

Title: AGR-2 Pre-Test Prediction Analyses using the PARFUME Code for U.S. Fuel Particles

ECAR No.: 1020

ECAR Rev. No.: 2

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1. Index Codes			
Building/Type: N/A	SSC ID: N/A	Site Area: N/A	
2. Quality Level and Determination #:			
QL 3, MSA-000014			
3. Objective/Purpose:			
This report documents analyses that were performed to predict fuel particle behavior and the probability of fuel particle failure during the second planned irradiation test of the Advanced Gas Reactor program (otherwise referred to as the AGR-2 test). These analyses were completed using the particle fuel performance computer code known as PARFUME.			
4. Conclusions/Recommendations:			
The particle failure probability results of two U.S. fuel types, UCO and UO ₂ , have been calculated based upon projected AGR-2 irradiation conditions. Compared to the the 427 μm UCO fuel in Capsules 2, 5 and 6, the 508 μm UO ₂ fuel in Capsule 3 exhibited a higher SiC particle failure probability due to asphericity and higher internal pressures.			

5. Review (R) and Approval (A) and Acceptance (Ac) ¹ :			
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Quality Assurance	R	K. J. Armour/Q580	<i>K. J. Armour for</i>
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1 Review and Approval are required. See LWP-10200 for definitions and responsibilities.

2 Electronic Change Request (ECR) numbers in lieu of signatures on this page indicate electronic final review, approval and acceptance by the listed individuals.

3 If Required, per LWP-10200.

Title: AGR-2 Pre-Test Prediction Analyses using the PARFUME Code for U.S. Fuel Particles

ECAR No.: 1020

ECAR Rev. No.: 2

Project File No.: 23841

Date: 05/29/2012

CONTENTS

SCOPE AND BRIEF DESCRIPTION.....	3
DESIGN OR TECHNICAL PARAMETER INPUT AND SOURCES.....	3
RESULTS OF LITERATURE SEARCHES AND OTHER BACKGROUND DATA.....	3
ASSUMPTIONS.....	4
DISCUSSION/ANALYSIS.....	4
Modeling.....	4
Boundary/Initial Conditions.....	6
Input Parameters.....	8
Multidimensional Stress.....	10
Material Properties.....	11
Physico-Chemical Behavior.....	11
Failure Mechanisms Considered.....	11
Solver Settings.....	12
RESULTS.....	14
COMPUTER CODE VALIDATION.....	26
PE STAMP.....	28
REFERENCES.....	28
APPENDIXES.....	30
Appendix A – Reference 8.....	31
Appendix B – Graphical Results.....	33
Appendix C – Input Data Decks.....	56

Title: AGR-2 Pre-Test Prediction Analyses using the PARFUME Code for U.S. Fuel Particles

ECAR No.: 1020

ECAR Rev. No.: 2

Project File No.: 23841

Date: 05/29/2012

SCOPE AND BRIEF DESCRIPTION

This report documents analyses that were performed to predict fuel particle behavior and the probability of fuel particle failure during the second planned irradiation test of the Advanced Gas Reactor program (otherwise referred to as the AGR-2 test). These analyses were completed using the particle fuel model computer code known as PARFUME. It should be noted that this ECAR revision includes changes to the input data decks, to reflect the correct particle number, and additional analyses (computed independent of PARFUME) which reflect an improved estimate of release rate to birth rate ratio (R/B) for capsules in which PARFUME predicts particle failures.

PARFUME, which is under development at Idaho National Laboratory (INL), is an integrated mechanistic code that evaluates the thermal, mechanical, and physico-chemical behavior of fuel particles during irradiation and the probability for fuel failure given the particle-to-particle statistical variations in physical dimensions and material properties that arise from the fuel fabrication process. A more detailed description of the code is available in References 1 through 3. Most calculations were performed on a Sun x86_64 workstation running SUSE LINUX using PARFUME Version 2.18⁴ as configured in the Revision Control System (RCS).⁵ Post-processing of results was performed on desktop PCs using MS Excel.

Two U.S. fuel types, UCO and UO₂ with nominal kernel diameters of 426.7 μm and 507.7 μm respectively, were analyzed. The fuel is contained within four of the six AGR-2 capsules. Specifically, the U.S. fuel is contained in Capsules 6, 5, 3, and 2. Failure probabilities are calculated for both types of fuel kernels. Each fuel type produces a unique set of particle failure probabilities at selected temperatures versus burnup and fluence. (Note that the analyses of the South African and French, Capsules 4 and 1 respectively, fuel types irradiated in AGR-2 will be reported separately.)

DESIGN OR TECHNICAL PARAMETER INPUT AND SOURCES

1. Natural Phenomena Hazard (NPH) category and source (Performance Category per DOE-STD-1021 and/or Seismic Design Category per ANSI/ANS 2.26): N/A
2. Load scenarios and Acceptance Criteria: N/A
3. Quality Level Source: "Determining Quality Levels," LWP-13014 Revision 4, Idaho National Laboratory, January 2010.
4. Maki, J. T., "AGR-2 Irradiation Test Specification," SPC-1064, Revision 1, Idaho National Laboratory, June 2010.
5. Chang, G. S., and J. R. Parry, "Reactor Physics Analysis for the AGR-2 Experiment Irradiated in the ATR B-12 Position," ECAR-949, Revision 0, Idaho National Laboratory, May 2010.
6. Maki, J. T., data files transmitted via e-mail to K. D. Hamman and W. F. Skerjanc, Idaho National Laboratory, April 28 and 29, 2010. (Transmitted files contain "new AGR-2 fuel parameter list" and "AGR-2 pretest irradiation conditions.")

RESULTS OF LITERATURE SEARCHES AND OTHER BACKGROUND DATA

This information is addressed in the body of the report and the references section.

Title: AGR-2 Pre-Test Prediction Analyses using the PARFUME Code for U.S. Fuel Particles

ECAR No.: 1020

ECAR Rev. No.: 2

Project File No.: 23841

Date: 05/29/2012

ASSUMPTIONS

1. As specified in References 1, 6, and 7.
2. Each fuel type will be exposed to a constant temperature, specified in Table 1, consistent with the parameter specifications in Reference 6 and data specified in Reference 8.

DISCUSSION/ANALYSIS

Modeling

The AGR-2 test will be located in the large West “B” (B-12) position in the Advanced Test Reactor (ATR). The test includes a total of six capsules arranged vertically. A radial cross-section through a single capsule inside the “B” position is shown in Figure 1; Reference 7 provides additional information on the capsule components (e.g., SST Shroud and Through Tube). As indicated, capsules contain three fuel stacks, and each fuel stack consists of a vertical arrangement of fuel compacts. Except for Capsule 1, a total of 12 fuel compacts are contained in each capsule (three stacks per capsule with four compacts per stack). Capsule 1 contains two compacts per stack, resulting in a total of 6 compacts.

The capsule arrangement inside the “B” position is illustrated in the axial cross section provided in Figure 2. This figure shows two of the three vertical fuel stacks with each compact divided into halves for modeling purposes. Only two of the three fuel stacks in each capsule are shown (the third fuel stack in each capsule is hidden behind the two stacks that are shown). Note that the horizontal division of each fuel compact is an aspect of modeling only and should not be interpreted to represent a physical segmentation of the compacts.

Based on current specifications, typical fuel compacts are right circular cylinders measuring ~12.3 mm in diameter and ~25.1 mm tall. Each particle has a nominal diameter of ~850 μm and contains either a UCO fuel kernel or a UO_2 fuel kernel. The UCO compacts contain ~3,200 fuel particles uniformly disbursed in a carbon-based substrate; the UO_2 compacts contain ~1,500 fuel particles uniformly disbursed in a carbon-based substrate. The kernel is coated with a porous buffer layer to accommodate fission product accumulation, a SiC layer to retain the fission products, and inner and outer pyrocarbon layers to protect the SiC as depicted in Figure 3. Capsule irradiation in ATR has been tentatively set at ~600 effective full power days (EFPD). Key aspects of the PARFUME modeling of these AGR-2 conditions are described below.

Title: AGR-2 Pre-Test Prediction Analyses using the PARFUME Code for U.S. Fuel Particles

ECAR No.: 1020

ECAR Rev. No.: 2

Project File No.: 23841

Date: 05/29/2012

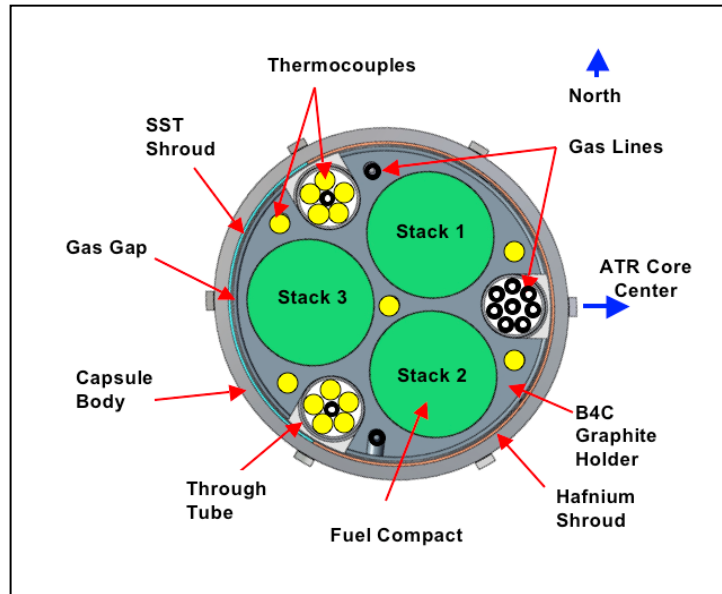


Figure 1. Radial cross section of a capsule in the AGR-2 test (not to scale).

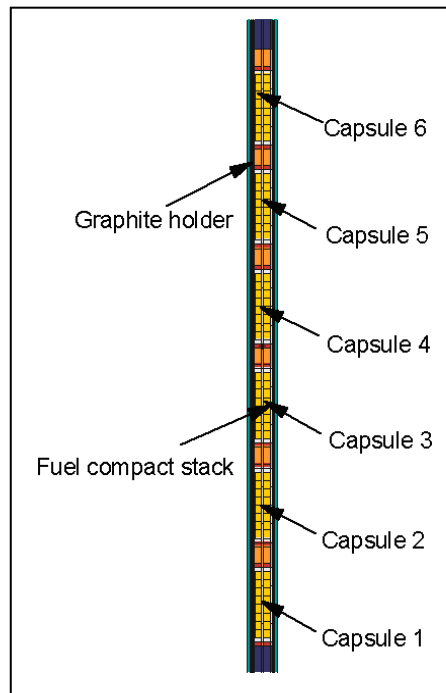


Figure 2. Axial cross section of the AGR-2 capsule (not to scale).

Title: AGR-2 Pre-Test Prediction Analyses using the PARFUME Code for U.S. Fuel Particles

ECAR No.: 1020

ECAR Rev. No.: 2

Project File No.: 23841

Date: 05/29/2012

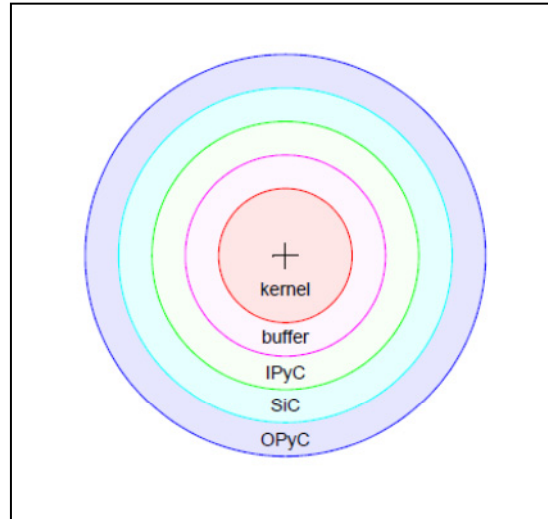


Figure 3. Cross section through a coated fuel particle (not to scale).

Boundary/Initial Conditions

PARFUME is designed to evaluate fuel performance based on user inputs for neutron fluence and burnup with a corresponding set of thermal conditions. Results from neutronics analyses and/or measured values are typical sources for fluence and burnup inputs. In this ECAR, capsule-specific fluence and burnup results from neutronics analyses performed as part of the AGR-2 design effort were used; fluence and burnup history is presented in Figure 4 and Figure 5, respectively. Thermal conditions are presented in Table 1.

PARFUME has considerable flexibility relative to the application of thermal conditions affecting fuel particles. A user may define thermal conditions for the outer surfaces of fuel bearing materials (i.e., the outer surface of a pebble in the case of a pebble bed reactor or the coolant channel surface of a unit cell containing fuel compacts in the case of a prismatic reactor) or the user may directly specify fuel bearing material temperatures at locations throughout the fuel element. Fuel bearing material temperatures can be defined directly as time-dependent values applicable to the entire material or the user may divide the material into regions and supply time-dependent temperatures for each region. The direct specification of fuel bearing material temperatures was applied here. Specifically, the entire fuel bearing material was specified to be at the same temperature. A geometric modeling limitation in PARFUME requires this type of thermal modeling since AGR-2 capsule specific geometry is not a user option.³

The direct specification of fuel bearing material temperatures, presented in Table 1, was based on AGR-2 irradiation test specifications and data provided in References 6 and 8. In general, the temperature predictions were determined by keeping temperatures less than the time average peak temperature, consistent with capsule thermocouple measurement uncertainty.

Three types of capsule-specific PARFUME calculations were completed with respect to the temperature data specified in Table 1. Specifically, calculations were made assuming each of the six capsules followed a constant maximum temperature, volume average temperature, and minimum temperature throughout the entire irradiation. Note that all fuel particles (in a given capsule) share the

Title: AGR-2 Pre-Test Prediction Analyses using the PARFUME Code for U.S. Fuel Particles

ECAR No.: 1020

ECAR Rev. No.: 2

Project File No.: 23841

Date: 05/29/2012

same outer (OPyC) surface temperature in these calculations. Additionally, note that the potential effects of an ATR high power (PALM) cycle were not considered in these analyses.

Table 1. Capsule thermal conditions.

Capsule Number	Temperatures (°C)		
	Maximum	Volume Avg.	Minimum
6	1240	1075	910
5	1240	1075	910
3	1140	970	800
2	1390	1225	1060

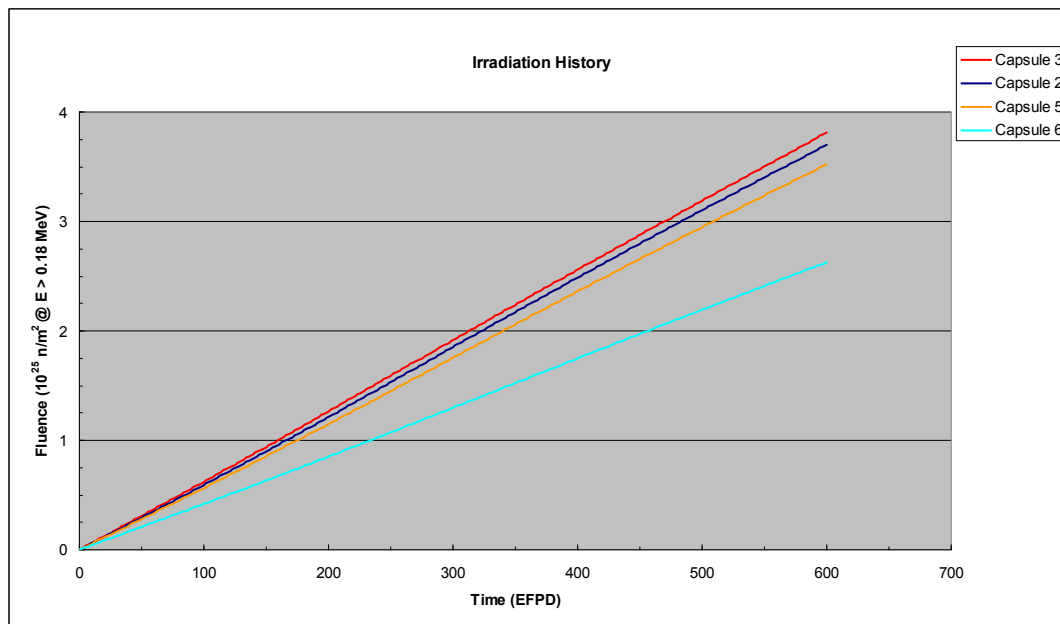


Figure 4. Fluence as a function of time from AGR-2 neutronics analyses.⁷

Title: AGR-2 Pre-Test Prediction Analyses using the PARFUME Code for U.S. Fuel Particles

ECAR No.: 1020

ECAR Rev. No.: 2

Project File No.: 23841

Date: 05/29/2012

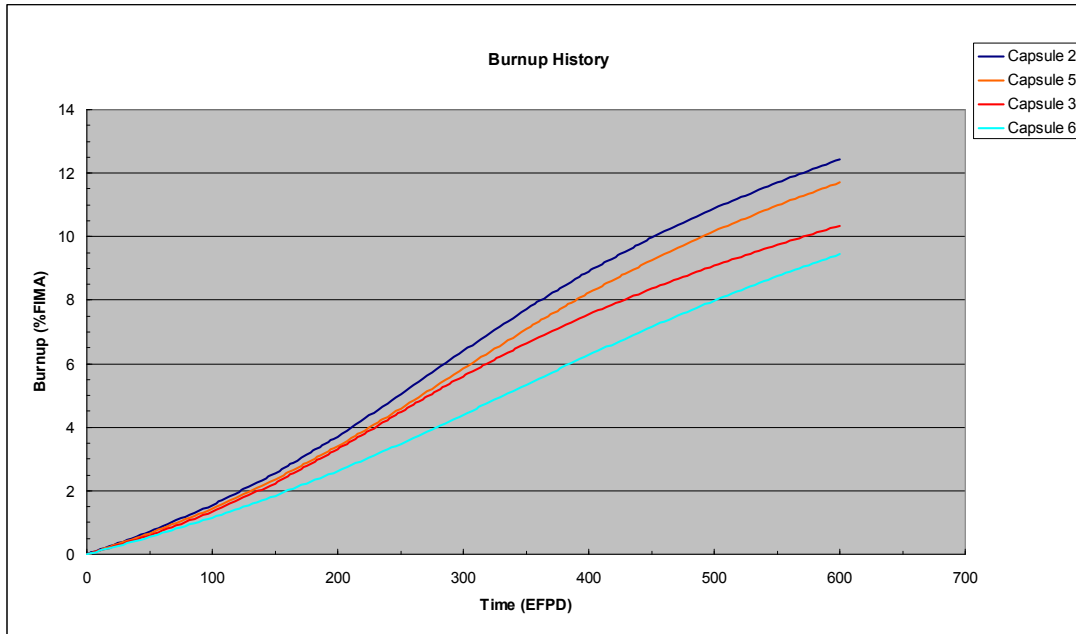


Figure 5. Burnup as a function of time from AGR-2 neutronics analyses.⁷

Input Parameters

PARFUME input parameters, needed to model the AGR-2, test were obtained from References 7 and 8. As previously mentioned, two fuel types were evaluated. Capsules 6, 5, and 2 contain UCO fuel; Capsule 3 contain UO₂. Irradiation conditions are presented in Table 2.

Table 2. Irradiation Conditions

Attribute	Units	UCO (Capsules 6, 5, 2)	UO ₂ (Capsule 3)
Irradiation duration	Effective Full Power Days	600, 600, 600	600
End-of-life burnup	% FIMA	9.45, 11.71, 12.43	10.34
End-of-life fluence	10 ²⁵ n/m ² [E _n >0.18 MeV]	2.63, 3.52, 3.70	3.81
Irradiation temperature	°C	(see Table 1)	(see Table 1)
Ambient pressure	MPa	0.1	0.1

As shown in Table 3 and Table 4, statistical variations were considered relative to fuel particle geometry and some fuel particle properties. PARFUME also has the capability to address statistical variations in several parameters. However, results from sensitivity calculations indicate that those variations (which are small by specification) have little impact on the probability of fuel particle failures.¹⁴

Title: AGR-2 Pre-Test Prediction Analyses using the PARFUME Code for U.S. Fuel Particles

ECAR No.: 1020

ECAR Rev. No.: 2

Project File No.: 23841

Date: 05/29/2012

Table 3. Fuel Particle Geometry

Attribute	Units	UCO		UO ₂	
		Mean Value	St. Dev.	Mean Value	St. Dev
Kernel Diameter	μm	426.7	8.8	507.7	11.9
Buffer Thickness	μm	98.9	8.4	97.7	9.9
IPyC Thickness	μm	40.4	2.5	41.9	3.2
SiC Thickness	μm	35.2	1.2	37.5	1.2
OPyC Thickness	μm	43.4	2.9	45.6	2.4
Particle Sphericity	aspect ratio	1.052	0.017 ^a	1.052	0.016 ^a
Fuel Particle Number	Particles per Capsule	38,052	--	18,660	--

Note (a) The theoretical minimum limit for particle sphericity is "1". Since PARFUME evaluates some attributes over a range of 4 standard deviations; the standard deviation for particle sphericity input was changed from 0.017 and 0.016, for UCO and UO₂ respectively, to 0.013 for both UCO and UO₂ to prevent particle sphericity from being evaluated at values <1 .

Table 4. Fuel Particle Material Properties

Attribute	Units	UCO		UO ₂	
		Mean Value	St. Dev.	Mean Value	St. Dev
Kernel Density	Mg/m ³	10.97	--	10.86	--
Buffer Density	Mg/m ³	1.04	--	0.99	--
IPyC Density	Mg/m ³	1.89	0.01	1.89	0.02
OPyC Density	Mg/m ³	1.91	0.01	1.88	0.01
IPyC BAF		1.047	0.005	1.047	0.004
OPyC BAF		1.043	0.002	1.037	0.002
IPyC Weibull modulus		9.5	--	9.5	--
OPyC Weibull modulus		6.0	--	6.0	--
SiC Characteristic Strength	MPa-μm ^{3/6}	9.64	--	9.64	--
IPyC/SiC Bond Strength	MPa	100	--	100	--
PyC Poisson's Ratio in Creep		0.5	--	0.5	--
U-235 Enrichment	weight %	14.03	--	9.60	--
Oxygen-to-Uranium	atom ratio	1.43	--	2.00	--
Carbon-to-Uranium	atom ratio	0.39	--	0.00	--
U Contamination Fraction		9.74E-6	--	8.55E-6	--

Title: AGR-2 Pre-Test Prediction Analyses using the PARFUME Code for U.S. Fuel Particles

ECAR No.: 1020

ECAR Rev. No.: 2

Project File No.: 23841

Date: 05/29/2012

Multidimensional Stress

In addition to the one-dimensional (1-D) behavior of a symmetrical spherical fuel particle, PARFUME considers multidimensional behavior, including 1) an aspherical geometry, 2) cracking of the IPyC layer, and 3) partial debonding of the IPyC from the SiC. To model such effects, PARFUME utilizes the results of detailed finite element analyses for cracked, debonded, and/or aspherical particles in conjunction with results from the PARFUME closed form one-dimensional solution to make a statistical approximation of the stress levels in any particle. Version 6.7-5 of ABAQUS was used to perform the finite element stress analyses to capture the multi-dimensional effects. The corresponding mean strength values are presented in Table 5, and the corresponding statistical parameters are listed in the input data decks in Appendix C.

Note that the asphericity mean strength values shown in Table 5, computed using ABAQUS results, show erratic behavior in that the trends from capsule-to-capsule are not consistent. The reasons for this behavior are that: (1) the tensile stress spatial distribution, in these cases, is concentrated in local areas of the aspherical geometry, shown in Figure 6; and (2) the magnitude of the stresses are low enough (as low as 7 MPa) that the location of the maximum stress can vary from one capsule to another. (Note that at higher tensile stress levels, the tensile stresses are distributed over more of the SiC volume.)

It is noted that the SiC failure probabilities due to pressure are very low for all UCO cases, and follow the correct trends.

Table 5. Multi-dimensional Mean Strength Values

	Mean Strength (MPa)		
	Cracking	Asphericity	Debonding
Capsule 6			
High	1084	1037	b
Average	1084	891	b
Low	1085	802	b
Capsule 5			
High	1085	1936	b
Average	1085	1046	b
Low	1085	894	b
Capsule 3			
High	1035	1183	b
Average	1035	1246	b
Low	1035	1022	b
Capsule 2			
High	1085	1384	b
Average	1085	1849	b
Low	1085	1038	b

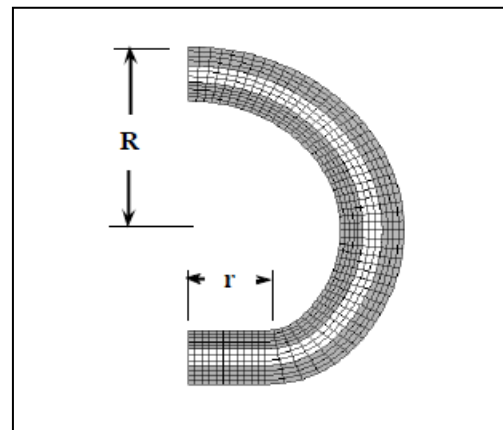


Figure 6. Aspherical ABAQUS geometry.

Note (b) Partial debonding of the IPyC from the SiC was not predicted, so a debonding mean strength was not computed.

Title: AGR-2 Pre-Test Prediction Analyses using the PARFUME Code for U.S. Fuel Particles

ECAR No.: 1020

ECAR Rev. No.: 2

Project File No.: 23841

Date: 05/29/2012

Material Properties

Material properties used in PARFUME are discussed in Reference 1. As such, the elastic moduli and swelling strains for the IPyC and OPyC are treated as functions of fluence. The effective range for these properties extends to a fluence of 3.96×10^{25} n/m². As discussed in Reference 1, there is significant uncertainty in the physical properties of the coating layers. The accuracy of failure probability predictions from any fuel performance code relies on the accuracy of these properties.

Physico-Chemical Behavior

The internal gas pressure is calculated in PARFUME as a function of time according to the Redlich-Kwong equation of state. Parameters utilized in this equation are derived from the critical temperature and pressure of each gas specie occupying the void volume within the particle. PARFUME considers the generation of CO and the release of the noble gas fission products, xenon and krypton, in this pressure calculation.

CO production is calculated in PARFUME using an algorithm derived from thermochemical free energy minimization calculations performed by the HSC computer code.¹ PARFUME calculates fission product gas release (e.g. krypton and xenon) caused by both recoil and diffusion. Direct fission recoil from the kernel to the buffer is accounted for by geometrical considerations and fission fragment ranges derived from compiled experimental data. Diffusive release is calculated according to the Booth equivalent sphere diffusion model, which utilizes an effective diffusion coefficient formulated by Turnbull¹⁵. This effective diffusion coefficient accounts for intrinsic, athermal, and irradiation-enhanced diffusion.

A model accounting for release of short-lived fission product gases from failed particles and from uranium contamination in the fuel bearing material is incorporated into PARFUME¹⁵. This model calculates release rate to birth rate (R/B) ratios for several prominent fission product nuclides. Also, based upon the Booth equivalent sphere gas release model, this model uses different reduced diffusion coefficients for release from failed particles and from uranium contamination.

Details of physico-chemical behavior can be found in References 1, 2, and 15.

Failure Mechanisms Considered

Four potential failure mechanisms are currently considered in PARFUME. The first is a pressure vessel failure caused by the buildup of gases (e.g. fission product gases and CO). Stresses for this failure mechanism are determined using the one-dimensional solution in PARFUME for a three-layer (IPyC-SiC-OPyC) particle. Because of asphericity in the particle shape, these stresses are modified based on results of finite element analysis of aspherical particles. Stress modification was based on coefficients included in the input data decks located in Appendix C. Some particle internal pressures were found to trigger this failure mechanism in AGR-2 test calculations, especially at the high temperatures.

