Collin, “AGR-2 Irradiation Test Final As-Run Report”, INL/EXT-14-32277, Rev. 2, August 2014.
- P.A. Demkowicz, J.D. Hunn, R.N. Morris, I.J. van Rooyen, T.J. Gerczak, J.M. Harp, and S.A. Ploger, “AGR-1 Post Irradiation Examination Final Report”, INL/EXT-15-36407, August 2015a.
- P.A. Demkowicz, “Test Plan for the Safety Test of AGR-1 Fuel Compacts 1-4-2, 1-1-1, and 1-1-3”, PLN-4731, November 2015b.
- D. Freis, “Störfallsimulationen und Nachbestrahlungsuntersuchungen an kugelförmigen Brennelementen für Hochtemperaturreaktoren“, PhD Thesis, 2009.
- M.A. Fütterer, H. Lohner, R. Conrad, K. Bakker, S. de Groot, and C. M. Sciolla, “HFR-Eu1bis Design and Safety Report”, HTR-F-04/07-D-2.1.3, July 2004.
- G.L. Hawkes, “AGR-1 Daily As-run Thermal Analyses,” ECAR-968, Rev. 3, May 2012.
- G.L. Hawkes, “AGR-2 Daily As-Run Thermal Analyses,” ECAR-2476, Rev. 1, August 2014.
- IAEA, “Fuel performance and fission product behaviour in gas cooled reactors”, TECDOC-978, November 1997.
- IAEA, “Advances in High Temperature Gas Cooled Reactor Fuel Technology”, TECDOC-1674, June 2012.
- J.T. Maki, “AGR-1 Irradiation Experiment Test Plan”, INL/EXT-05-00593, Rev. 3, October 2009.
- H. Nabielek, K. Verfondern, and H. Werner, “Selection of benchmark cases for mechanical failure prediction”, HTR-F1-04/08-D3.1.1, January 2005.
- M. Pelletier, H. Nabielek, T. Abram, and D. Martin, “HTR-F Project: Selection of properties and models for the coated particle – Fuel kernel”, Technical Note CEA SESC/LSC 03-028, August 2003.
- K. Verfondern, Private communication, November 2013.