The second mechanism considered is failure of the SiC layer caused by partial debonding of the IPyC from the SiC. Debonding, if it occurs, results from IPyC shrinking inward away from the SiC during irradiation. PARFUME first determines whether debonding between the IPyC/SiC layers occurs by comparing the radial stress between layers with the bond strength between layers. If debonding is determined to occur, then the code estimates the stress in the SiC layer accounting for multidimensional effects using a previously documented methodology. Because AGR-2 particle fabrication was based on German processes, the bond strength was set at a value that is considered to be representative for German particles (i.e., 100 MPa). At this bond strength, IPyC/SiC debonding was not predicted, and therefore debonding did not contribute to particle failures in the AGR-2 test.

Title: AGR-2 Pre-Test Prediction Analyses using the PARFUME Code for U.S. Fuel Particles

ECAR No.: 1020

ECAR Rev. No.: 2

Project File No.: 23841

Date: 05/29/2012

The third failure mechanism considered in PARFUME is migration of the fuel kernel into the SiC layer, or the amoeba effect. This failure mechanism has the potential to occur if the particles are subjected to a global temperature gradient. However, the amoeba effect made no contribution to particle failures in these analyses because migration coefficients were very small.

The fourth and final failure mechanism currently considered in PARFUME is failure of the SiC layer caused by irradiation-induced shrinkage and the associated cracking of the IPyC layer. The presence of a crack in the IPyC layer creates a stress concentration in the SiC layer. To treat the multi-dimensional effects of this stress concentration, PARFUME estimates stresses in the SiC layer resulting from the presence of a crack based on a previously documented methodology.¹ The input data decks, located in Appendix C, contain coefficients used to apply that methodology in the AGR-2 test. In evaluating failures caused by IPyC cracking, PARFUME first determines whether the IPyC layer cracks using the Weibull statistical theory. If the IPyC layer is predicted to crack, the particle is evaluated for failure of the SiC layer due to the presence of the crack. Some fuel particle failure probability results, in AGR-2 test calculations, were found to be caused by this mechanism.

Chemical attack of the SiC (primarily) by palladium (Pd) represents another potential failure mechanism. Although PARFUME does not fully simulate this mechanism, scoping calculations have shown that fuel particle failure occurs when penetration through the thickness of the SiC is complete, leading to the direct release of fission products. Based on Pd penetration rates, however, SiC failure would not occur in the AGR-2 test even if particle temperatures were assumed to remain fixed at the maximum calculated value for the entire irradiation period.¹⁴

PARFUME uses the Weibull statistical theory to determine whether particles fail, using a mean strength for the SiC layer based on a stress distribution corresponding to the failure mechanism under consideration. The failure modes are implemented such that a particle fails only in the mode of failure that would occur first for that particle. The code retains the time at which failures occur, allowing for the construction of a time evolution of the failure probability for a batch of fuel particles. Weibull parameters used to evaluate failures of the SiC layer and cracking of the IPyC layer are discussed in References 1 and 2.

Solver Settings

All results were calculated with the fast integration solver. Although the full integration solver or Monte Carlo solver could have been chosen, the introduction of several variables with corresponding standard deviations significantly increases the computer run-time under full-loop integration. Additionally, the Monte Carlo method, as currently implemented in PARFUME Version 2.18, requires large statistical samples to capture small failure probabilities. For these reasons, 2-loop integration was used for the simulation runs. Reference 14 demonstrates that time-saving simplifications using the fast integration scheme (i.e., 2-loop integration) do not adversely affect the accuracy of simulation results.

Title: AGR-2 Pre-Test Prediction Analyses using the PARFUME Code for U.S. Fuel Particles

ECAR No.: 1020

ECAR Rev. No.: 2

Project File No.: 23841

Date: 05/29/2012

Table 6. Summary of probability results.

CAPSULE 6 (UCO)				
Temperature (°C)	1240 (High)	1075 (Average)	910 (Low)	
Fluence (x 10²⁵ n/m²)	2.63	2.63	2.63	
Burnup (% FIMA)	9.45	9.45	9.45	
Probability Summary				Estimated No. Particle Failures
Probability of SiC failure	<u>2.3878E-08</u>	<u>7.9748E-07</u>	<u>3.9248E-05</u>	0
Contribution due to amoeba effect	0.0000E+00	0.0000E+00	0.0000E+00	
Contribution due to IPyC cracking	2.3878E-08	7.9748E-07	3.9248E-05	
Contribution due to IPyC debonding	0.0000E+00	0.0000E+00	0.0000E+00	
Contribution due to pressure	1.4658E-20	0.0000E+00	0.0000E+00	
Probability of IPyC cracking (Note c)	5.0519E-03	3.8125E-02	3.6767E-01	
Probability of IPyC debonding	0.0000E+00	0.0000E+00	0.0000E+00	
CAPSULE 5 (UCO)				
Temperature (°C)	1240 (High)	1075 (Average)	910 (Low)	
Fluence (x 10²⁵ n/m²)	3.52	3.52	3.52	
Burnup (% FIMA)	11.71	11.71	11.71	
Probability Summary				Estimated No. Particle Failures
Probability of SiC failure	<u>2.3896E-08</u>	<u>5.7371E-07</u>	<u>3.9130E-05</u>	0
Contribution due to amoeba effect	0.0000E+00	0.0000E+00	0.0000E+00	
Contribution due to IPyC cracking	2.3776E-08	5.7371E-07	3.9130E-05	
Contribution due to IPyC debonding	0.0000E+00	0.0000E+00	0.0000E+00	
Contribution due to pressure	1.2006E-10	0.0000E+00	0.0000E+00	
Probability of IPyC cracking (Note c)	5.0479E-03	3.8083E-02	3.6670E-01	
Probability of IPyC debonding	0.0000E+00	0.0000E+00	0.0000E+00	
CAPSULE 3 (UO₂)				
Temperature (°C)	1140 (High)	970 (Average)	800 (Low)	
Fluence (x 10²⁵ n/m²)	3.81	3.81	3.81	
Burnup (% FIMA)	10.34	10.34	10.34	
Probability Summary				Estimated No. Particle Failures
Probability of SiC failure	<u>2.3395E-02</u>	<u>4.6367E-04</u>	<u>2.2716E-04</u>	114
Contribution due to amoeba effect	0.0000E+00	0.0000E+00	0.0000E+00	
Contribution due to IPyC cracking	2.1979E-07	1.0655E-05	2.2716E-04	
Contribution due to IPyC debonding	0.0000E+00	0.0000E+00	0.0000E+00	
Contribution due to pressure	2.3395E-02	4.5302E-04	3.3333E-13	
Probability of IPyC cracking (Note c)	1.8067E-02	1.7794E-01	8.5693E-01	
Probability of IPyC debonding	0.0000E+00	0.0000E+00	0.0000E+00	
CAPSULE 2 (UCO)				
Temperature (°C)	1390 (High)	1225 (Average)	1060 (Low)	
Fluence (x 10²⁵ n/m²)	3.70	3.70	3.70	
Burnup (% FIMA)	12.43	12.43	12.43	
Probability Summary				Estimated No. Particle Failures
Probability of SiC failure	<u>3.5134E-06</u>	<u>3.2816E-08</u>	<u>1.0987E-06</u>	0
Contribution due to amoeba effect	0.0000E+00	0.0000E+00	0.0000E+00	
Contribution due to IPyC cracking	1.6233E-09	3.2496E-08	1.0987E-06	
Contribution due to IPyC debonding	0.0000E+00	0.0000E+00	0.0000E+00	
Contribution due to pressure	3.5118E-06	3.1995E-10	0.0000E+00	
Probability of IPyC cracking (Note c)	1.4087E-03	6.0369E-03	4.5931E-02	
Probability of IPyC debonding	0.0000E+00	0.0000E+00	0.0000E+00	

Title: AGR-2 Pre-Test Prediction Analyses using the PARFUME Code for U.S. Fuel Particles

ECAR No.: 1020

ECAR Rev. No.: 2

Project File No.: 23841

Date: 05/29/2012

RESULTS

The fuel particle failure probability analyses for the AGR-2 test of two U.S. fuel types, UCO and UO₂, have identified irradiation condition ranges where an increased number of particle failures are expected. Compared to the the 427 μm UCO fuel in Capsules 2, 5 and 6, the 508 μm UO₂ fuel in Capsule 3 exhibited a higher SiC particle failure probability due to apshericity and higher internal pressures caused by greater amounts of CO produced by the UO₂ fuel. Irradiation conditions for the 508 μm UO₂ fuel in Capsule 3 include analysis temperatures of 1140, 970, and 800°C; a maximum fluence of 3.81×10^{25} n/m² (E>0.18 MeV); and a maximum burnup of 10.3 % FIMA. Irradiation condition ranges for the 427 μm UCO fuel in Capsule 2 include analysis temperatures of 1390, 1225, and 1060°C; a maximum fluence of 3.7×10^{25} n/m² (E>0.18 MeV); and a maximum burnup of 12.4% FIMA. The remaining capsule irradiation conditions are presented in Table 2 above.

The analyses were completed using PARFUME, its associated models, and user developed calculations for failed particle R/B as discussed in previous sections of this report¹⁵. Corresponding failure probability results, including the estimated number of particle failures, from those analyses are summarized in Table 6. The results were generated assuming the outer surfaces of all fuel particles in each capsule are at capsule-specific temperature as shown in Table 1. The SiC failure probabilities due to IPyC cracking and pressure loading of apshpherical particles were the two mechanisms leading to potential fuel particle failures under these conditions; furthermore, the calculated fuel particle failure probabilities vary depending on the fuel type. The estimated final number of particle failures is zero for Capsules 2, 5, and 6 with 114 estimated particle failures in Capsule 3. A time-history plot of the number of Capsule 3 particle failures is shown in Figure 7. The particle failure estimate [see Equation (1)] was computed assuming that the fuel particles were evenly distributed between the high and low analysis temperatures and that the total failure probability varied piece-wise linearly between the analysis points.

$$N_{\text{total}} = \text{ROUND}(w_{\text{high}} \times P_{\text{high}} \times N_{\text{PC}}) + \text{ROUND}(w_{\text{avg}} \times P_{\text{avg}} \times N_{\text{PC}}) + \text{ROUND}(w_{\text{low}} \times P_{\text{low}} \times N_{\text{PC}}) \quad \text{Equ. (1)}$$

where:

N_{total} = total number of particle failures per capsule

N_{PC} = number of particles per capsule

P_{high} = total probability of SiC failure at the high temperature

P_{avg} = total probability of SiC failure at the average temperature

P_{low} = total probability of SiC failure at the low temperature

w_k = weighting factor for each analysis temperature 'k', where $w_{\text{high}} = 0.25$, $w_{\text{avg}} = 0.50$, and $w_{\text{low}} = 0.25$

and 'ROUND' is a MS Excel function which returns a whole number to reflect that "fractions" of particles do not exist (e.g. 1.76 particles).

It should be noted that the computed failure probability results, and in general all results, are only approximations. They are approximations because the compacts in each capsule will never be at a given uniform temperature (as assumed in the calculations). Instead, fuel particles in each capsule will be exposed to some distribution of temperatures in space and time. Consequently, the results strictly apply only if all fuel particles in the capsules are exposed to the assumed uniform temperatures, and will only be approximations otherwise.

Title: AGR-2 Pre-Test Prediction Analyses using the PARFUME Code for U.S. Fuel Particles

ECAR No.: 1020

ECAR Rev. No.: 2

Project File No.: 23841

Date: 05/29/2012

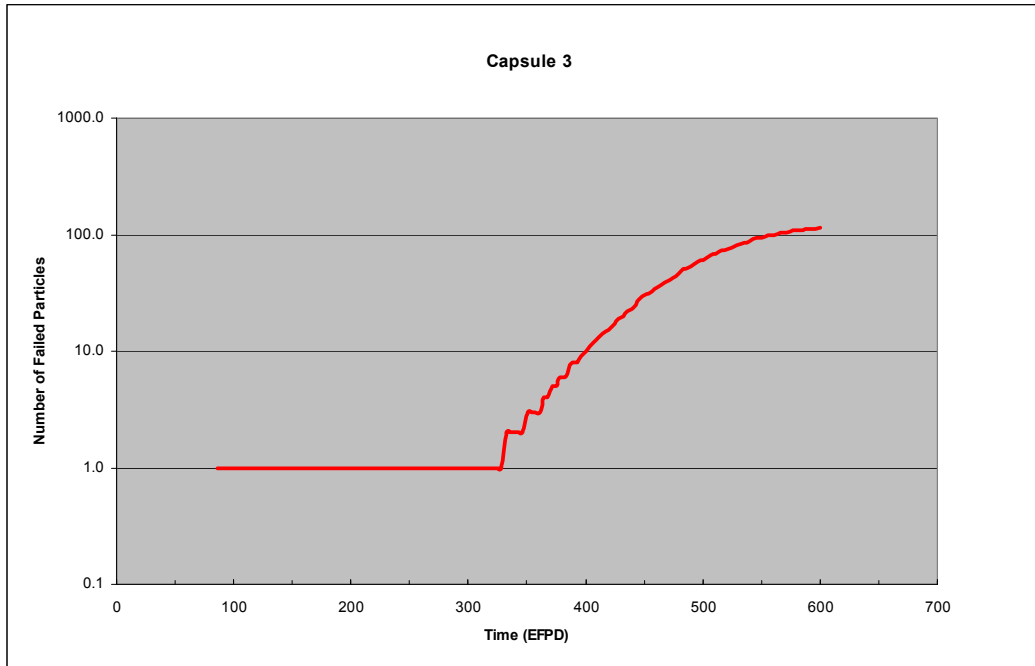


Figure 7. Estimated number of failed particles (Capsule 3).

The remainder of this section contains a description of predicted parameters and conditions leading to the results described. This discussion is offered as a way to provide further insights into the AGR-2 test. (Note that capsule-to-capsule comparisons are presented in Appendix B.)

Irradiation can lead to the development of a gap between the buffer and the IPyC. The gap can develop as a result of the combined effects of kernel swelling; shrinkage, and creep in the buffer, IPyC, and OPyC layers; the effects of particle internal pressure, and the kernel/buffer contact pressure. However, difference in density between the buffer and the IPyC is a primary factor in the process. The buffer, which is much more porous than the dense IPyC layer, shrinks more during irradiation. The growth rate for the gap size slows, however, as the buffer becomes denser during irradiation. The size of this gap is shown in Figure 8 and Figure 9 for nominal particles, assuming the outer surfaces of those particles follow capsule-specific volume-averaged temperatures. Note the comparison of the gap width as a function of temperature in these figures. The gap width tends to increase with temperature as indicated because irradiation-induced shrinkage is temperature-dependent.

The buffer-to-IPyC gap can be a significant fraction of the thermal resistance in a fuel particle. Consequently, if other conditions are equal, temperature differentials (from the kernel centerline to the outer surface of the OPyC) are higher across particles with larger gaps. This trend is apparent in Figure 10 and Figure 11. The discontinuities in Figure 10 and associated figures in Appendix B are due to the discrete nature of the PARFUME input (i.e., irradiation time, burnup, fluence, and temperature).

Title: AGR-2 Pre-Test Prediction Analyses using the PARFUME Code for U.S. Fuel Particles

ECAR No.: 1020

ECAR Rev. No.: 2

Project File No.: 23841

Date: 05/29/2012

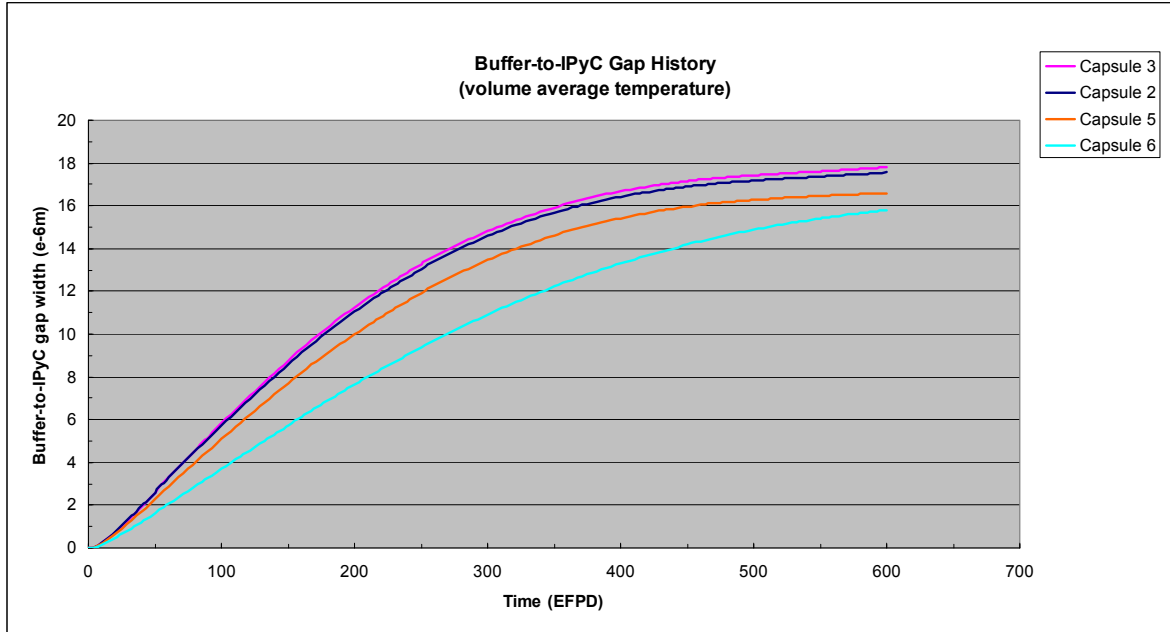


Figure 8. Buffer-to-IPyC gap width in nominal particles (Capsules 3, 2, 5, 6).

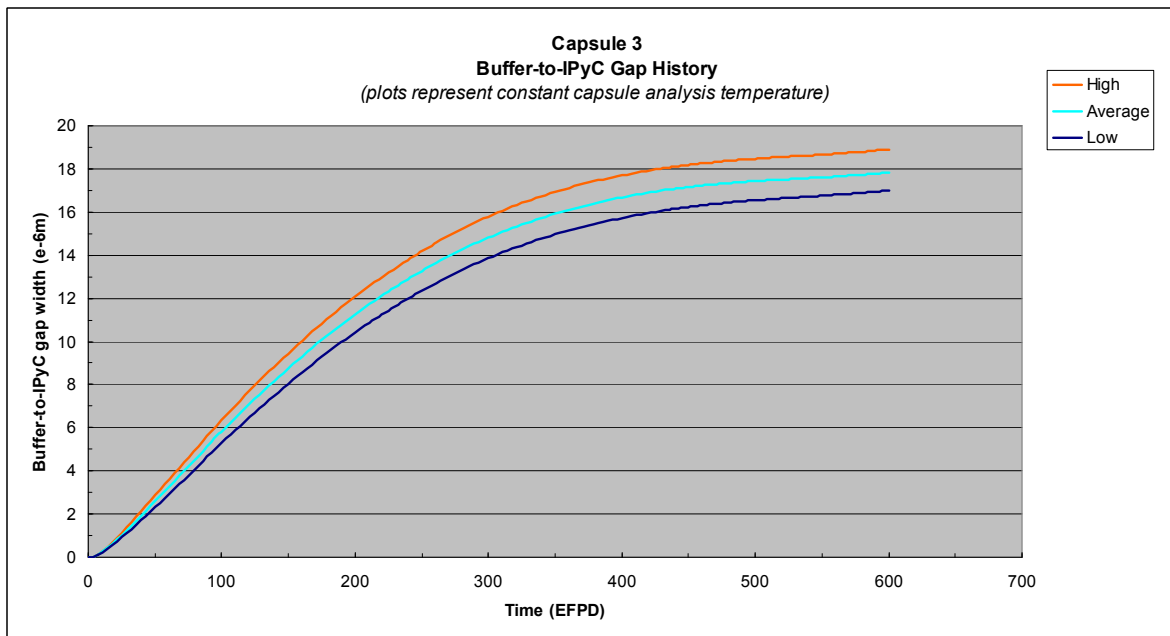


Figure 9. Buffer-to-IPyC gap width in nominal particles (Capsules 3).

Title: AGR-2 Pre-Test Prediction Analyses using the PARFUME Code for U.S. Fuel Particles

ECAR No.: 1020

ECAR Rev. No.: 2

Project File No.: 23841

Date: 05/29/2012

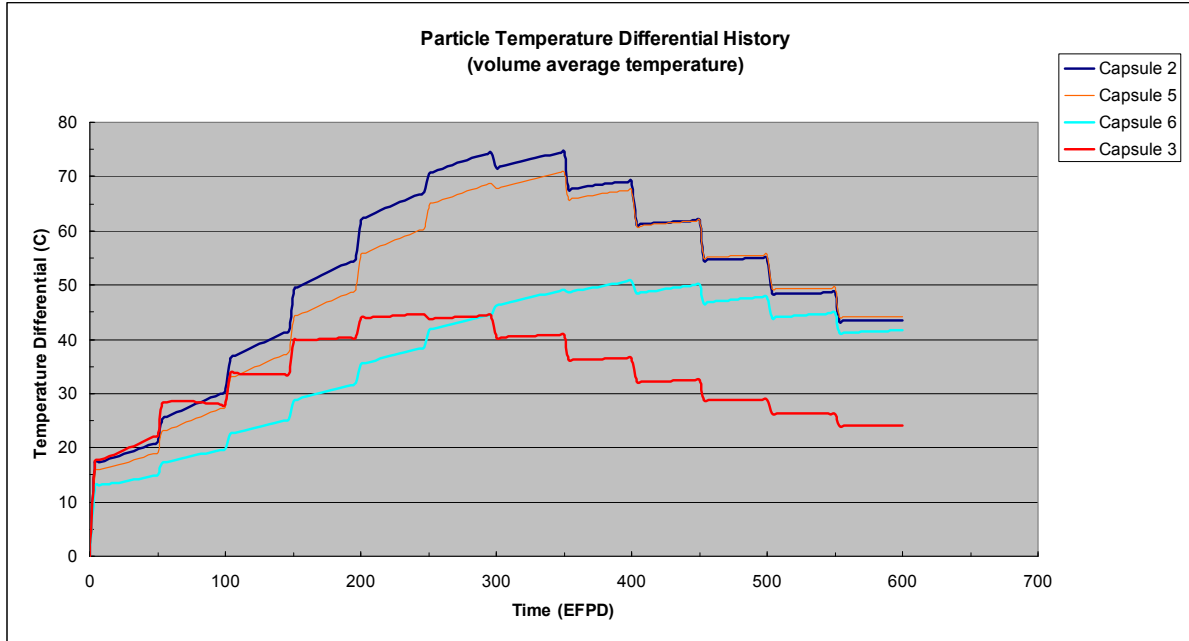


Figure 10. Particle temperature differentials (Capsules 2, 3, 5, 6).

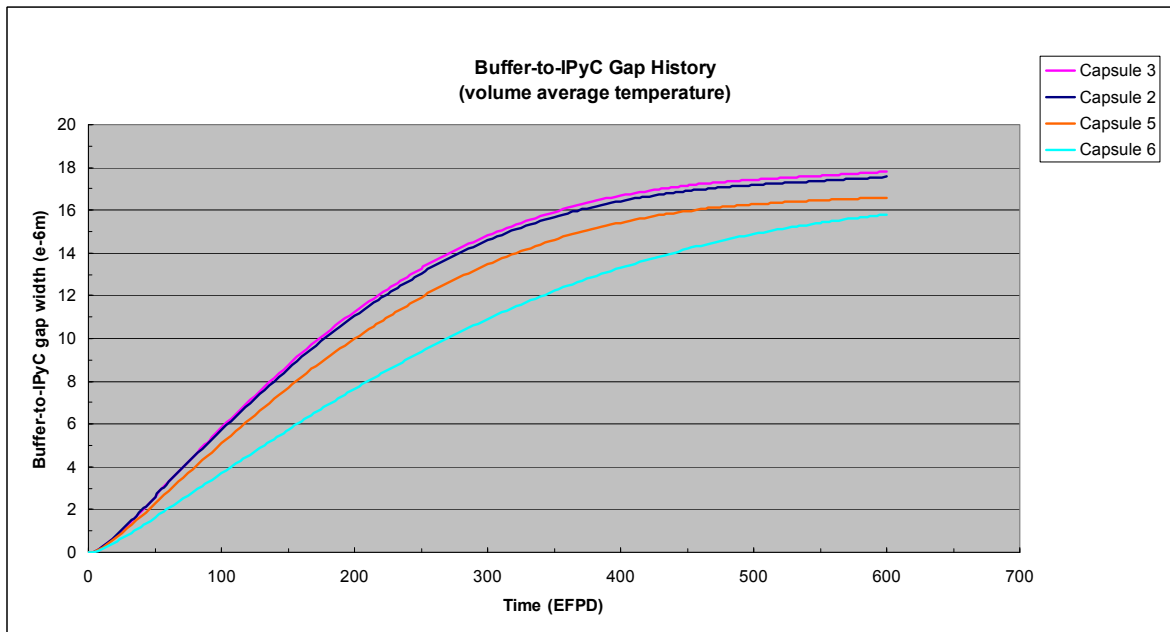


Figure 11. Buffer-to-IPyC gap width in nominal particles (Capsules 3, 2, 5, 6).

For a given fuel type, particle internal pressures tend to increase as temperatures increase because fission product release and the pressure of confined gases both increase with temperature. This trend is apparent in Figure 12 with Capsules 2, 5, and 6 (the UCO fuel particles), where capsule temperature increases from Capsule 6 (lowest temperature) to Capsule 2 (highest temperature). Figure 13 shows a

Title: AGR-2 Pre-Test Prediction Analyses using the PARFUME Code for U.S. Fuel Particles

ECAR No.: 1020

ECAR Rev. No.: 2

Project File No.: 23841

Date: 05/29/2012

similar effect for Capsule 3 (UO₂ fuel). Note that the pressure in Capsule 3 exceeds that of the other capsules due to greater production of CO.

Figure 14 and Figure 15 show SiC inner tangential stresses for Capsules 2, 5, and 6, in addition to Capsule 3. As indicated, stresses decrease as temperatures increase. Although internal pressures, shrinkage, creep, and thermal effects all contribute to the stress in a particle, the stress magnitude decreases as temperatures increase because higher pyrocarbon creep at higher temperature more than offsets the increased shrinkage. For this reason, stress magnitudes in hotter particles tend to be less than those in cooler particles.

Ultimately, particle failures are directly related to particle stresses. Calculated failure probabilities for all capsules at volume-averaged temperatures are presented in Figure 16 through Figure 19. Because shrinkage of the pyrocarbons has the greatest effect relatively early during irradiation, failure probabilities driven by shrinkage-induced IPyC cracking reach a local maximum well before the fluence has reached 1×10^{25} n/m².

Release rate to birth rate ratio (R/B) results presented in Figure 20 through Figure 24 are consistent with the failure probability predictions. Specifically, Capsules 2, 5, and 6 volume average temperature results are consistent with release from uranium contamination only and differences in irradiation temperature. For example, the higher R/B rates for Capsule 2 are a result of its higher volume average irradiation temperature. The Capsule 3 results, containing failed fuel particles, are consistent with the failure fraction trends previously predicted by Equation (1).

Due to the input assumption of constant analysis temperature throughout each capsule, off-line calculations were used to determine expected R/B results when failed particles are predicted to be present in the capsule. An overview of these calculations is presented below.

$$R/B_{\text{total}} = f_{\text{U-cont}} * R/B_{\text{U-cont}} + (f_{\text{fail-high}} * R/B_{\text{fail-high}} + f_{\text{fail-avg}} * R/B_{\text{fail-avg}} + f_{\text{fail-low}} * R/B_{\text{fail}}) \quad \text{Equ. (2)}$$

$$f_{\text{fail-k}} = \text{ROUND}(w_k * P_{\text{fail-k}} * N_{\text{PC}}) / N_{\text{PC}} \quad \text{Equ. (3)}$$

where:

$f_{\text{U-cont}}$ = uranium contamination fraction

$f_{\text{fail-k}}$ = particle failure fraction for each analysis temperature 'k'

$R/B_{\text{U-cont}}$ = release rate to birth rate due to uranium contamination evaluated at the volume average temperature

$R/B_{\text{fail-k}}$ = release rate to birth rate due to particle failure for each analysis temperature 'k'

w_k = weighting factor for each analysis temperature 'k', where $w_{\text{high}} = 0.25$, $w_{\text{avg}} = 0.50$, and $w_{\text{low}} = 0.25$

N_{PC} = number of particles per capsule

$P_{\text{fail-k}}$ = total probability of SiC failure at each analysis temperature 'k'

and 'ROUND' is a function which returns a whole number to reflect that "fractions" of particles do not exist (e.g. 1.76 particles).

Title: AGR-2 Pre-Test Prediction Analyses using the PARFUME Code for U.S. Fuel Particles

ECAR No.: 1020

ECAR Rev. No.: 2

Project File No.: 23841

Date: 05/29/2012

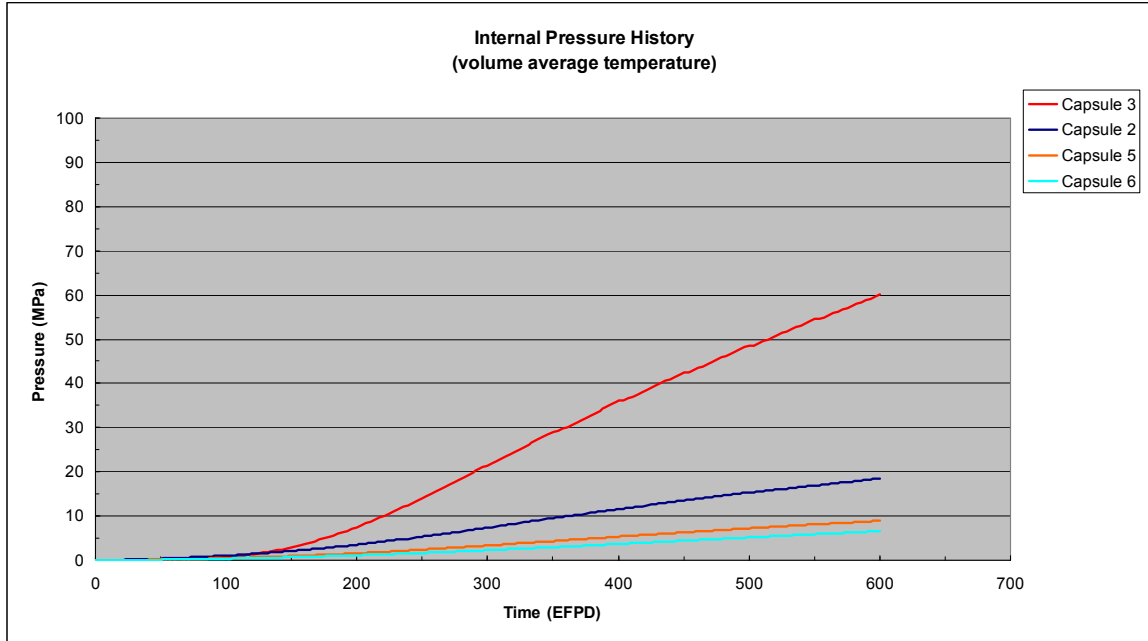


Figure 12. Particle internal pressure (Capsules 2, 3, 5, 6).

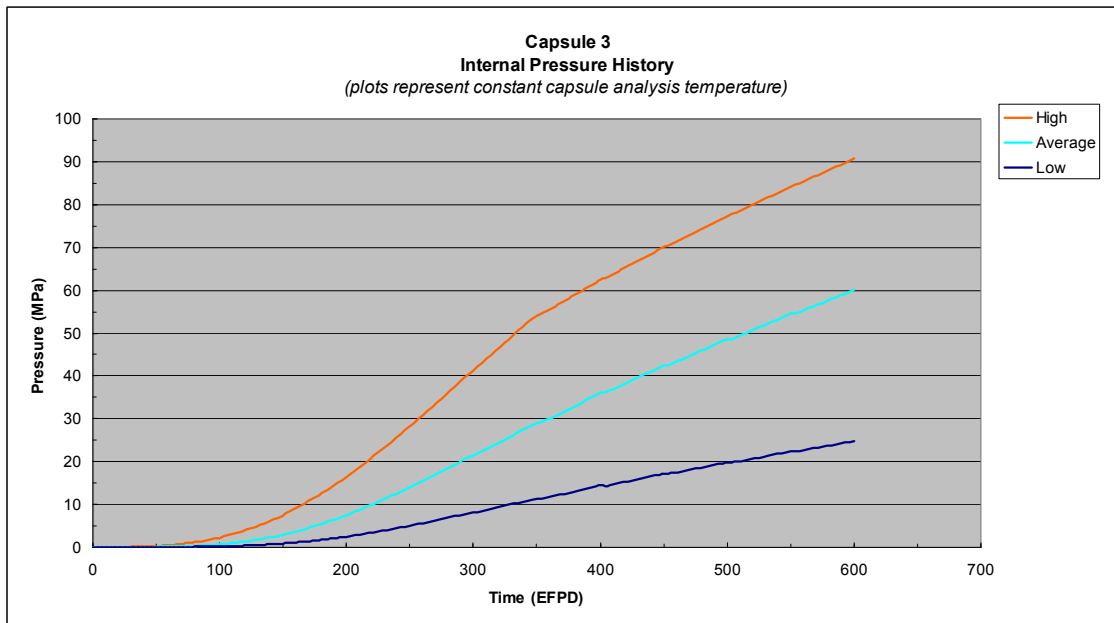


Figure 13. Particle internal pressure (Capsule 3).

Title: AGR-2 Pre-Test Prediction Analyses using the PARFUME Code for U.S. Fuel Particles

ECAR No.: 1020

ECAR Rev. No.: 2

Project File No.: 23841

Date: 05/29/2012

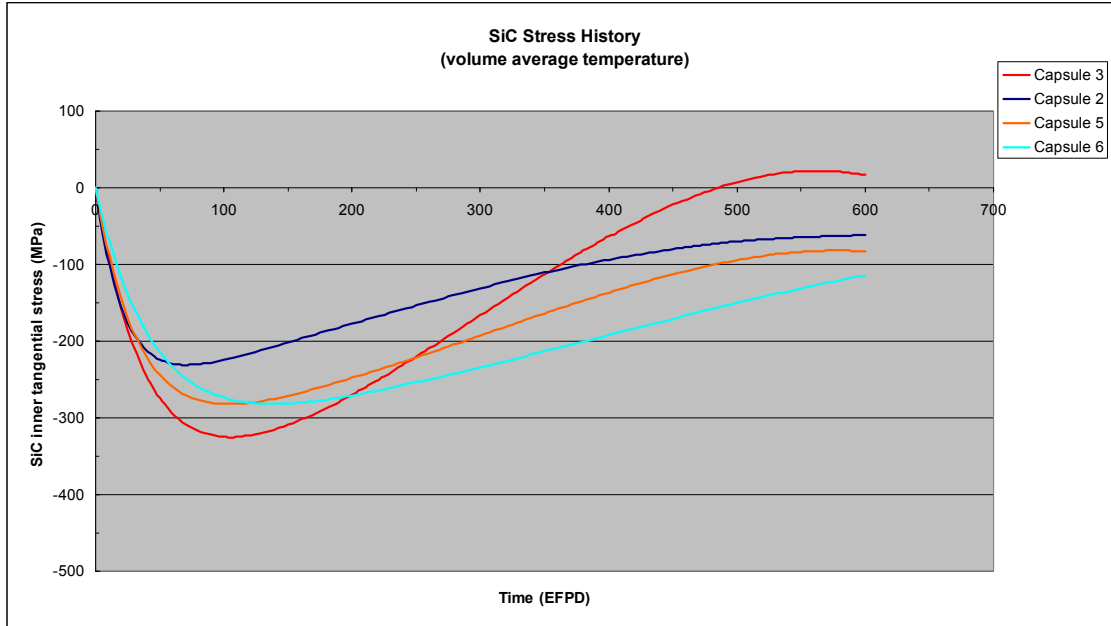


Figure 14. SiC inner tangential stress (Capsules 2, 3, 5, 6).

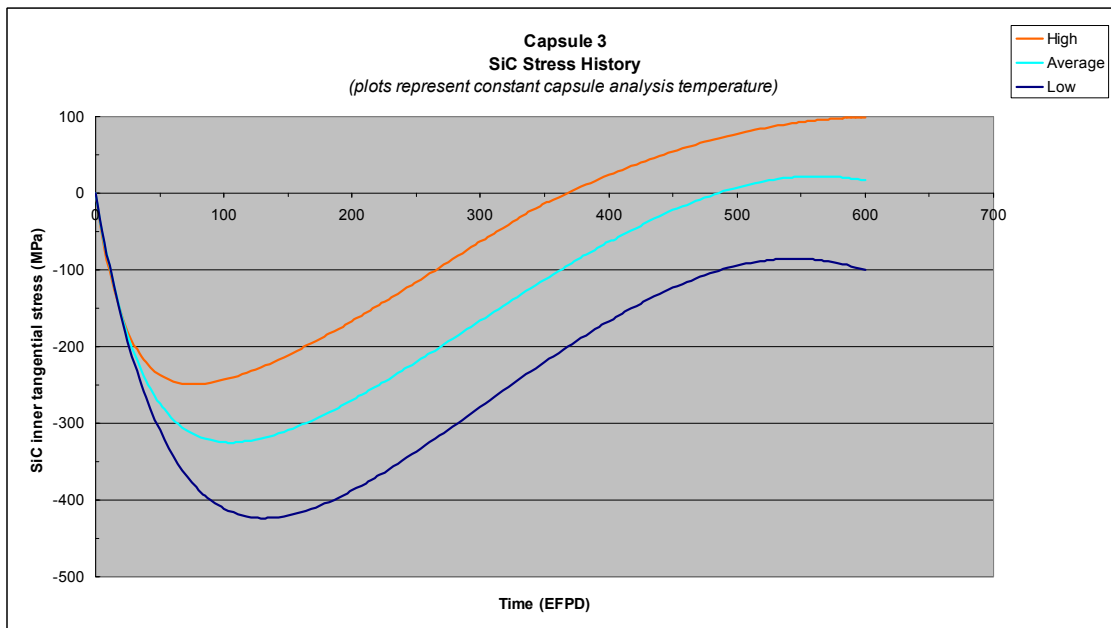


Figure 15. SiC inner tangential stress (Capsule 3).

Title: AGR-2 Pre-Test Prediction Analyses using the PARFUME Code for U.S. Fuel Particles

ECAR No.: 1020

ECAR Rev. No.: 2

Project File No.: 23841

Date: 05/29/2012

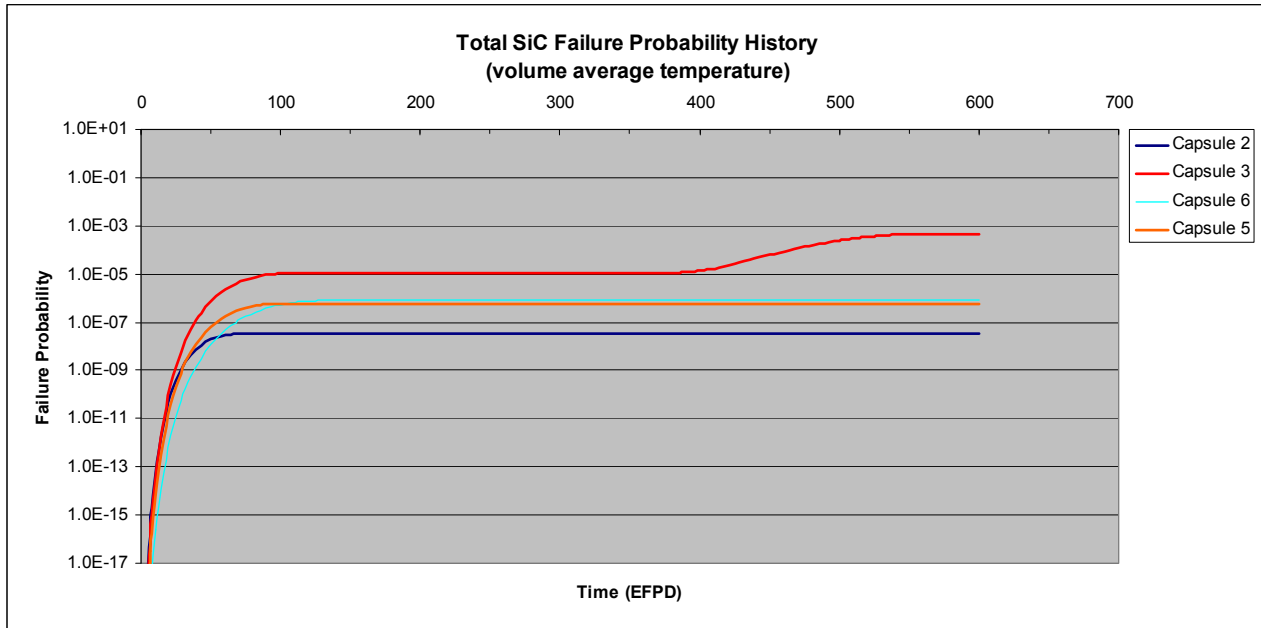


Figure 16. Total SiC fuel particle failure probabilities (Capsules 2, 3, 5, 6).

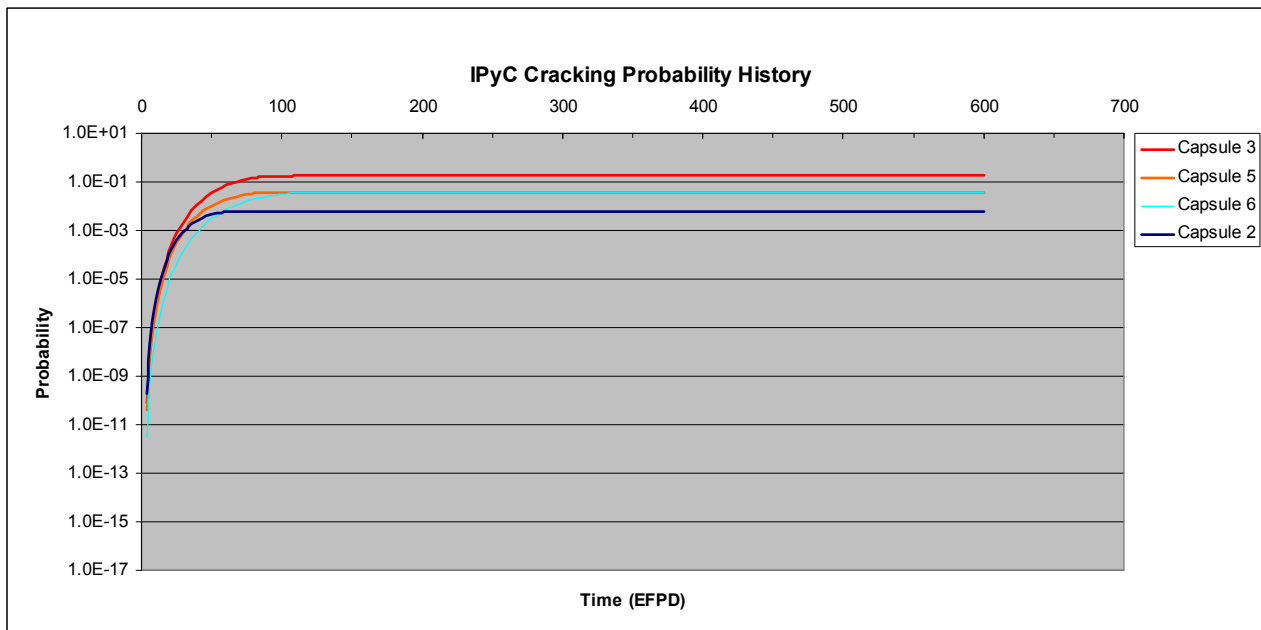


Figure 17. IPyC cracking probabilities (Capsules 2, 3, 5, 6).

Title: AGR-2 Pre-Test Prediction Analyses using the PARFUME Code for U.S. Fuel Particles

ECAR No.: 1020

ECAR Rev. No.: 2

Project File No.: 23841

Date: 05/29/2012

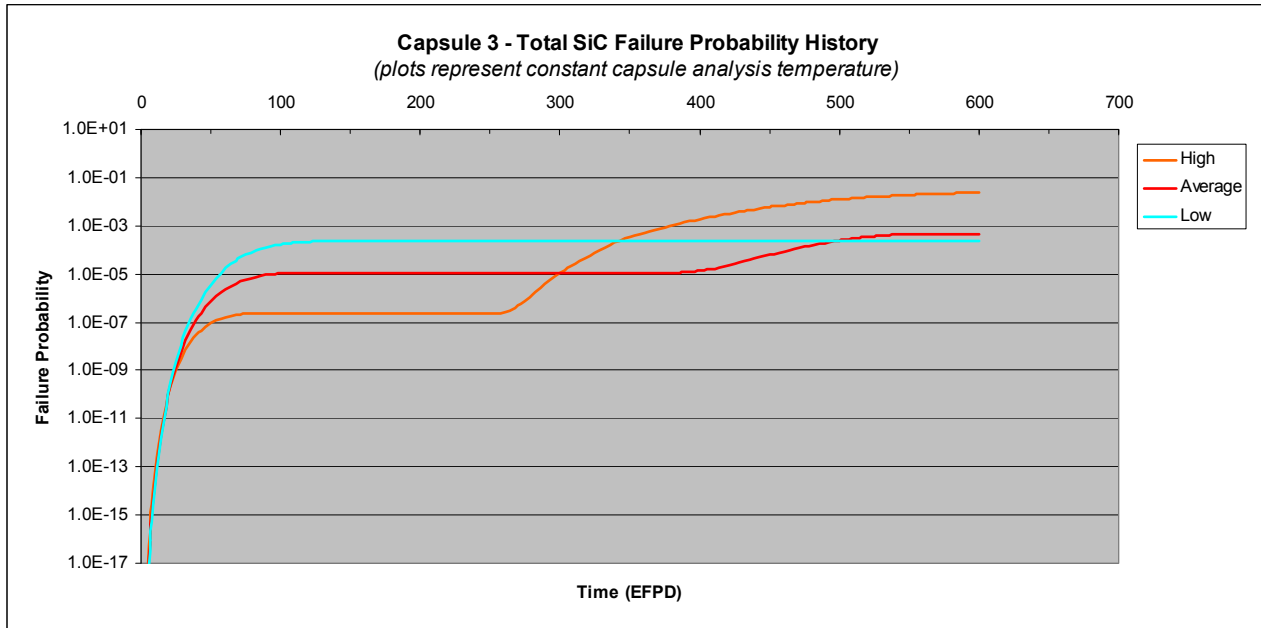


Figure 18. Total SiC Failure Probability (Capsule 3).

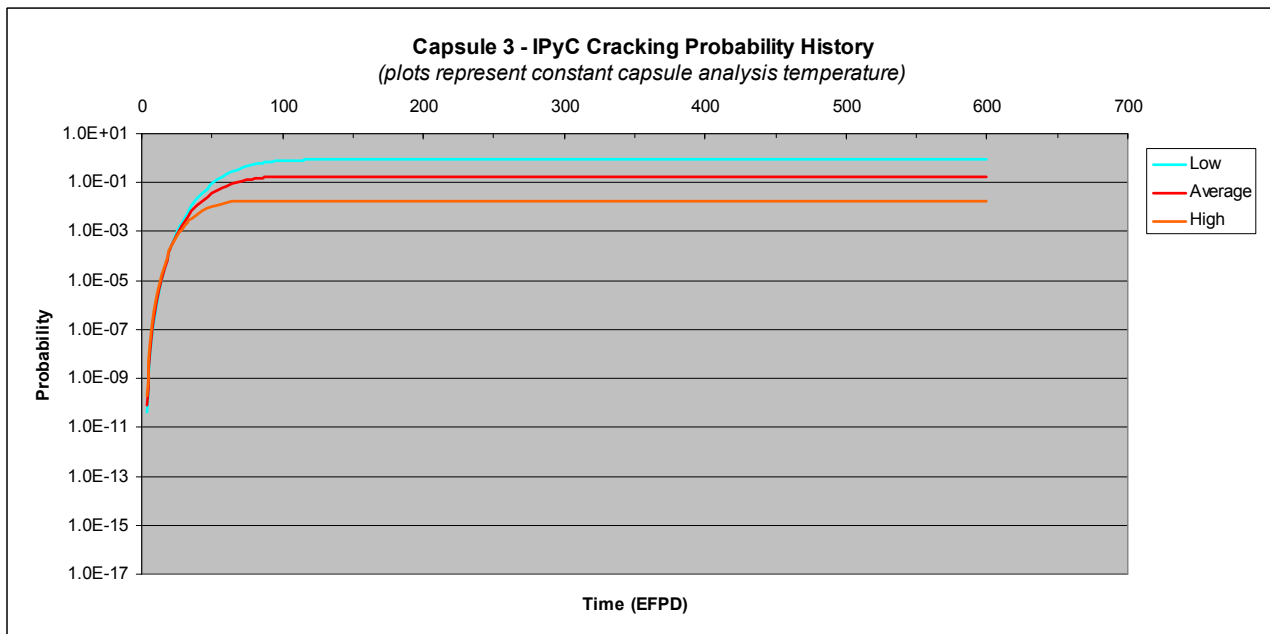


Figure 19. IPyC Cracking Probabilities (Capsule 3).

Title: AGR-2 Pre-Test Prediction Analyses using the PARFUME Code for U.S. Fuel Particles

ECAR No.: 1020

ECAR Rev. No.: 2

Project File No.: 23841

Date: 05/29/2012

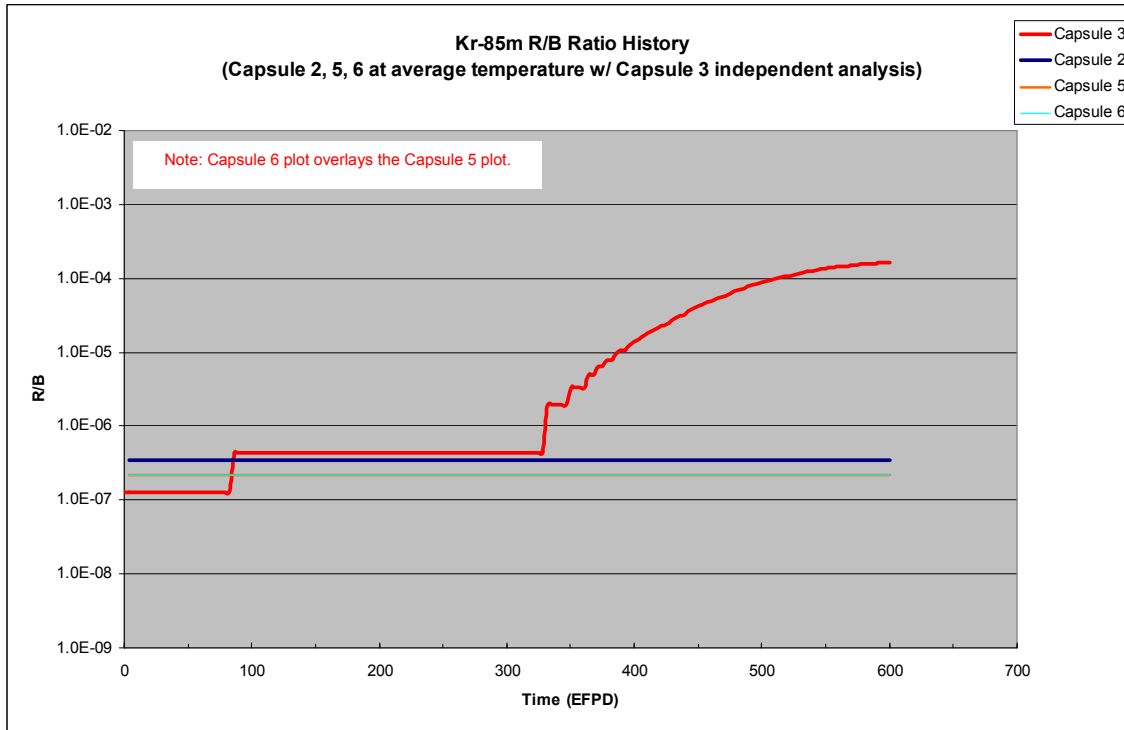


Figure 20. Kr-85m R/B Ratio (Capsules 2, 3, 5, 6).

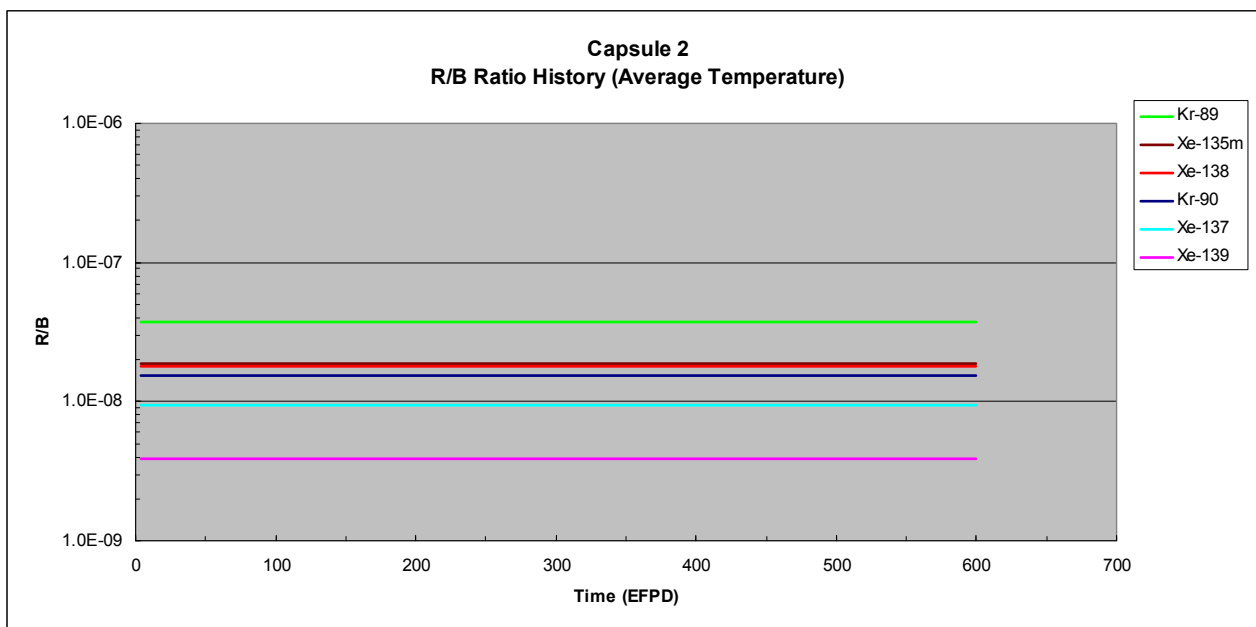


Figure 21. Capsule 2 R/B for fission products with relatively short (<1000 s) half-lives.

Title: AGR-2 Pre-Test Prediction Analyses using the PARFUME Code for U.S. Fuel Particles

ECAR No.: 1020

ECAR Rev. No.: 2

Project File No.: 23841

Date: 05/29/2012

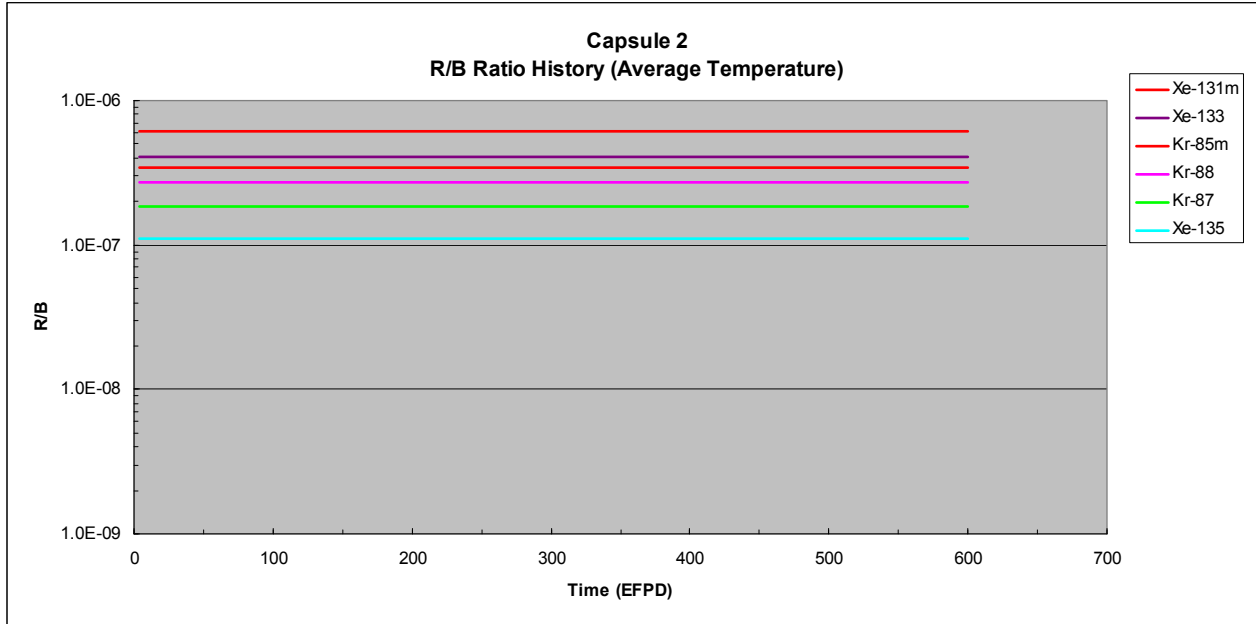


Figure 22. Capsule 2 R/B for fission products with relatively long (>1000 s) half-lives.

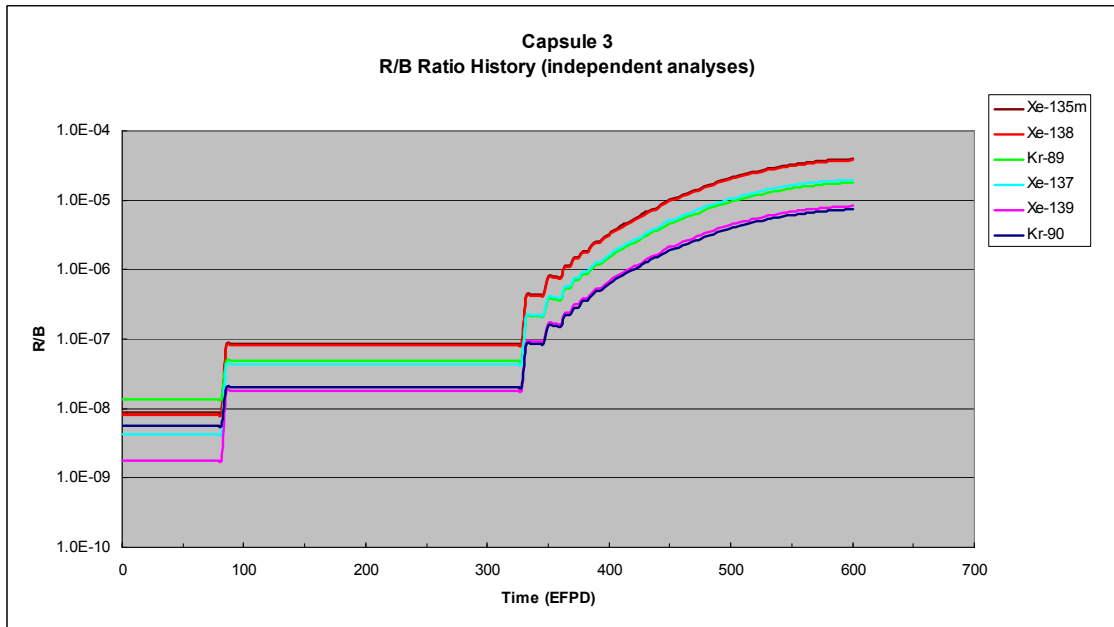


Figure 23. Capsule 3 R/B for fission products with relatively short (<1000 s) half-lives.

Title: AGR-2 Pre-Test Prediction Analyses using the PARFUME Code for U.S. Fuel Particles

ECAR No.: 1020

ECAR Rev. No.: 2

Project File No.: 23841

Date: 05/29/2012

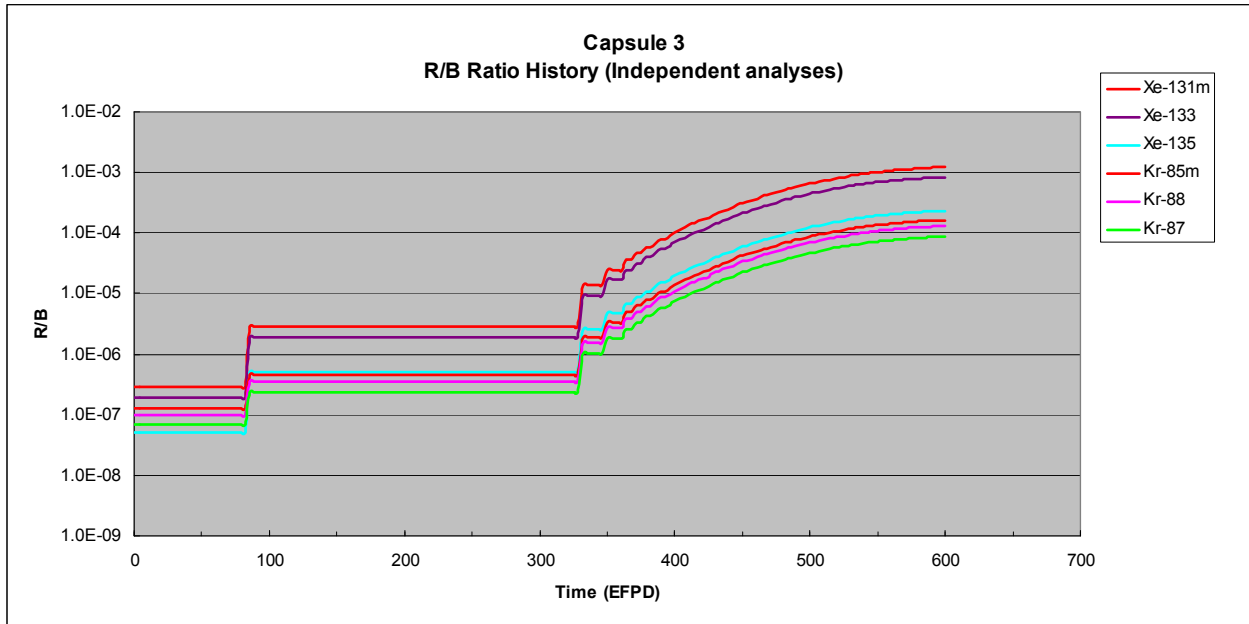


Figure 24. Capsule 3 R/B for fission products with relatively long (>1000 s) half-lives.

CONCLUSIONS

Fuel particle failure analyses of the AGR-2 test were completed using PARFUME for UCO and UO₂ U.S. fuels located in Capsules 2, 3, 5, and 6. The following summarizes conclusions derived as a result of this work.

1. The SiC failure due to IPyC cracking and pressure loading of aspherical particles were the two mechanisms leading to potential fuel particle failures.

The calculated fuel particle failure probabilities varied depending on the fuel type. The estimated final number of particle failures for Capsule 3, the UO₂ fuel type, is 114; while no particle failures are predicted for Capsules 2, 5, and 6, the UCO fuel type.

The fuel particles are exposed to relatively mild to extreme conditions, such that some of the failure mechanisms are triggered. Both fuel types do show some cracking of the IPyC layer, and irradiation temperatures are at levels where these cracks induce significant SiC stresses. Irradiation-induced shrinkage of the IPyC layer induces tensile stresses in the IPyC. Because of the Weibull distribution in IPyC strength, these stresses result in cracking of the IPyC for a nominal percentage of particles. For these cracked particles, the presence of the crack induces tensile stresses in the SiC layer in the region of the crack tip. With a Weibull distribution in SiC strengths, a fraction of these cracked particles are predicted to fail.

2. No failures due to IPyC debonding or failures as the result of the amoeba effect were predicted.

Title: AGR-2 Pre-Test Prediction Analyses using the PARFUME Code for U.S. Fuel Particles

ECAR No.: 1020

ECAR Rev. No.: 2

Project File No.: 23841

Date: 05/29/2012

Because a strong bond is assumed at the IPyC/SiC interface, the predictions indicate that debonding between these layers does not occur in either fuel type. Therefore, partial debonding of the IPyC does not contribute to the predicted failure probability. Finally, the amoeba effect did not contribute to particle failures because UCO and UO₂ kernel migration coefficients are too small.

3. R/B ratio trends are consistent.

For Capsules 2, 5 and 6, which contain no failed particles, R/B results are low ($<1 \times 10^{-6}$) and consistent with release from uranium contamination only and differences in irradiation temperature. For Capsule 3, R/B results are relatively low (e.g. $<1 \times 10^{-6}$) early in the irradiation reflecting release from only uranium contamination. After approximately 82 EFPD, R/B values begin to increase due to additional release from failed particles. With increasing number of failed particle, R/B continues to increase, reaching a maximum value of approximately 1.2×10^{-3} at 600 EFPD.

It is worth noting that design and specification constraints were important in limiting fuel particle failures in these analyses. For example, higher anisotropy and greater asphericity would lead to higher particle failure probabilities; but anisotropy and asphericity were limited by fuel specifications. Test train design incorporated boron carbide in the sample holders to simulate nominal conditions in a high temperature gas reactor. As a result, beginning of life power densities and thermal gradients were reduced. Therefore, constraints imposed by fuel and test specifications along with design considerations are reflected in PARFUME results such that predicted AGR-2 fuel particle failures are expected to be low in some capsules and higher in capsules exposed to harsher conditions.

The number of predicted UO₂ particle failures may be considered as a conservative upper bound estimate. This conservatism arises from the chemical equilibrium based CO model used in PARFUME which may overestimate its production and hence, overestimate particle internal pressures. Also, the number and severity of faceted particles may be over estimated by PARFUME given that the asphericity input is based upon quality control data that reflects aspect ratios for both ellipsoidal and faceted particles. For a given aspect ratio, faceted particles have a higher probability of failure than ellipsoidal particles; hence, PARFUME may over predict failures due to asphericity.

Ultimately, the computed failure probabilities, and in general all results, are only approximations. They are approximations because the compacts in each capsule will never be at a given uniform temperature (as assumed in the calculations). Instead, fuel particles in each capsule will be exposed to some distribution of temperatures in space and time. Consequently, the results strictly apply only if all fuel particles in the capsules are exposed to the assumed uniform temperatures, and will only be approximations otherwise.

COMPUTER CODE VALIDATION

The solution process, depicted in Figure 25 below and implemented in PARFUME Version 2.18, involves preparing input data, processing the input data using the PARFUME code, and subsequent post-processing of the output (i.e., generation of results).

Title: AGR-2 Pre-Test Prediction Analyses using the PARFUME Code for U.S. Fuel Particles

ECAR No.: 1020

ECAR Rev. No.: 2

Project File No.: 23841

Date: 05/29/2012

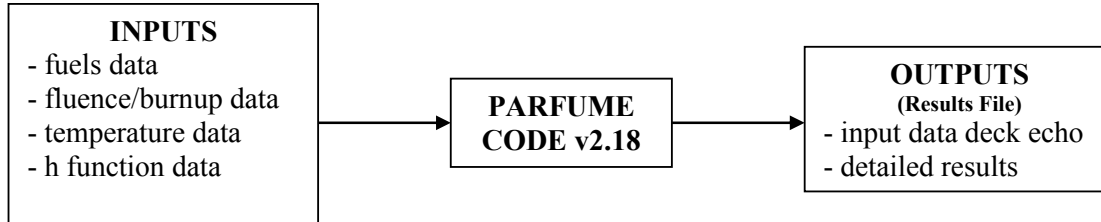


Figure 25. PARFUME solution process.

The PARFUME executable used for the analyses was compiled on the Sun hardware platform using an Intel compiler using the default compiler optimization setting. A description of the compiler and the settings used to compile PARFUME Version 2.18 are presented in Reference 9. Most calculations were performed on the Sun x86_64 workstation running SUSE LINUX using PARFUME Version 2.18⁴ as configured in the Revision Control System (RCS).⁵ Analysis software and hardware descriptions for this step in the analysis process are presented in Table 7 and Table 8 below.

All of the input data, except for the “h function” inputs were obtained from References 7 and 8. The “h function” input was computed using the following analysis software: PARFUME Version 2.18 and ABAQUS Version 6.7-5, a commercial structural analysis code.^{11,12} The underlying theory of “h functions” is presented in References 1 and 2. The data obtained from the “h function” analysis was post-processed using simple Fortran 90/95 programs (“haspher.exe” and “hipycr.exe”), which were compiled on Icestorm.¹⁰ A formal verification and validation (V&V) of these two programs was not conducted, although results were reviewed and confirmed, using ABAQUS Viewer and MS Excel 2007, to be satisfactory. Additional raw data (e.g. fluence and burnup) from Reference 7 was post-processed using MS Excel 2003. Collectively this information is entered into what is referred to as an “input data deck”, which is the primary data input into PARFUME. The input data decks are presented in Appendix C, and an input data summary is presented in Table 1 through Table 5.

The data output by PARFUME is generated in a results file which includes an input data deck echo; the echo enables the user to verify the parameters that were input into PARFUME. The detailed results were post-processed (i.e., graphical plot development) using MS Excel 2003. Selected output data is presented in Table 6, Figure 7 through Figure 24, and Appendix B.

Although PARFUME results have been compared with hand calculations and with results from codes that have been subjected to formal V&V methodologies, the V&V of PARFUME is not considered complete. This situation is unavoidable given that the code is still in the development stage. This is mentioned only as an indication of the current code status and should not be interpreted to mean that PARFUME results are unreliable or unusable. Comparisons against independent results have instilled a good level of confidence in the code.^{13, 14}

Due to the nature of the raw data (e.g. h functions and reactor physics analysis results⁷) required for input into PARFUME in addition to the raw data output by PARFUME, MS Excel is used extensively for processing this data. Although a formal validation report has not been performed, documenting the current validation status of MS Excel, data transfer among worksheets and some results computed by MS Excel were checked with hand calculations to provide some level of confidence in the post-processing results. Note that hundreds of calculations are performed using MS Excel, making it impractical to check all MS Excel results using hand calculations.

Title: AGR-2 Pre-Test Prediction Analyses using the PARFUME Code for U.S. Fuel Particles

ECAR No.: 1020

ECAR Rev. No.: 2

Project File No.: 23841

Date: 05/29/2012

User developed calculations to support failed particle R/B analyses were computed using MS Excel 2003 on PC #2. Some of the spreadsheet R/B results were compared with hand calculations; the spreadsheet and hand calculations agreed. Note that hundreds of R/B calculations are performed using MS Excel, making it impractical to check all of the spreadsheet results using hand calculations.

Table 7. Analysis software and hardware platforms.

Software Name	Software Version	Hardware Platform
PARFUME	2.18	Icestorm and Sun
ABAQUS	6.7-5	Icestorm
haspher/hipyccr	0	Icestorm
MS Excel	2007 SP2 (MSO)	PC #1
MS Excel	2003 SP3 (MSO)	PC #2

Table 8. Description of hardware used to run the analysis software.

Hardware	Model	Operating System	Processor
Icestorm	SGI Altix ICE 8200	SUSE Linux Enterprise Server 10 (x86_64)	Intel Xeon@2.66GHz
Sun	Sun W2100Z	SUSE Linux 2.6 (x86_64)	AMD Opteron 252@2.6GHz
PC #1	Dell Precision T5400	MS Windows XP 2002 SP3 (x86_32)	Intel Xeon E5430@2.66Hz
PC #2	Dell Precision 490	MS Windows XP 2002 SP3 (x86_32)	Intel Xeon 5150@2.66Hz

PE STAMP

N/A

REFERENCES

1. Miller, G. K., Petti, D. A., Maki, J. T., Knudson, D. L., "PARFUME Theory and Model Basis Report," INL/EXT-08-14497, Idaho National Laboratory, September 2009.
2. Miller, G. K., Petti, D. A., et al., "PARFUME Theory Overview," INL/MIS-10-18314, Idaho National Laboratory, April 2010.
3. PARFUME Development Team, "PARFUME User Guide," INL/EXT-10-18317 (DRAFT), Idaho National Laboratory, March 2010.
4. PARFUME, Version 2.18 in the Revision Control System, running on a Sun x86_64 workstation operating with SUSE LINUX, June 2010.

Title: AGR-2 Pre-Test Prediction Analyses using the PARFUME Code for U.S. Fuel Particles

ECAR No.: 1020

ECAR Rev. No.: 2

Project File No.: 23841

Date: 05/29/2012

5. Tichy, W. F., "RCS - A System for Version Control," Software Practice and Experience, 15, 7, pg. 637-654, July 1985.
6. Maki, J. T., "AGR-2 Irradiation Test Specification," SPC-1064, Revision 1, Idaho National Laboratory, June 2010.
7. Chang, G. S., and J. R. Parry, "Reactor Physics Analysis for the AGR-2 Experiment Irradiated in the ATR B-12 Position," ECAR-949, Revision 0, Idaho National Laboratory, May 2010.
8. Maki, J. T., data files transmitted via e-mail to K. D. Hamman and W. F. Skerjanc, Idaho National Laboratory, April 28 and 29, 2010. (Transmitted files contain "new AGR-2 fuel parameter list" and "AGR-2 pre-test irradiation conditions.")
9. Intel(R) Fortran Compiler for Intel(R) EM64T-based applications, Version 9.1, Build 20070510, Package ID: I_fc_c_9.1.051, Intel Corporation, 2007. (PARFUME v2.18 executable compiled under options: < ifort -fpe0 -V -check bounds -check uninit -traceback -o pf.x pf.f >.)
10. Intel(R) Fortran Intel(R) 64 Compiler Professional for applications running on Intel(R) 64, Version 11.1, Build 20090630, Package ID: I_cprof_p_11.1.046, Intel Corporation, 2009. (Both executables compiled under default options.)
11. ABAQUS User's Manual, Version 6.7-5, Hibbitt, Karlsson, and Sorenson, Inc., 2007.
12. Snow, S. D., "Software Validation Report for ABAQUS/Standard and ABAQUS/Explicit Version 6.7-5," ECAR-202, May 2008.
13. Miller, G. K., and D. L. Knudson, "PARFUME Benchmark for Coated Particle Fuel Performance Under Normal Operation," EDF-6036, Idaho National Laboratory, June 2005.
14. Miller, G. K. and Knudson D. L., "Advanced Gas Reactor-1 Pre-Test Prediction Analyses Using the PARFUME Code," EDF-5741, Revision 1, Idaho National Laboratory, April 2007.
15. Petti, D. A. (Lead Principal Investigator), "Development of Improved Models and Designs for Coated-Particle Gas Reactor Fuels," INEEL/EXT-05-02615, Idaho National Laboratory, December 2004.

Title: AGR-2 Pre-Test Prediction Analyses using the PARFUME Code for U.S. Fuel Particles

ECAR No.: 1020

ECAR Rev. No.: 2

Project File No.: 23841

Date: 05/29/2012

APPENDIXES

Title: AGR-2 Pre-Test Prediction Analyses using the PARFUME Code for U.S. Fuel Particles

ECAR No.: 1020

ECAR Rev. No.: 2

Project File No.: 23841

Date: 05/29/2012

Appendix A – Reference 8

AGR-2 Pre-test Irradiation Conditions					
For all cases, all fuel in each capsule is at the same temperature for 600 EFPD					
Capsule	Fuel	EOL Burnup (% FIMA)	EOL Fluence (1E25)	Case	Temperature (C)
6	UCO	9.45	2.63	Max temp	1240
				Vol ave temp	1075
				Min temp	910
5	UCO	11.71	3.52	Max temp	1240
				Vol ave temp	1075
				Min temp	910
3	UO2	10.34	3.81	Max temp	1140
				Vol ave temp	970
				Min temp	800
2	UCO	12.43	3.70	Max temp	1390
				Vol ave temp	1225
				Min temp	1060

Title: AGR-2 Pre-Test Prediction Analyses using the PARFUME Code for U.S. Fuel Particles

ECAR No.: 1020

ECAR Rev. No.: 2

Project File No.: 23841

Date: 05/29/2012

AGR-2 US Fuel Characteristics for Pre Test Prediction

Parameter	Unit	US UCO Fuel		US UO2 Fuel	
		Mean	Std. Dev.	Mean	Std. Dev.
Ambient pressure	MPa	0.1		0.1	
oxygen to uranium	atom ratio	1.43		2.00	
carbon to uranium	atom ratio	0.39		0.00	
U235 enrichment	wt. %	14.03		9.60	
Kernel diameter	um	426.7	8.8	507.7	11.9
Buffer thickness	um	98.9	8.4	97.7	9.9
IPyC thickness	um	40.4	2.5	41.9	3.2
SiC thickness	um	35.2	1.2	37.5	1.2
OPyC thickness	um	43.4	2.9	45.6	2.4
Kernel density	g/cc	10.97		10.86	
Buffer density	g/cc	1.04		0.99	
IPyC density	g/cc	1.89	0.01	1.89	0.02
SiC density	g/cc	3.20		3.20	
OPyC density	g/cc	1.91	0.01	1.88	0.01
Post-anneal IPyC BAF		1.047	0.005	1.047	0.004
Post-anneal OPyC BAF		1.043	0.002	1.037	0.002
Particle sphericity	OPyC aspect ratio	1.052	0.017	1.052	0.016
compact diameter	mm	12.29		12.27	
compact length	mm	25.14		25.13	
packing fraction	vol. %	37.1		23.7	
number particles per compact		3171		1555	
compacts/capsule		12		12	
U contamination	g U/g U in compact	9.74E-06		8.55E-06	

Title: AGR-2 Pre-Test Prediction Analyses using the PARFUME Code for U.S. Fuel Particles

ECAR No.: 1020

ECAR Rev. No.: 2

Project File No.: 23841

Date: 05/29/2012

Appendix B – Graphical Results

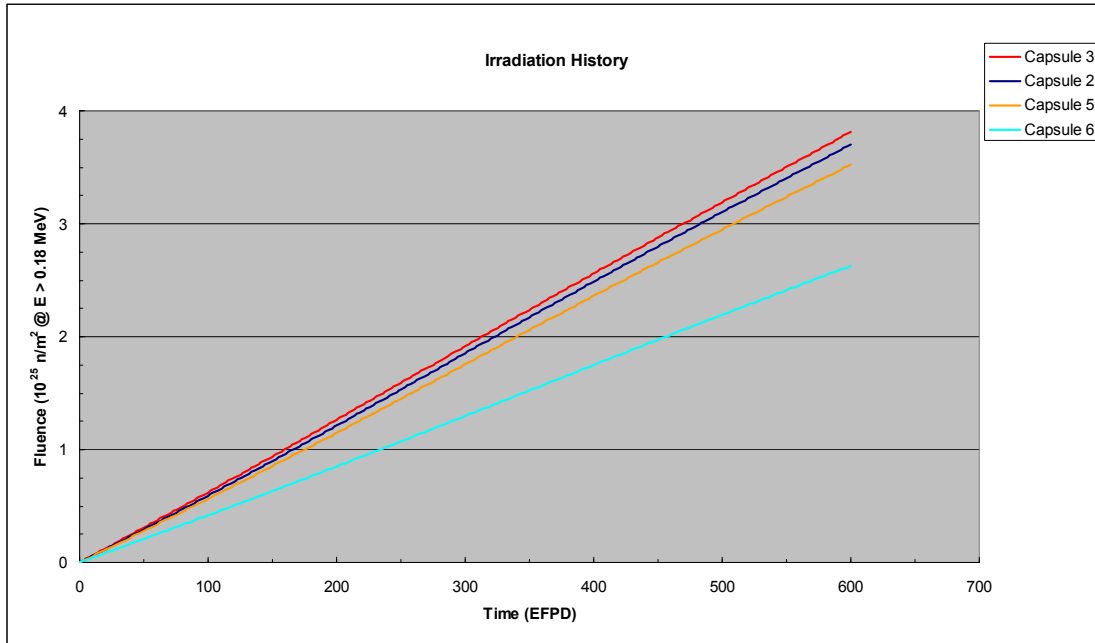


Figure B-1. Fluence as a function of time from AGR-2 neutronics analyses.⁷

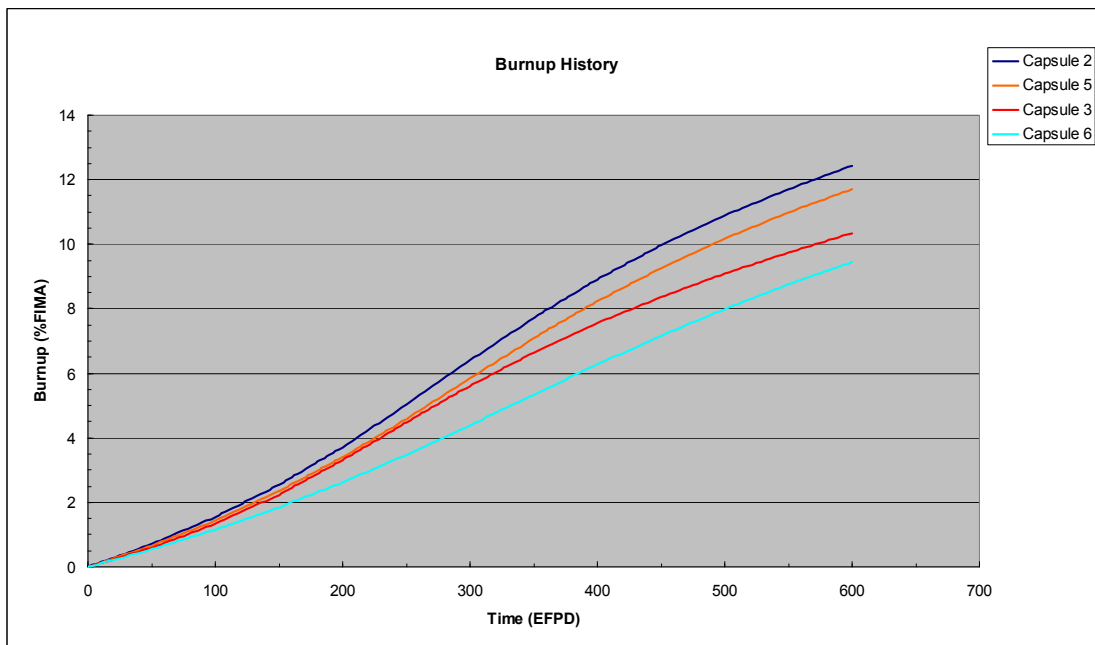


Figure B-2. Burnup as a function of time from AGR-2 neutronics analyses.⁷

Title: AGR-2 Pre-Test Prediction Analyses using the PARFUME Code for U.S. Fuel Particles

ECAR No.: 1020

ECAR Rev. No.: 2

Project File No.: 23841

Date: 05/29/2012

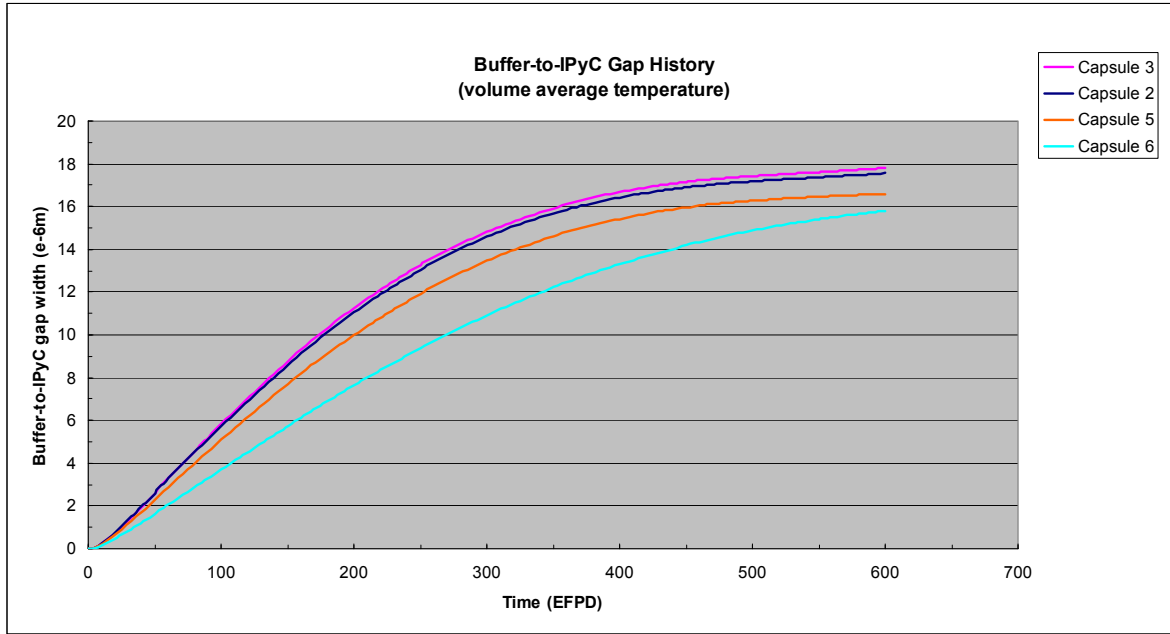


Figure B-3. Buffer-to-IPyC gap width in nominal particles (Capsules 3, 2, 5, 6).

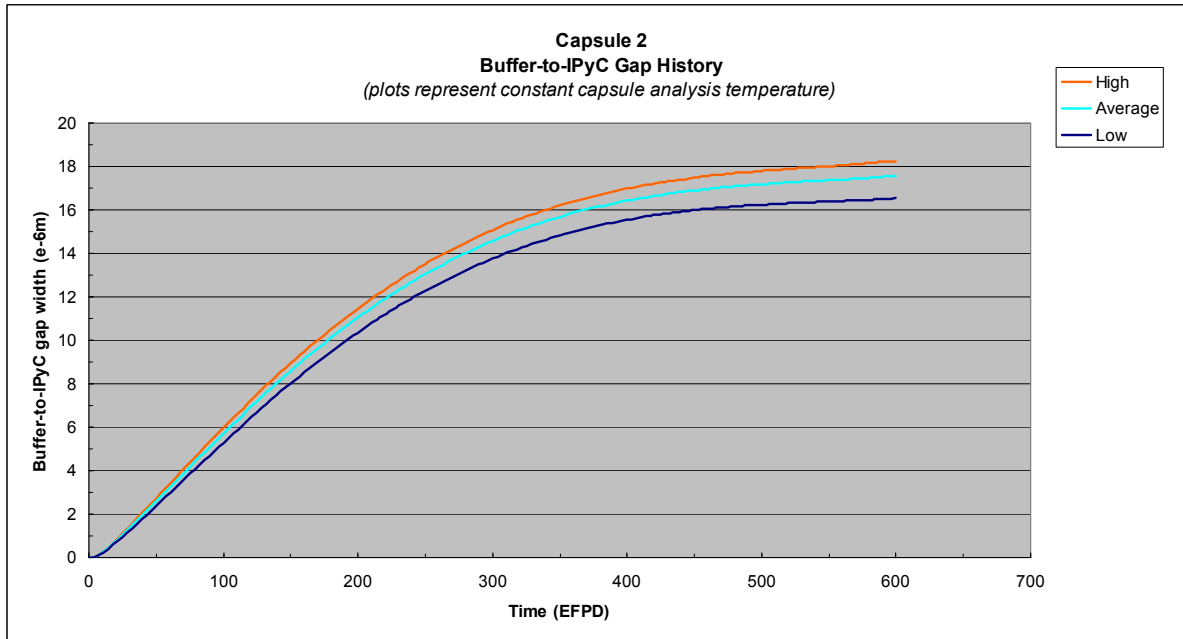


Figure B-4. Buffer-to-IPyC gap width in nominal particles (Capsule 2).

Title: AGR-2 Pre-Test Prediction Analyses using the PARFUME Code for U.S. Fuel Particles

ECAR No.: 1020

ECAR Rev. No.: 2

Project File No.: 23841

Date: 05/29/2012

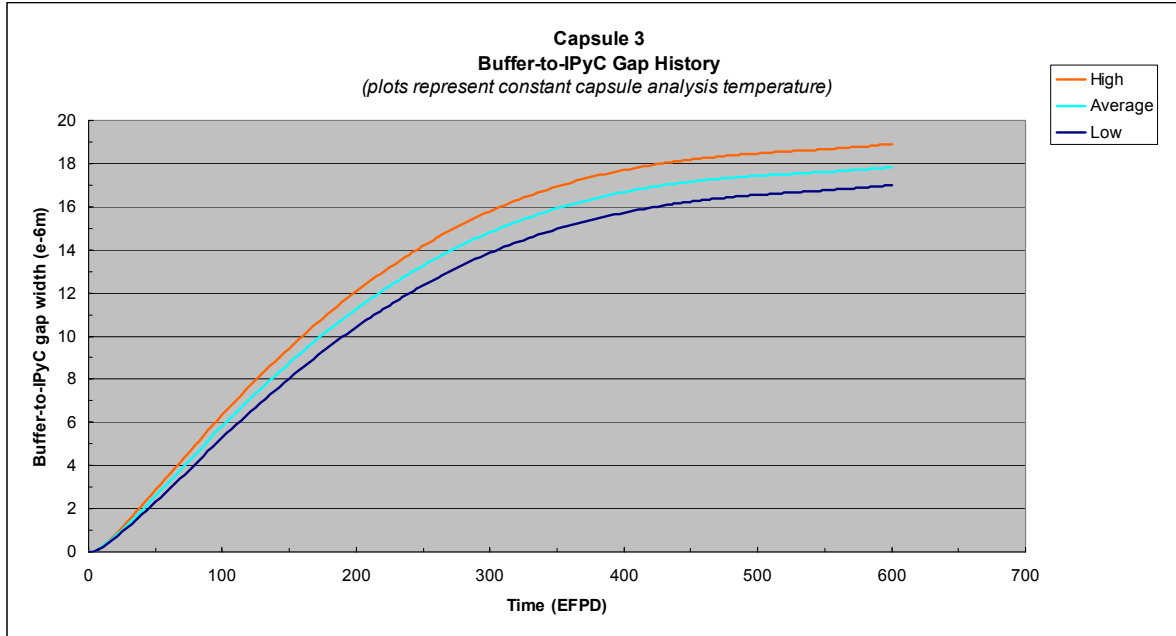


Figure B-5. Buffer-to-IPyC gap width in nominal particles (Capsule 3).

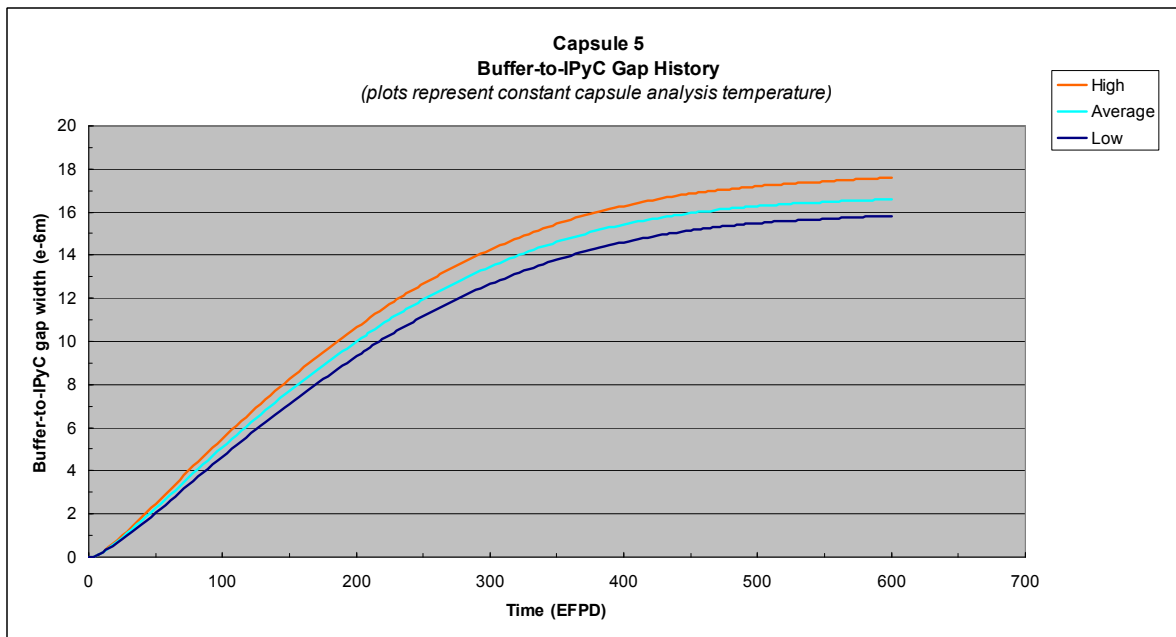


Figure B-6. Buffer-to-IPyC gap width in nominal particles (Capsule 5).

Title: AGR-2 Pre-Test Prediction Analyses using the PARFUME Code for U.S. Fuel Particles

ECAR No.: 1020

ECAR Rev. No.: 2

Project File No.: 23841

Date: 05/29/2012

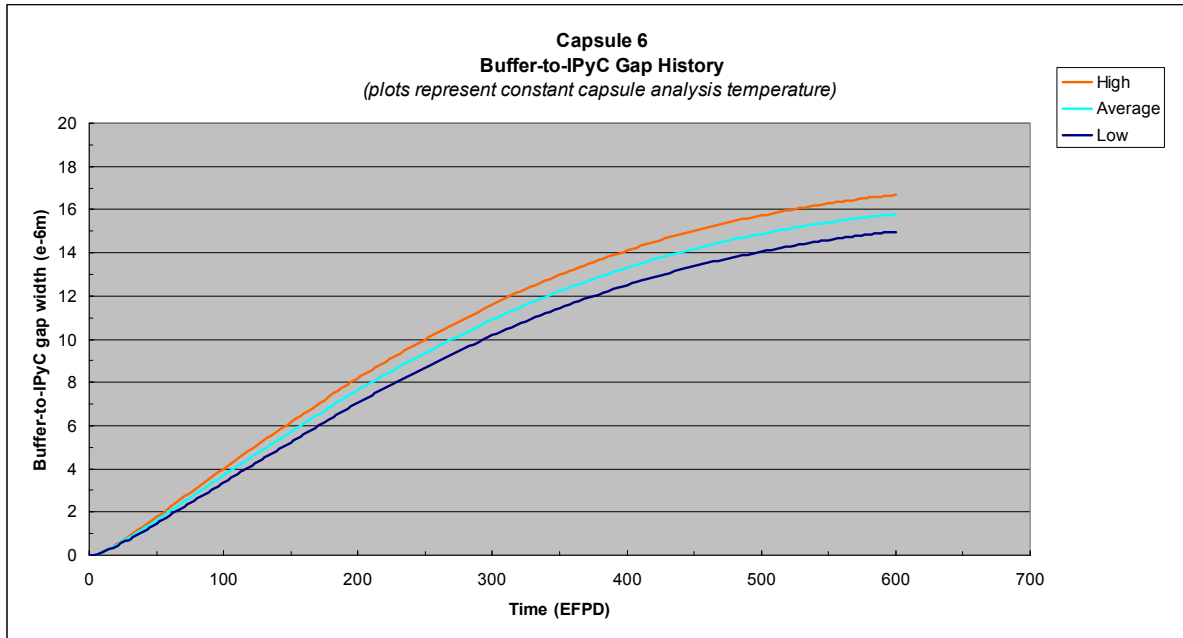


Figure B-7. Buffer-to-IPyC gap width in nominal particles (Capsule 6).

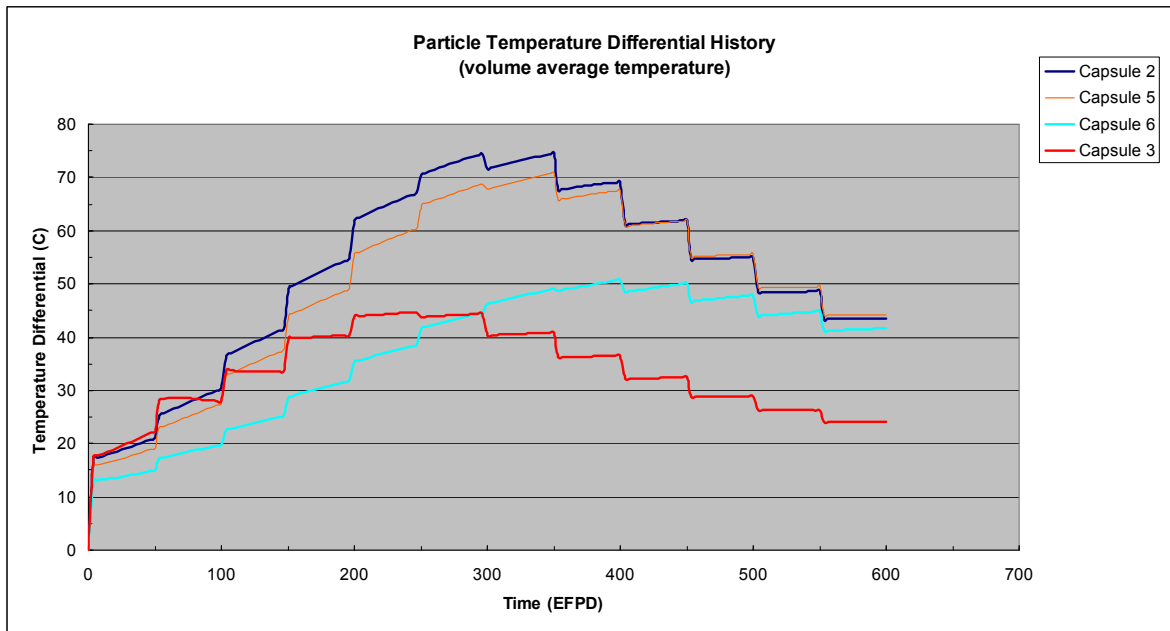


Figure B-8. Particle temperature differentials, kernel centerline to the outer surface of OPyC (Capsules 2, 3, 5, 6).

Title: AGR-2 Pre-Test Prediction Analyses using the PARFUME Code for U.S. Fuel Particles

ECAR No.: 1020

ECAR Rev. No.: 2

Project File No.: 23841

Date: 05/29/2012

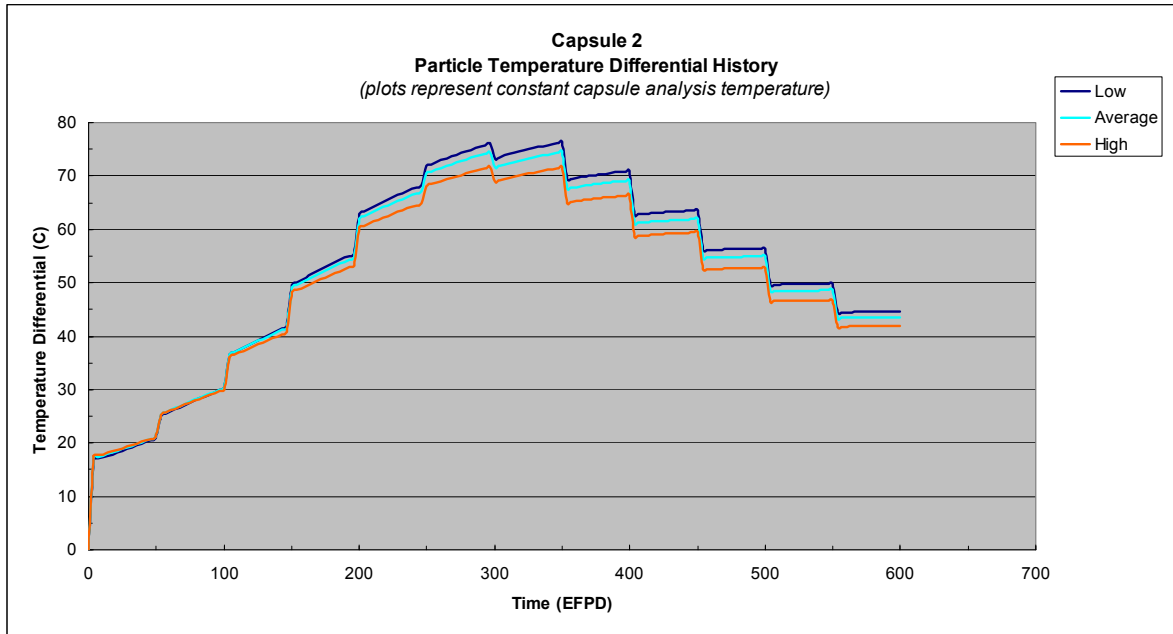


Figure B-9. Particle temperature differential, kernel centerline to the outer surface of the OPyC (Capsule 2).

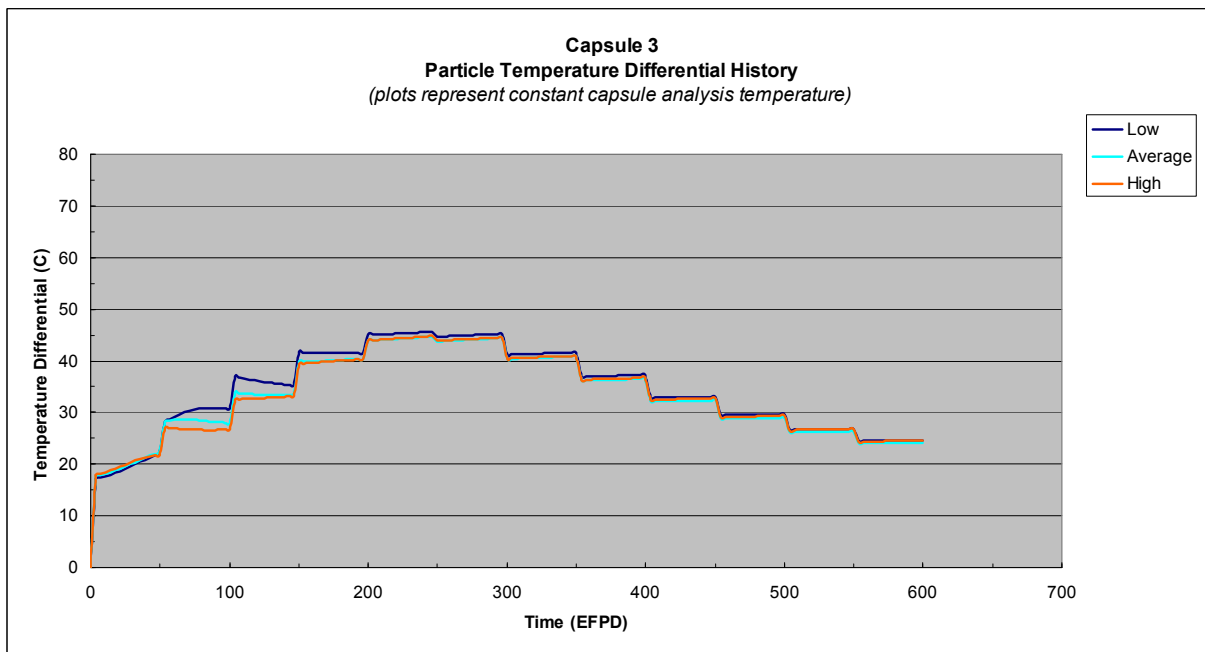


Figure B-10. Particle temperature differential, kernel centerline to the outer surface of the OPyC (Capsules 3).

Title: AGR-2 Pre-Test Prediction Analyses using the PARFUME Code for U.S. Fuel Particles

ECAR No.: 1020

ECAR Rev. No.: 2

Project File No.: 23841

Date: 05/29/2012

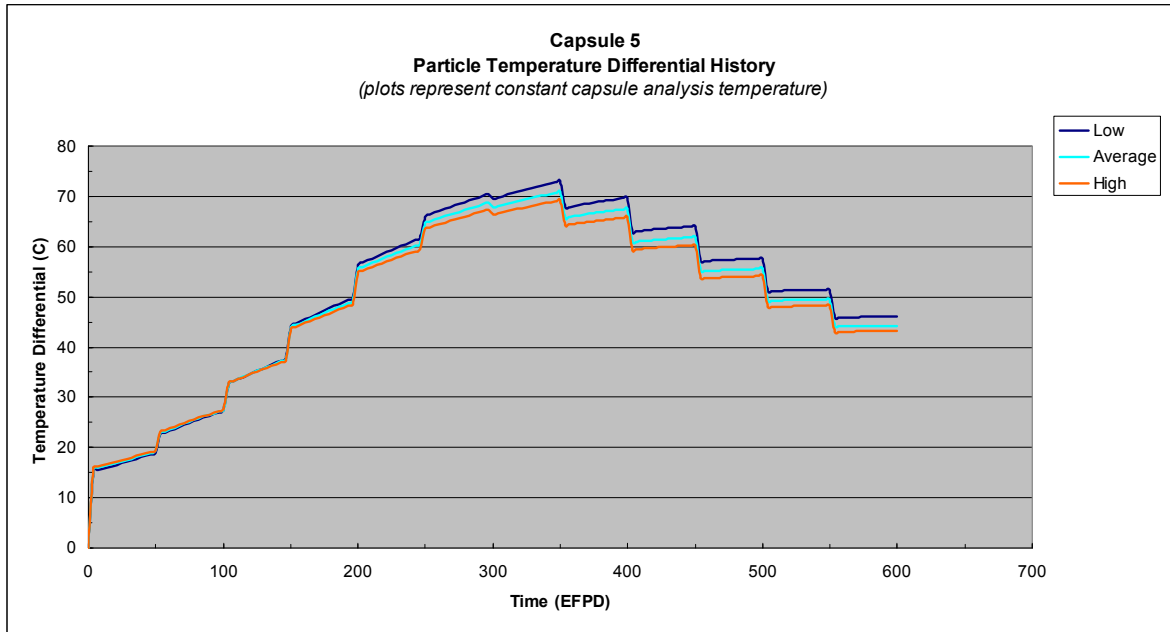


Figure B-11. Particle temperature differential, kernel centerline to the outer surface of the OPyC (Capsules 5).

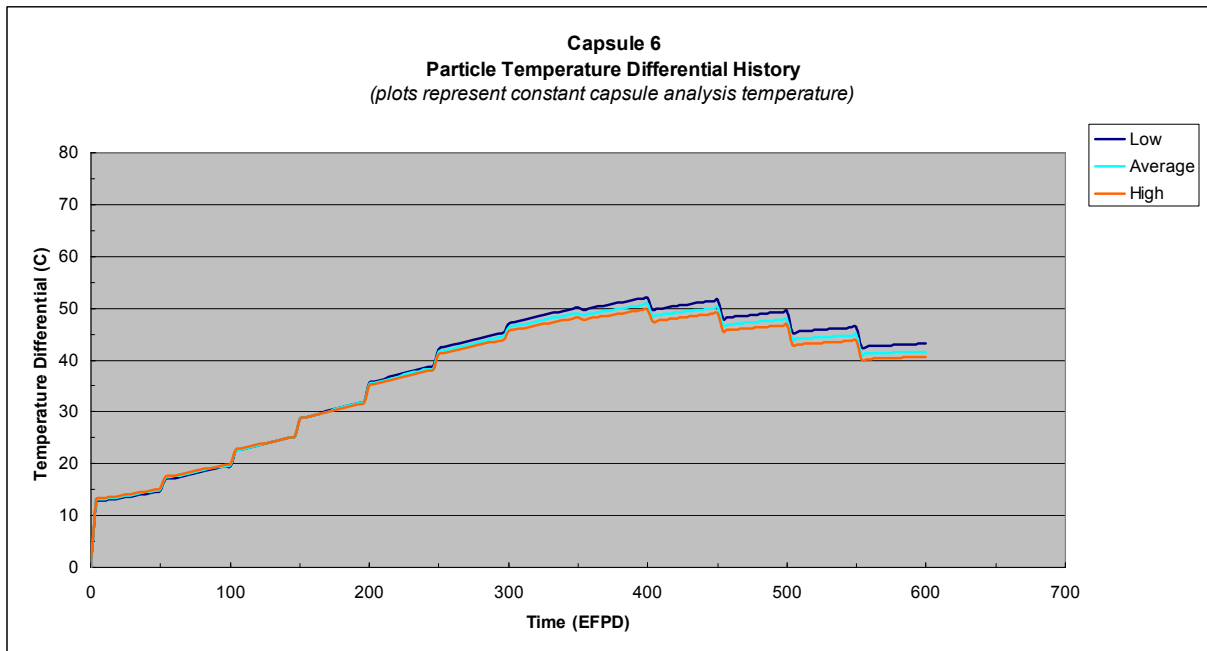


Figure B-12. Particle temperature differential, kernel centerline to the outer surface of the OPyC (Capsules 6).

Title: AGR-2 Pre-Test Prediction Analyses using the PARFUME Code for U.S. Fuel Particles

ECAR No.: 1020

ECAR Rev. No.: 2

Project File No.: 23841

Date: 05/29/2012

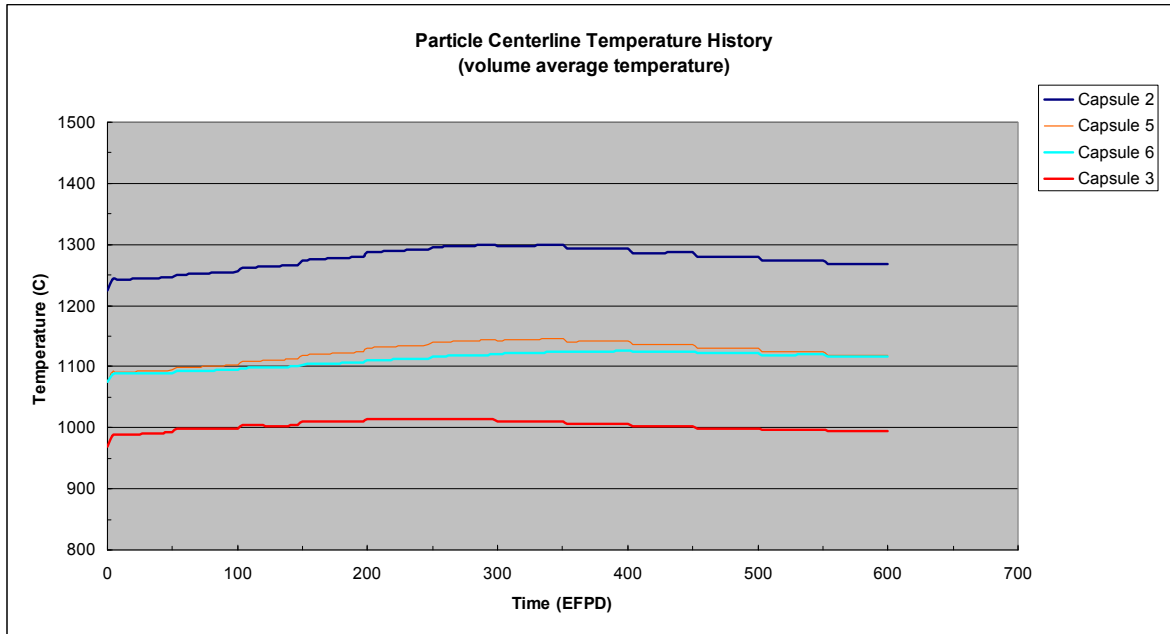


Figure B-13. Kernel centerline temperature (Capsules 2, 3, 5, 6).

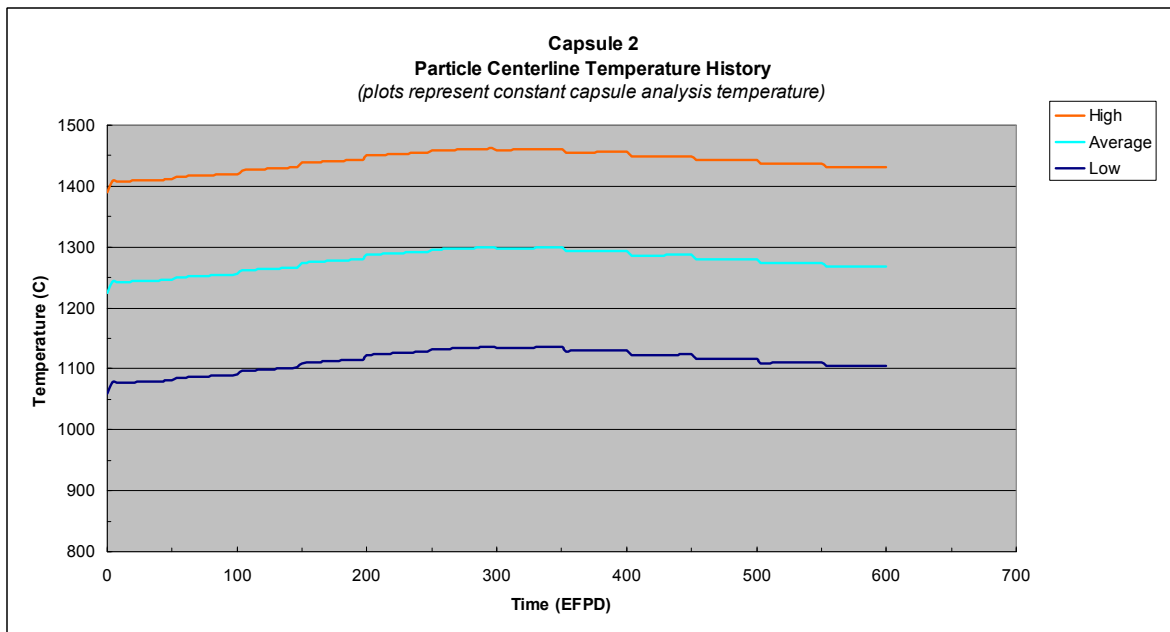


Figure B-14. Kernel centerline temperature (Capsules 2).

Title: AGR-2 Pre-Test Prediction Analyses using the PARFUME Code for U.S. Fuel Particles

ECAR No.: 1020

ECAR Rev. No.: 2

Project File No.: 23841

Date: 05/29/2012

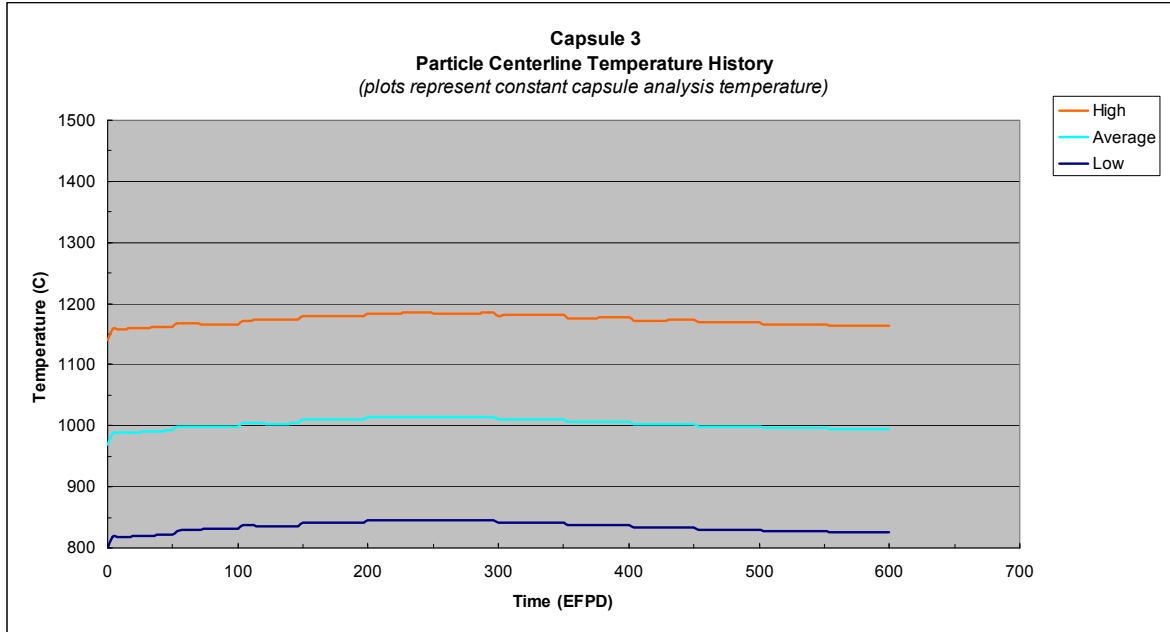


Figure B-15. Kernel centerline temperature (Capsules 3).

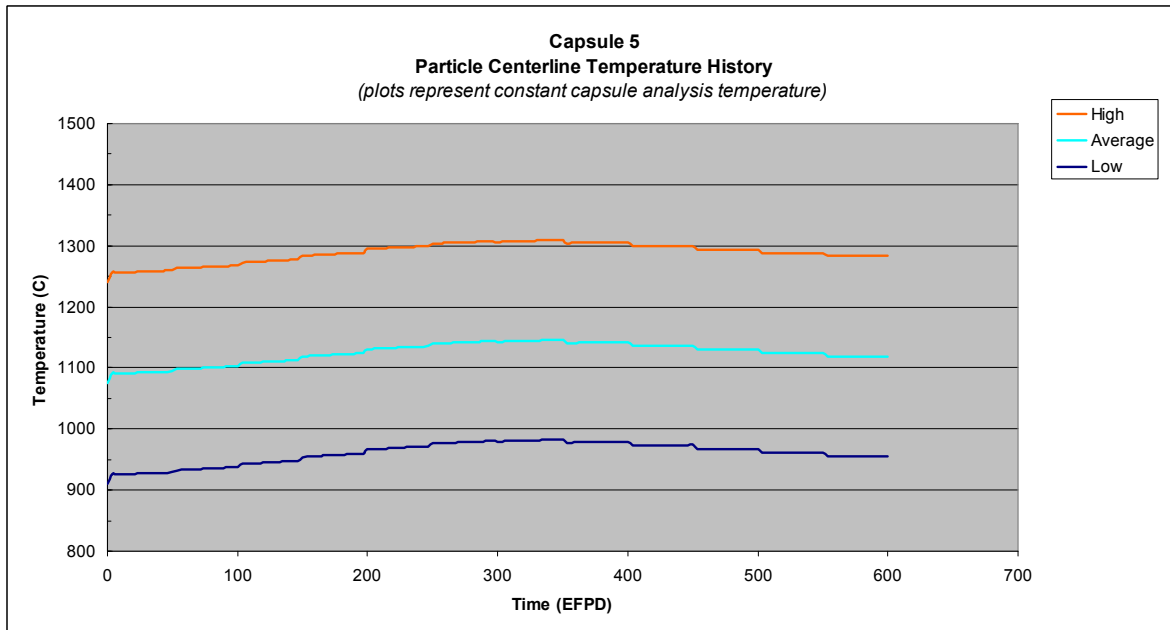


Figure B-16. Particle center line temperature (Capsules 5).

Title: AGR-2 Pre-Test Prediction Analyses using the PARFUME Code for U.S. Fuel Particles

ECAR No.: 1020

ECAR Rev. No.: 2

Project File No.: 23841

Date: 05/29/2012

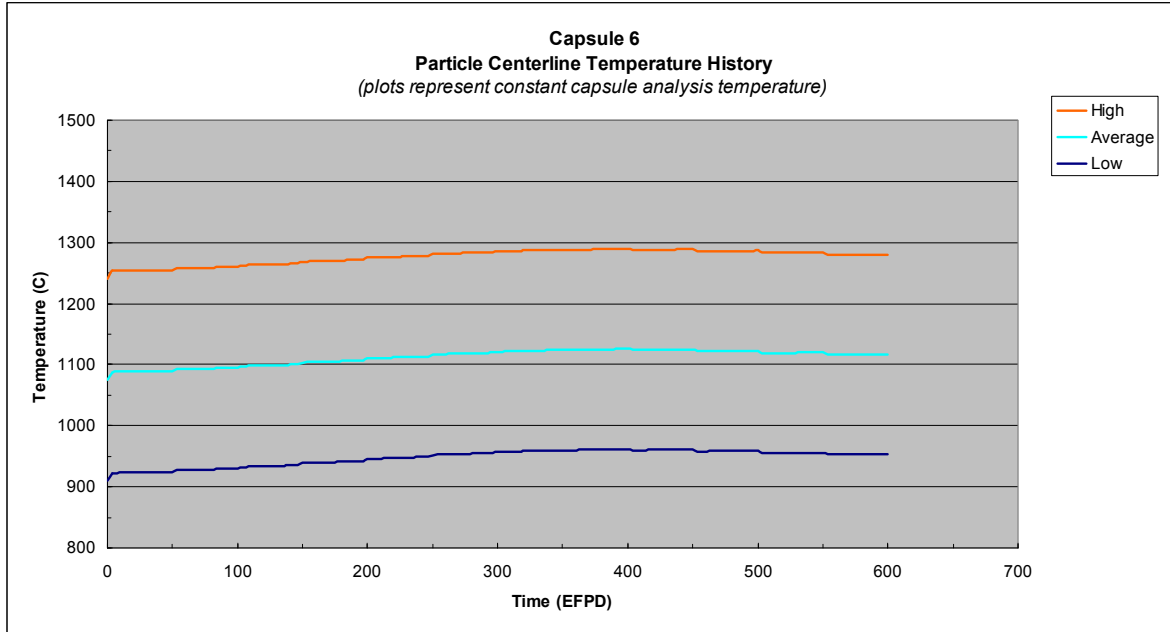


Figure B-17. Particle center line temperature (Capsules 6).

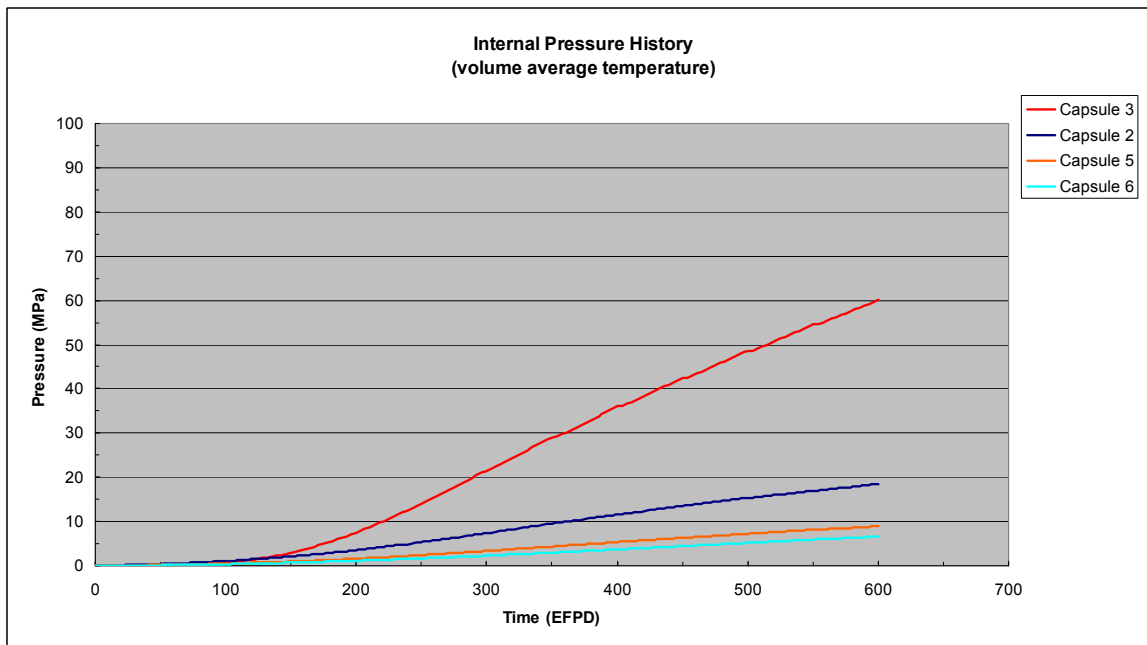


Figure B-18. Particle internal pressure (Capsules 2, 3, 5, 6)

Title: AGR-2 Pre-Test Prediction Analyses using the PARFUME Code for U.S. Fuel Particles

ECAR No.: 1020

ECAR Rev. No.: 2

Project File No.: 23841

Date: 05/29/2012

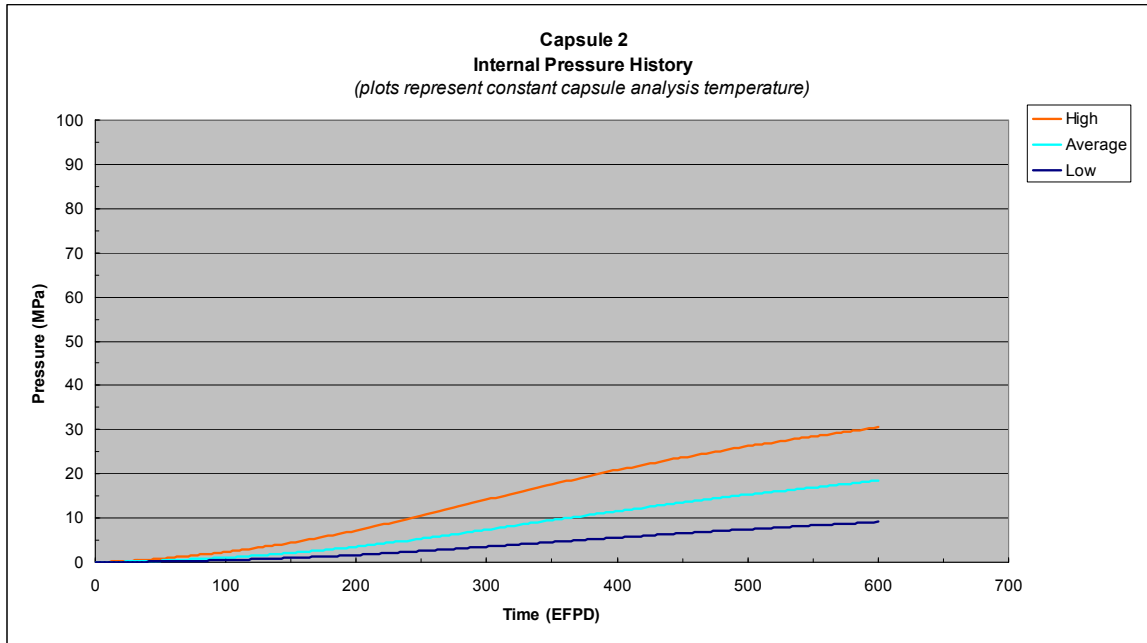


Figure B-19. Particle internal pressure (Capsules 2)

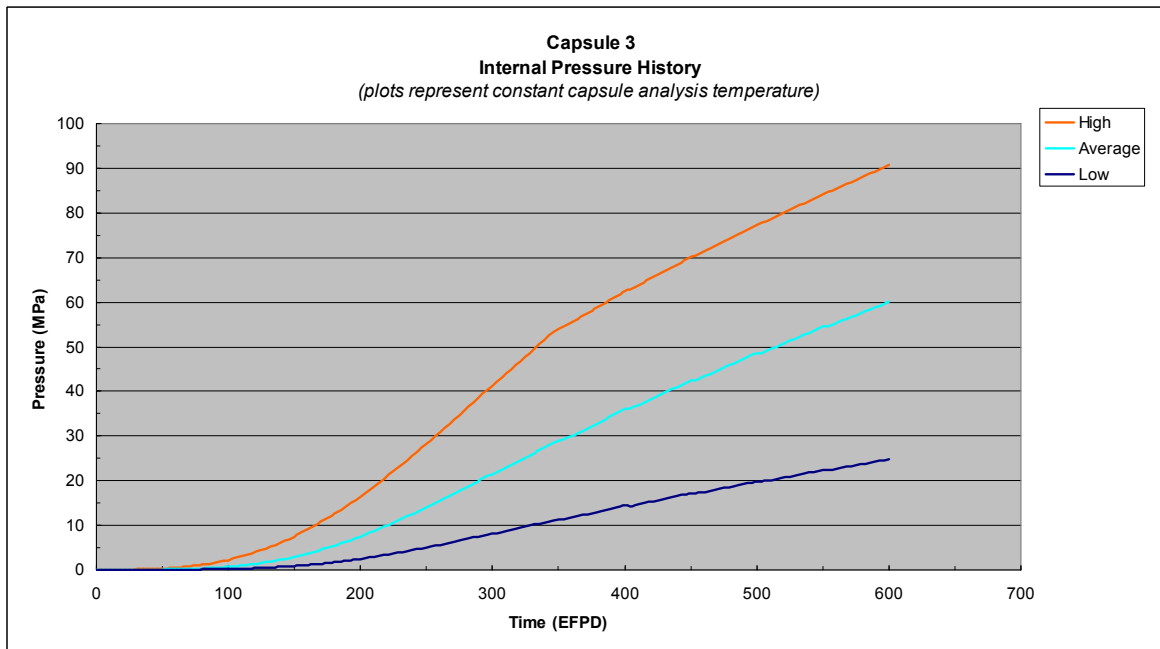


Figure B-20. Particle internal pressure (Capsules 3)

Title: AGR-2 Pre-Test Prediction Analyses using the PARFUME Code for U.S. Fuel Particles

ECAR No.: 1020

ECAR Rev. No.: 2

Project File No.: 23841

Date: 05/29/2012

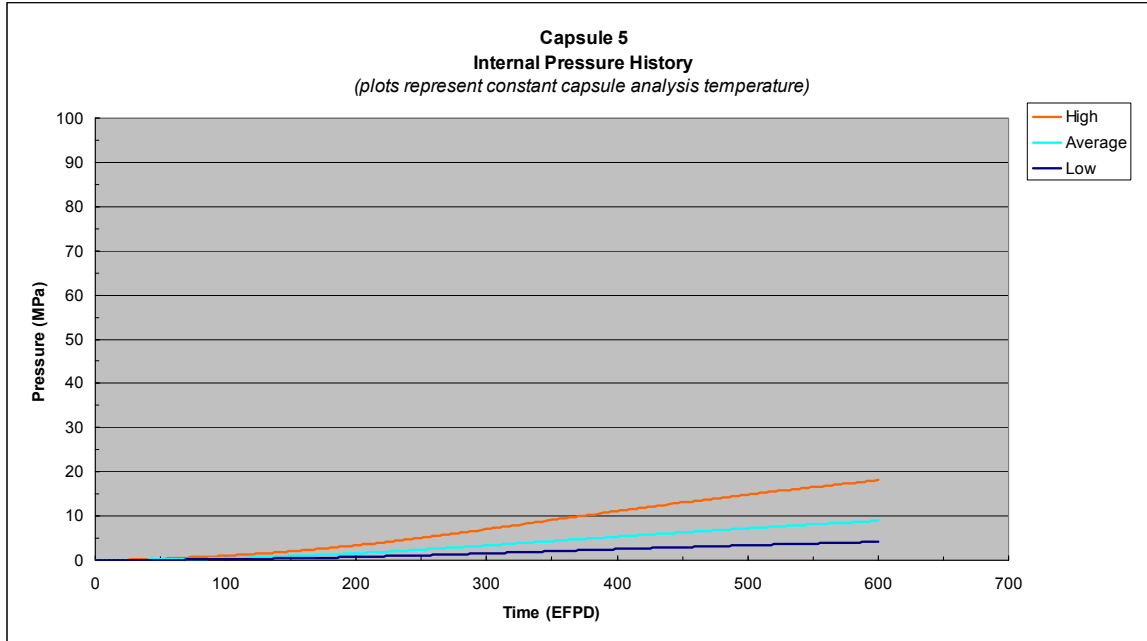


Figure B-21. Particle internal pressure (Capsules 5)

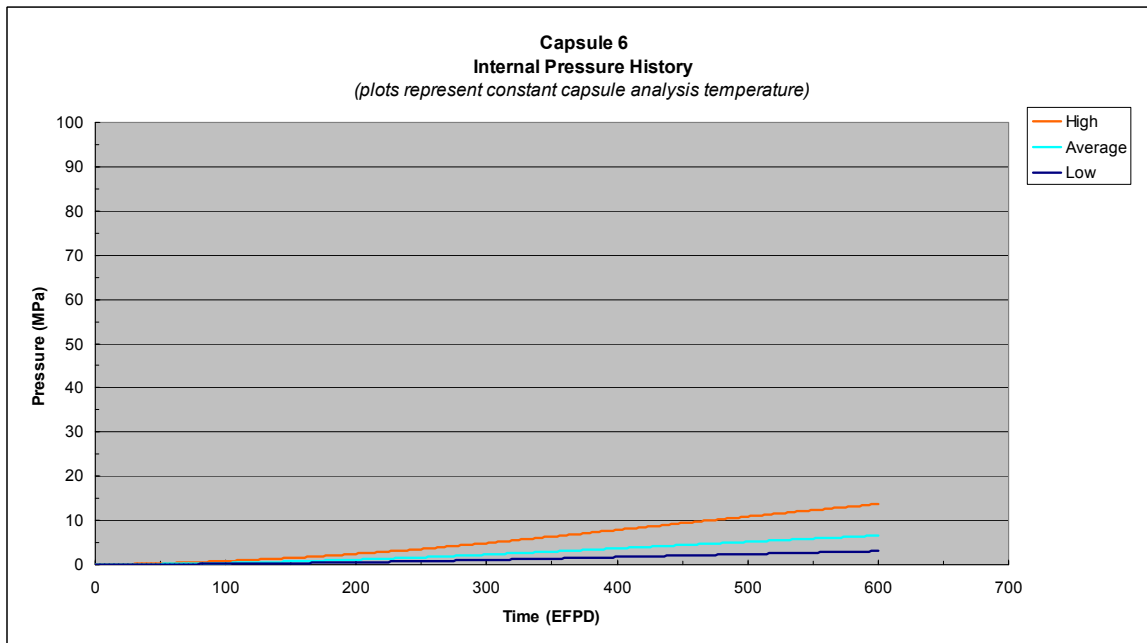


Figure B-22. Particle internal pressure (Capsules 6)

Title: AGR-2 Pre-Test Prediction Analyses using the PARFUME Code for U.S. Fuel Particles

ECAR No.: 1020

ECAR Rev. No.: 2

Project File No.: 23841

Date: 05/29/2012

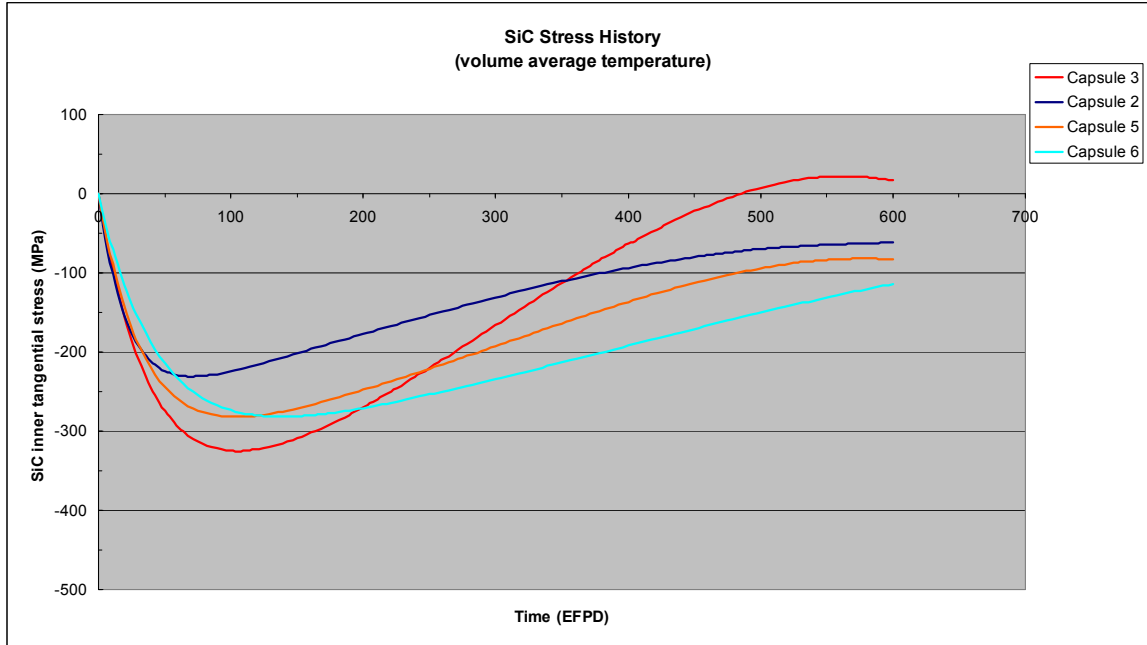


Figure B-23. SiC inner tangential stress (Capsules 2, 3, 5, 6).

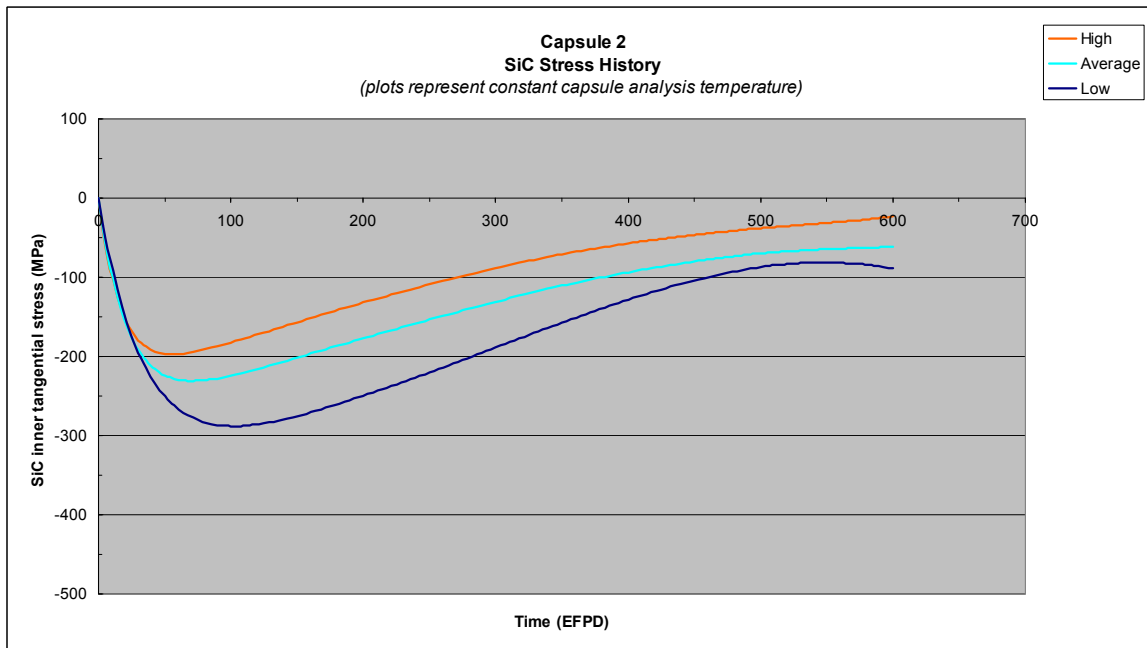


Figure B-24. SiC inner tangential stress (Capsule 2).

Title: AGR-2 Pre-Test Prediction Analyses using the PARFUME Code for U.S. Fuel Particles

ECAR No.: 1020

ECAR Rev. No.: 2

Project File No.: 23841

Date: 05/29/2012

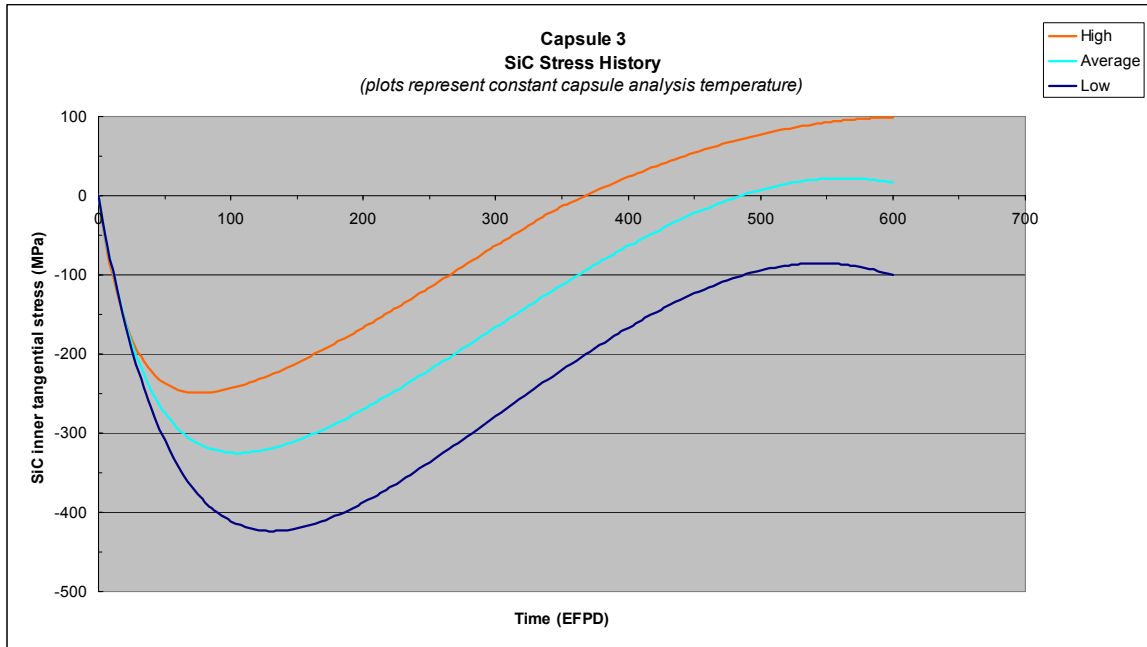


Figure B-25. SiC inner tangential stress (Capsule 3).

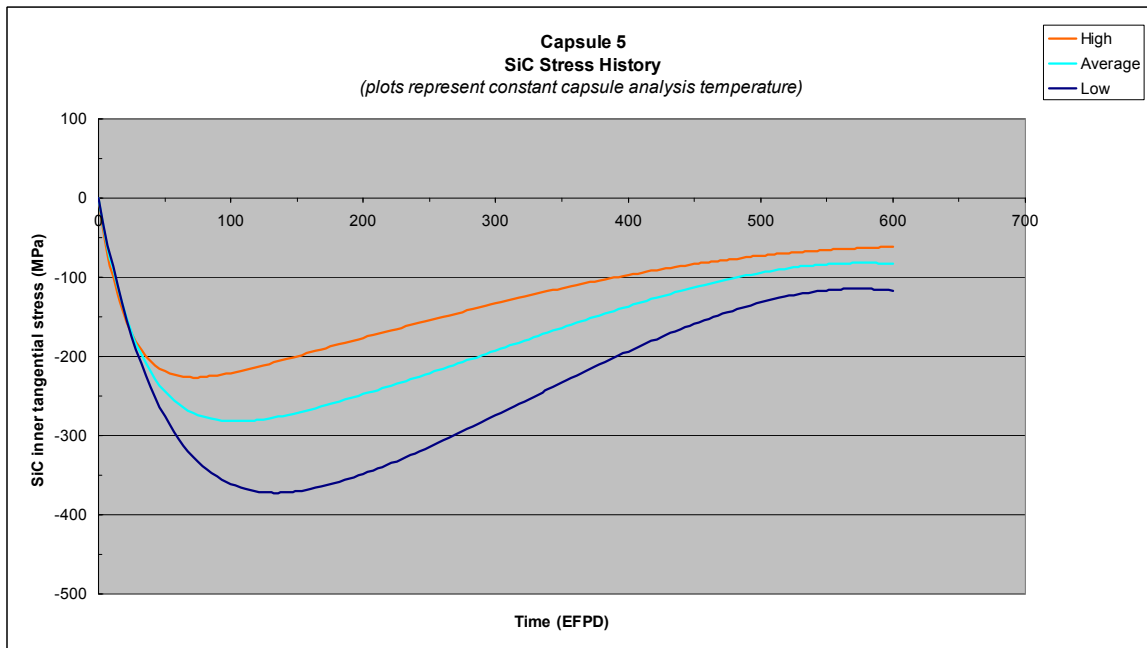


Figure B-26. SiC inner tangential stress (Capsule 5).

Title: AGR-2 Pre-Test Prediction Analyses using the PARFUME Code for U.S. Fuel Particles

ECAR No.: 1020

ECAR Rev. No.: 2

Project File No.: 23841

Date: 05/29/2012

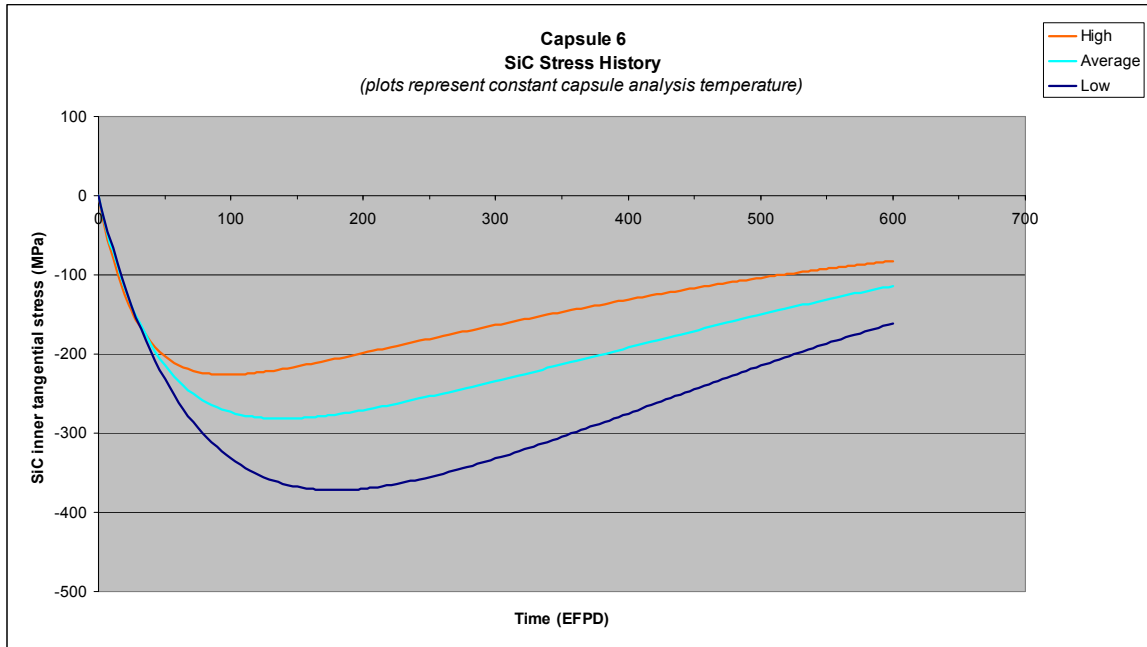


Figure B-27. SiC inner tangential stress (Capsule 6).

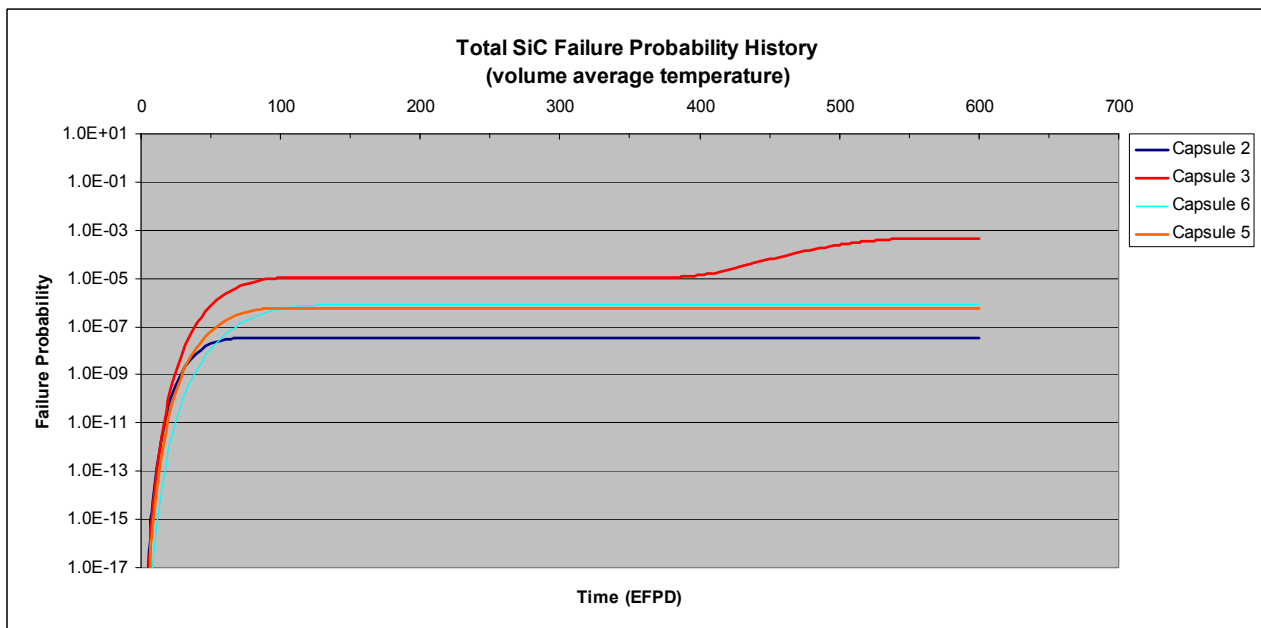


Figure B-28. Total SiC fuel particle failure probabilities (Capsules 2, 3, 5, 6).

Title: AGR-2 Pre-Test Prediction Analyses using the PARFUME Code for U.S. Fuel Particles

ECAR No.: 1020

ECAR Rev. No.: 2

Project File No.: 23841

Date: 05/29/2012

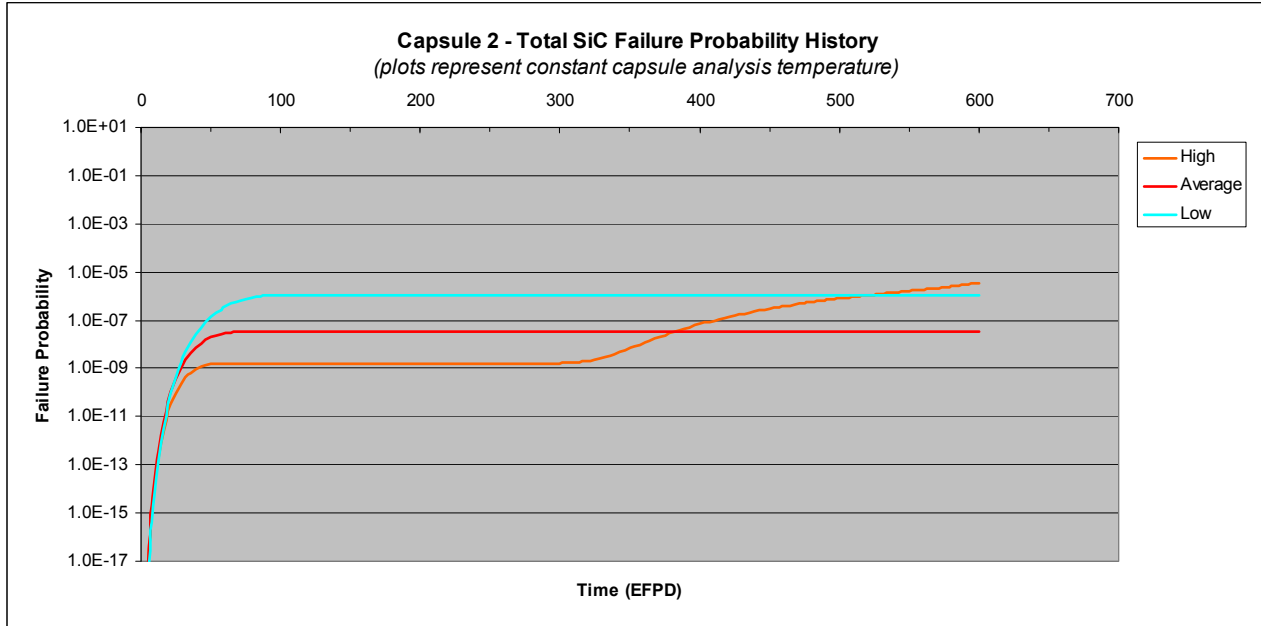


Figure B-29. Total SiC fuel particle failure probability (Capsules 2).

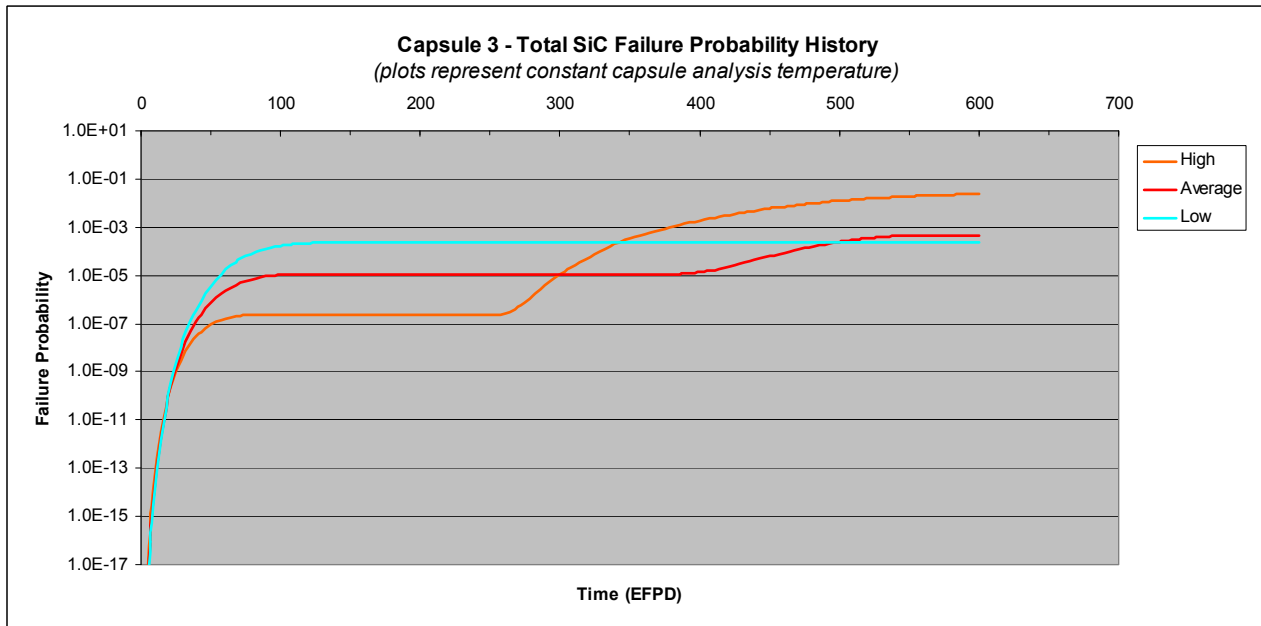


Figure B-30. Total SiC fuel particle failure probability (Capsules 3).

Title: AGR-2 Pre-Test Prediction Analyses using the PARFUME Code for U.S. Fuel Particles

ECAR No.: 1020

ECAR Rev. No.: 2

Project File No.: 23841

Date: 05/29/2012

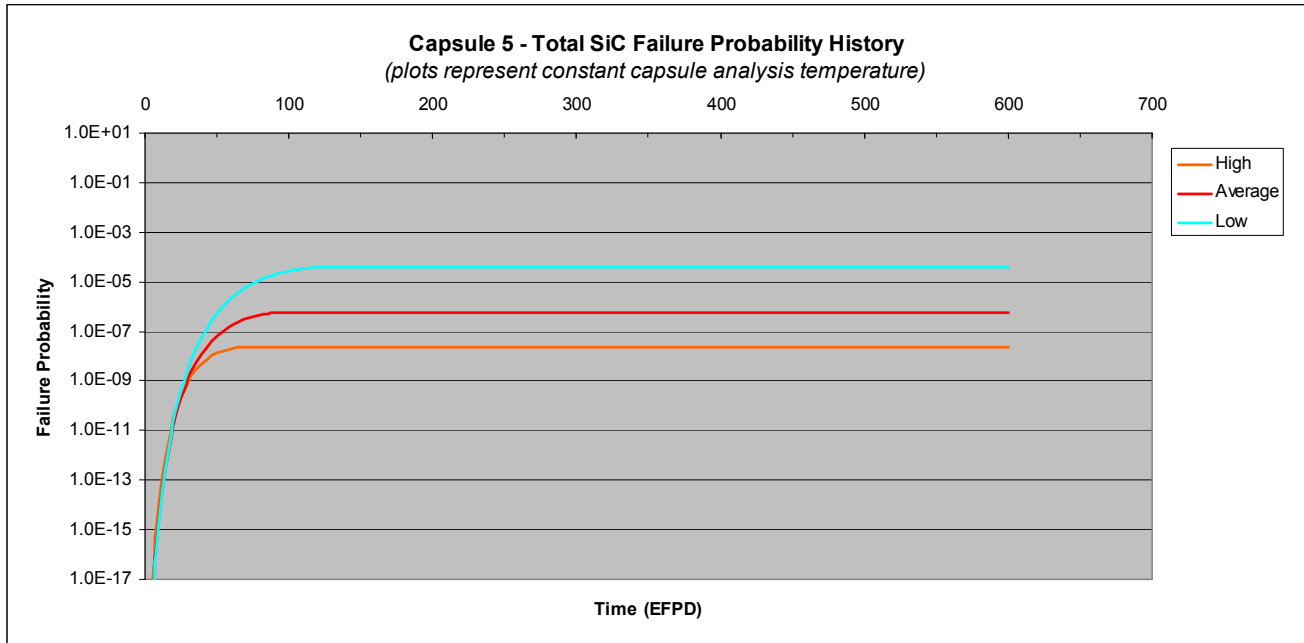


Figure B-31. Total SiC fuel particle failure probability (Capsules 5).

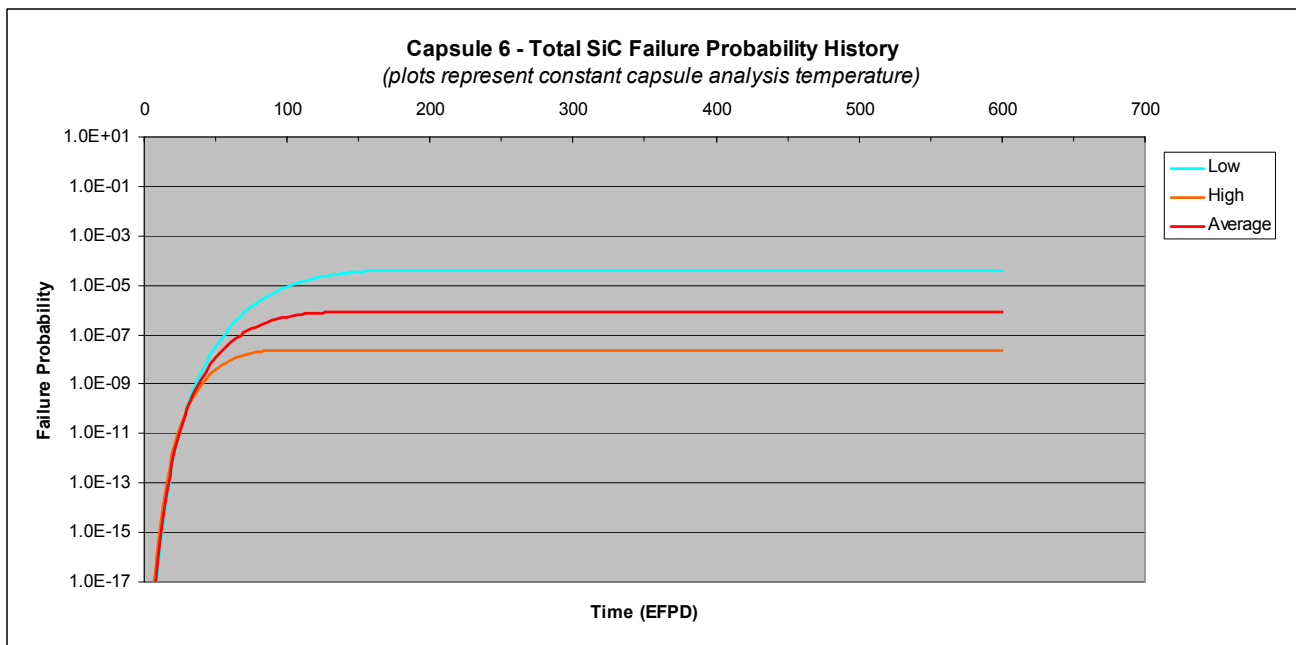


Figure B-32. Total SiC fuel particle failure probability (Capsules 6).

Title: AGR-2 Pre-Test Prediction Analyses using the PARFUME Code for U.S. Fuel Particles

ECAR No.: 1020

ECAR Rev. No.: 2

Project File No.: 23841

Date: 05/29/2012

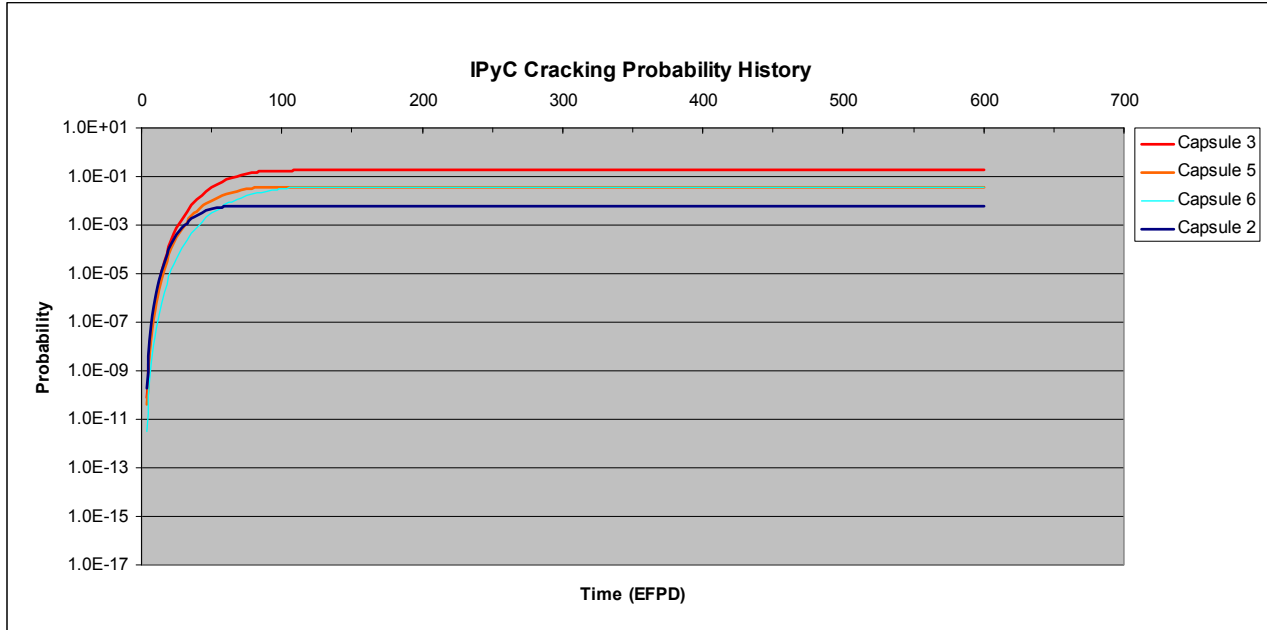


Figure B-33. IPyC cracking probabilities (Capsules 2, 3, 5, 6).

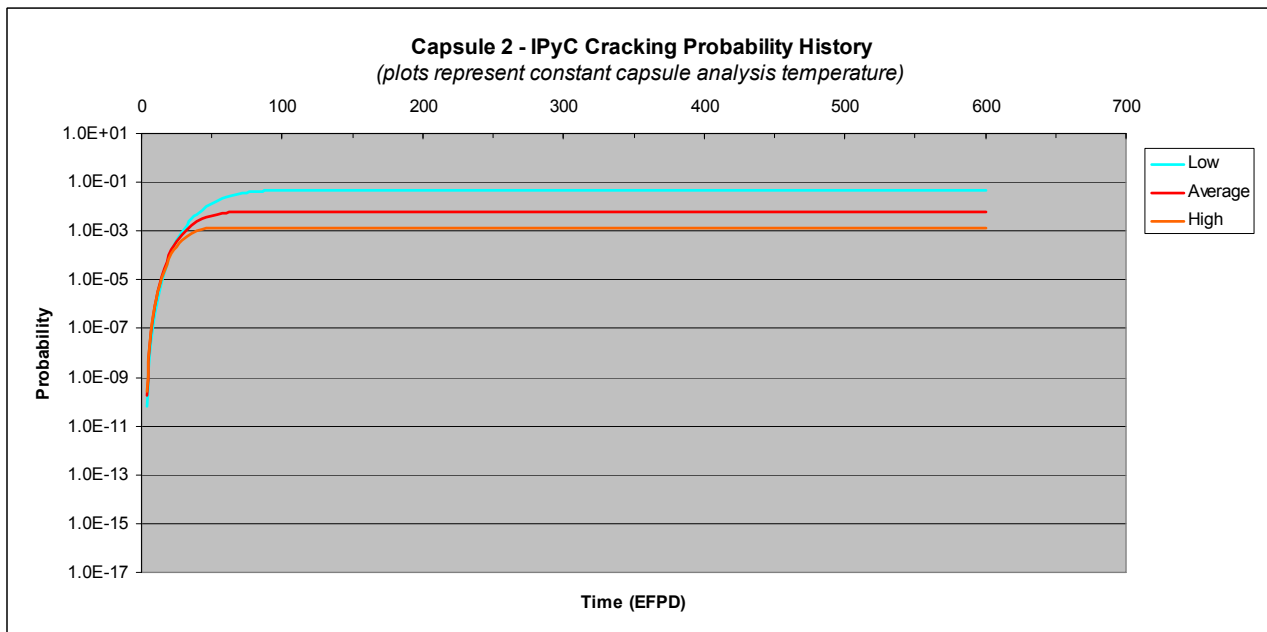


Figure B-34. IPyC cracking probabilities (Capsules 2).

Title: AGR-2 Pre-Test Prediction Analyses using the PARFUME Code for U.S. Fuel Particles

ECAR No.: 1020

ECAR Rev. No.: 2

Project File No.: 23841

Date: 05/29/2012

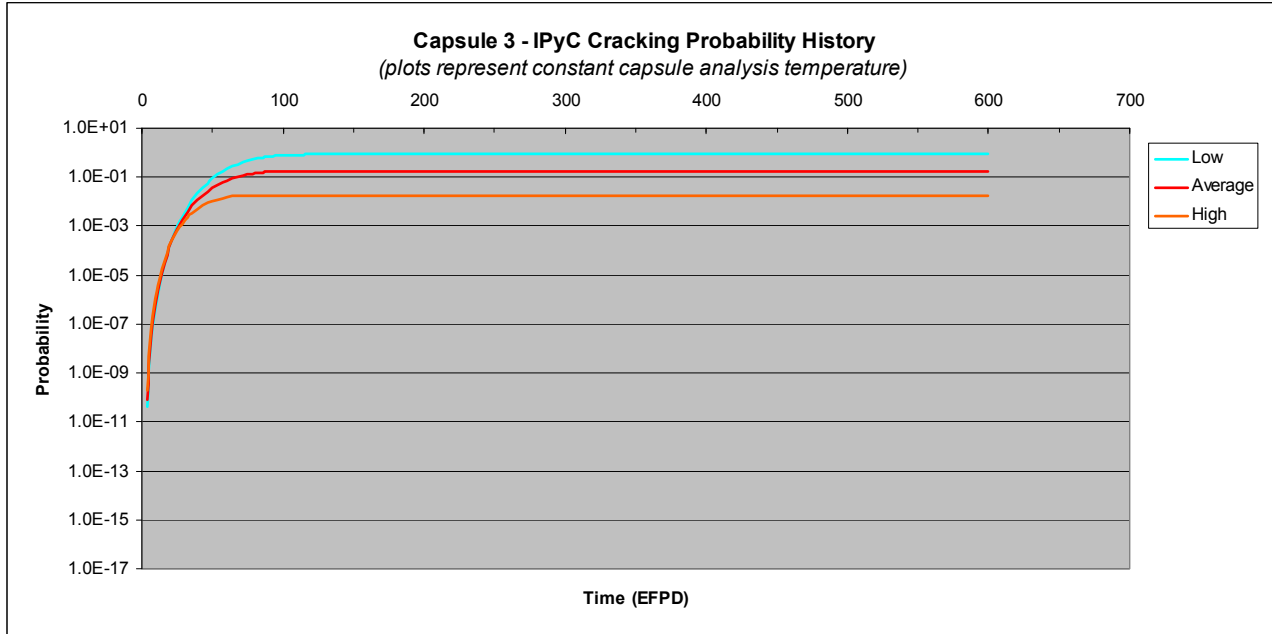


Figure B-35. IPyC cracking probabilities (Capsules 3).

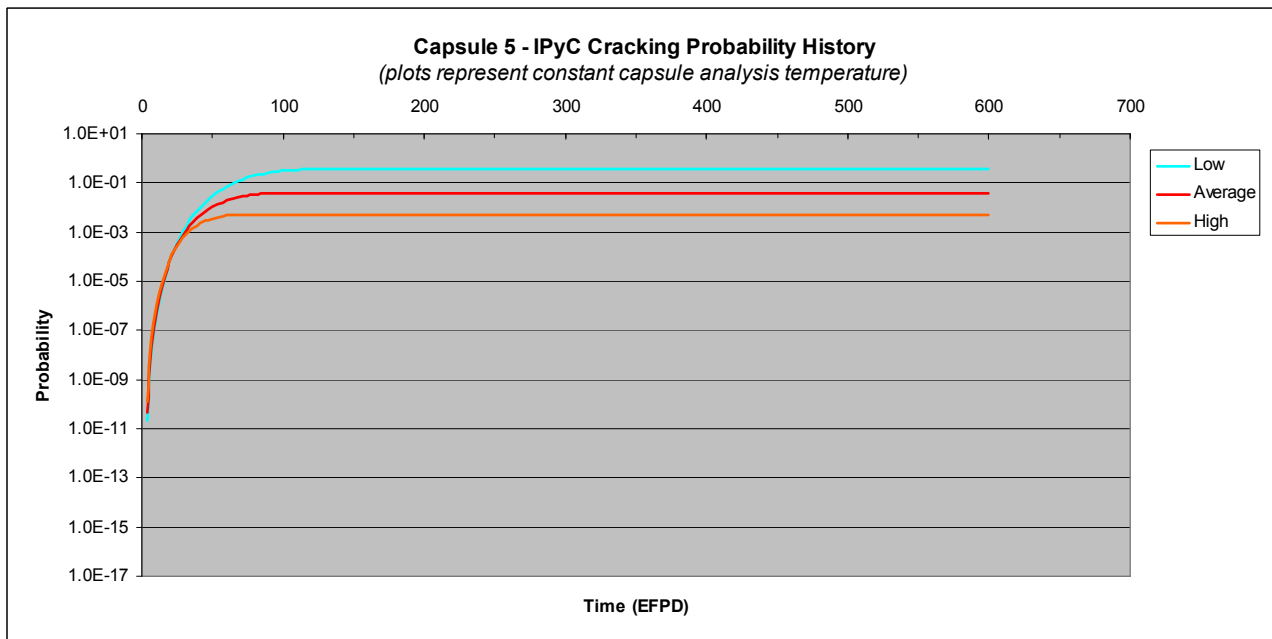


Figure B-36. IPyC cracking probabilities (Capsules 5).

Title: AGR-2 Pre-Test Prediction Analyses using the PARFUME Code for U.S. Fuel Particles

ECAR No.: 1020

ECAR Rev. No.: 2

Project File No.: 23841

Date: 05/29/2012

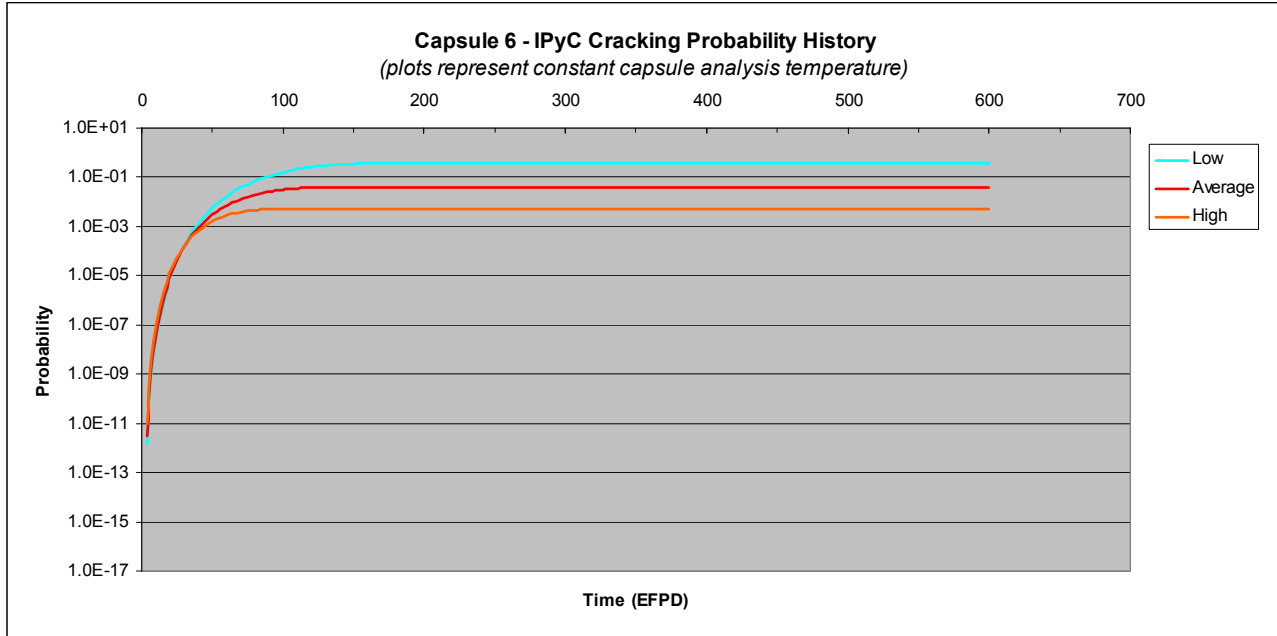


Figure B-37. IPyC cracking probabilities (Capsules 6).

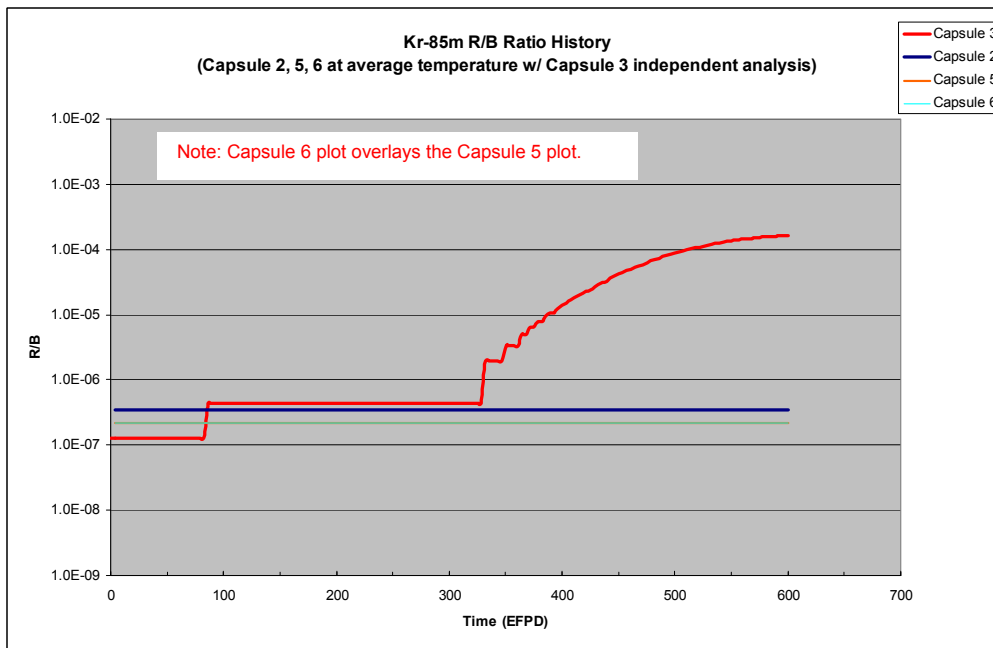


Figure B-38. Kr-85m R/B (Capsules 2, 3, 5, 6).

Title: AGR-2 Pre-Test Prediction Analyses using the PARFUME Code for U.S. Fuel Particles

ECAR No.: 1020

ECAR Rev. No.: 2

Project File No.: 23841

Date: 05/29/2012

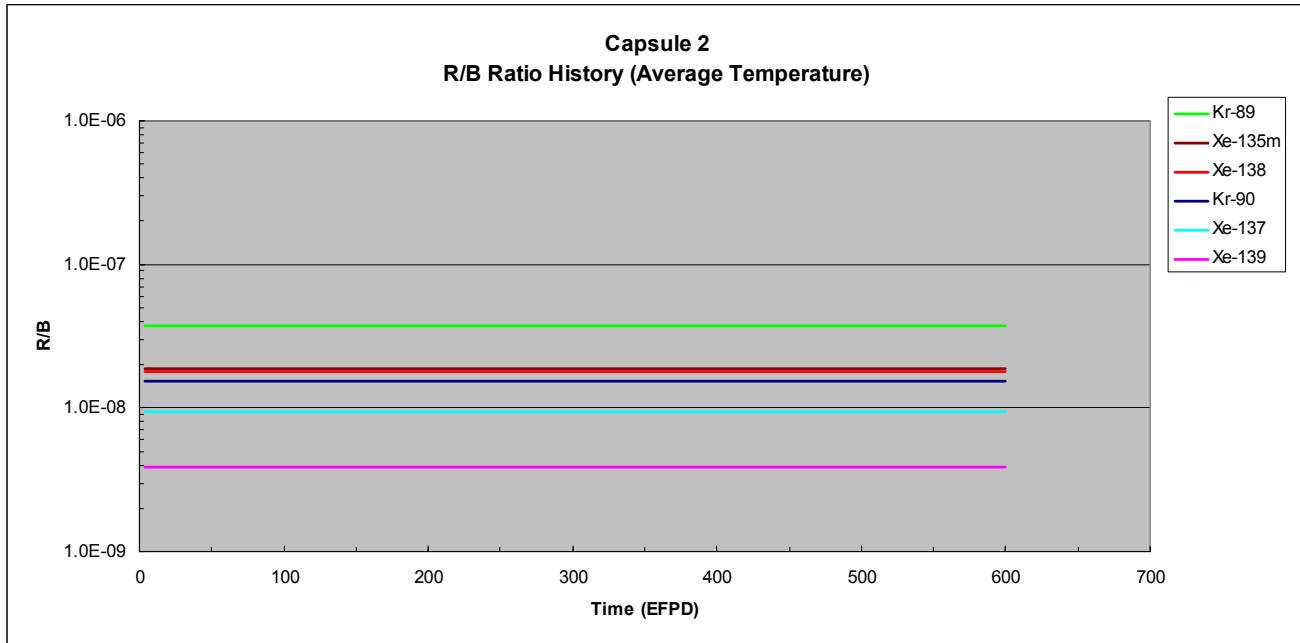


Figure B-39. Capsule 2 R/B for fission products with relatively short (<1000 s) half-lives.

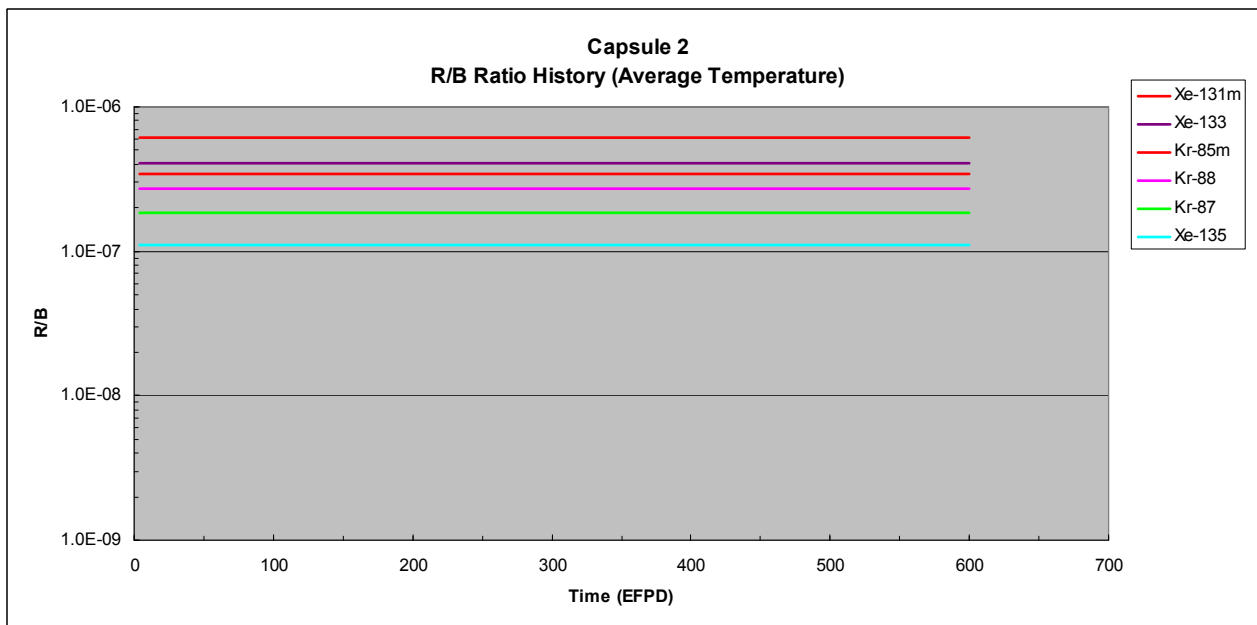


Figure B-40. Capsule 2 R/B for fission products with relatively long (>1000 s) half-lives.

Title: AGR-2 Pre-Test Prediction Analyses using the PARFUME Code for U.S. Fuel Particles

ECAR No.: 1020

ECAR Rev. No.: 2

Project File No.: 23841

Date: 05/29/2012

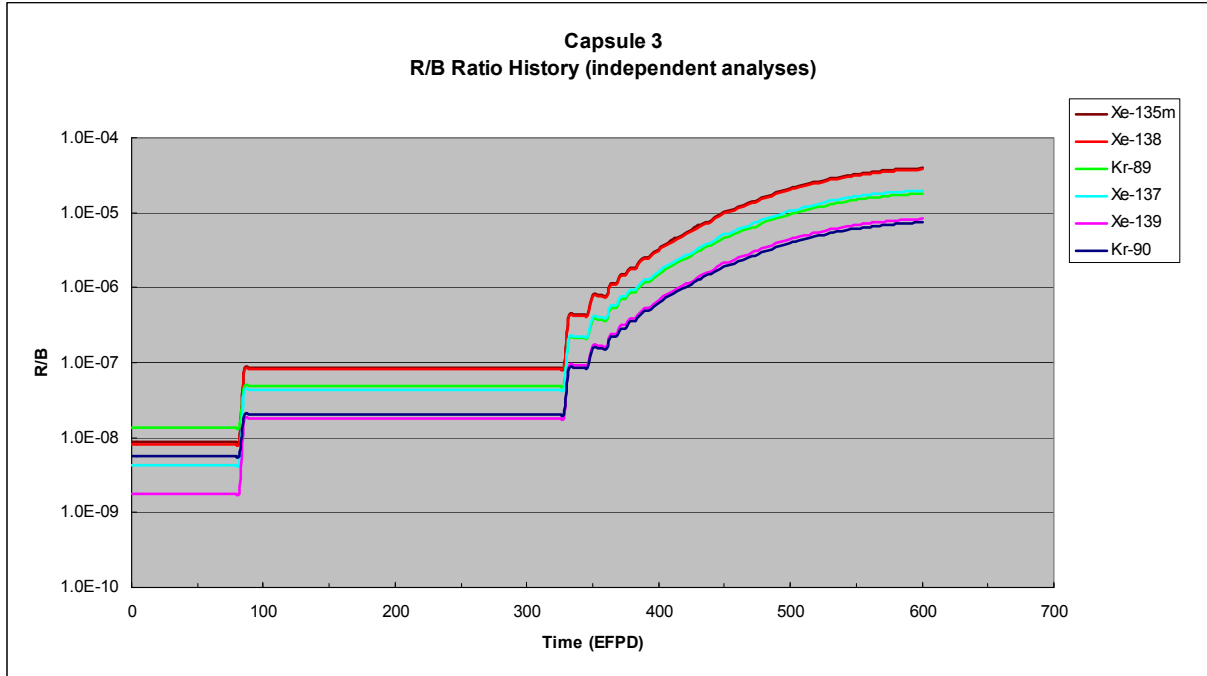


Figure B-41. Capsule 3 R/B for fission products with relatively short (<1000 s) half-lives.

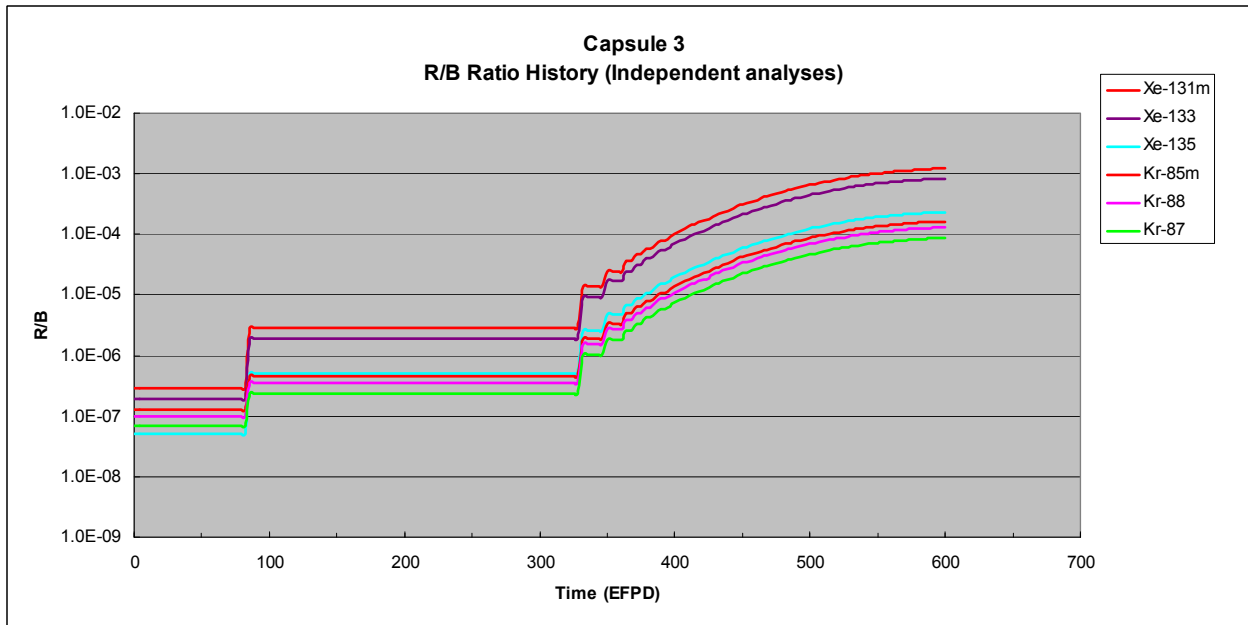


Figure B-42. Capsule 3 R/B for fission products with relatively long (>1000 s) half-lives.

Title: AGR-2 Pre-Test Prediction Analyses using the PARFUME Code for U.S. Fuel Particles

ECAR No.: 1020

ECAR Rev. No.: 2

Project File No.: 23841

Date: 05/29/2012

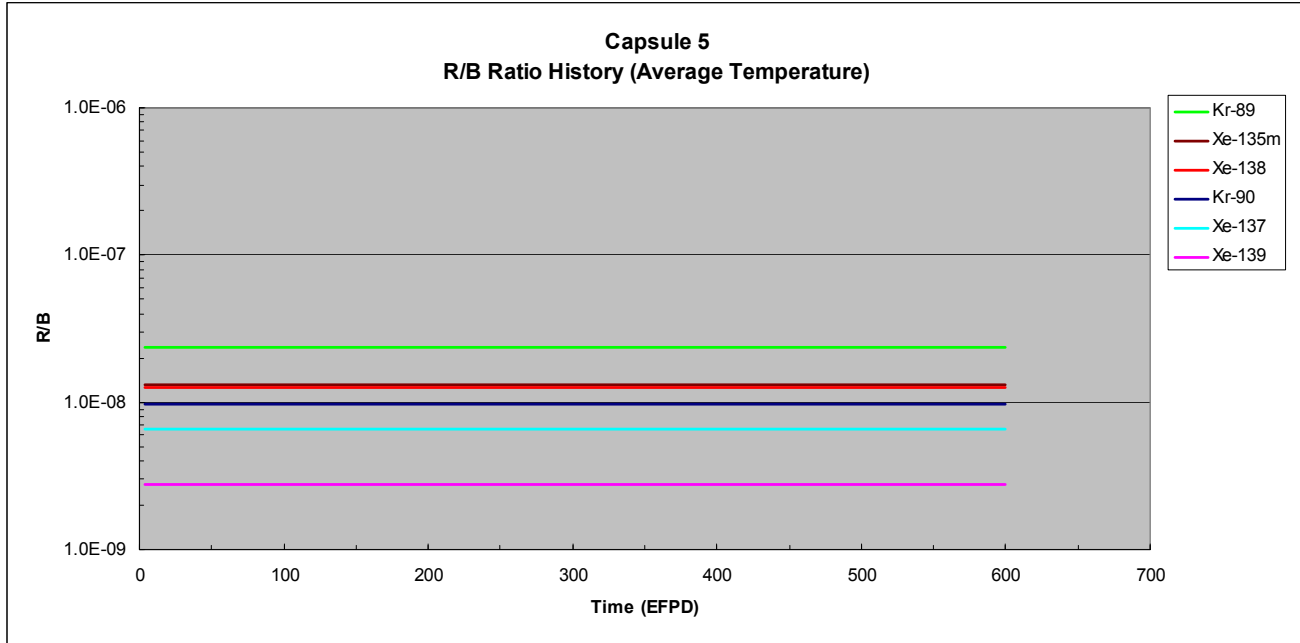


Figure B-43. Capsule 5 R/B for fission products with relatively short (<1000 s) half-lives.

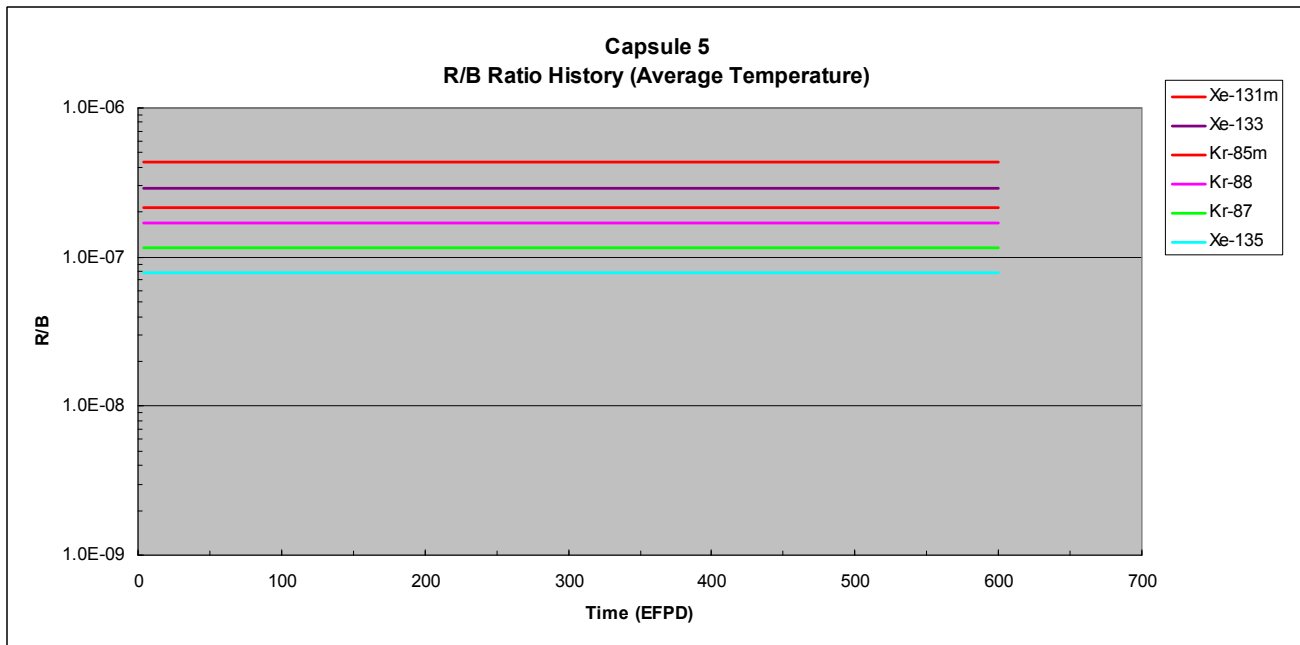


Figure B-44. Capsule 5 R/B for fission products with relatively long (>1000 s) half-lives.

Title: AGR-2 Pre-Test Prediction Analyses using the PARFUME Code for U.S. Fuel Particles

ECAR No.: 1020

ECAR Rev. No.: 2

Project File No.: 23841

Date: 05/29/2012

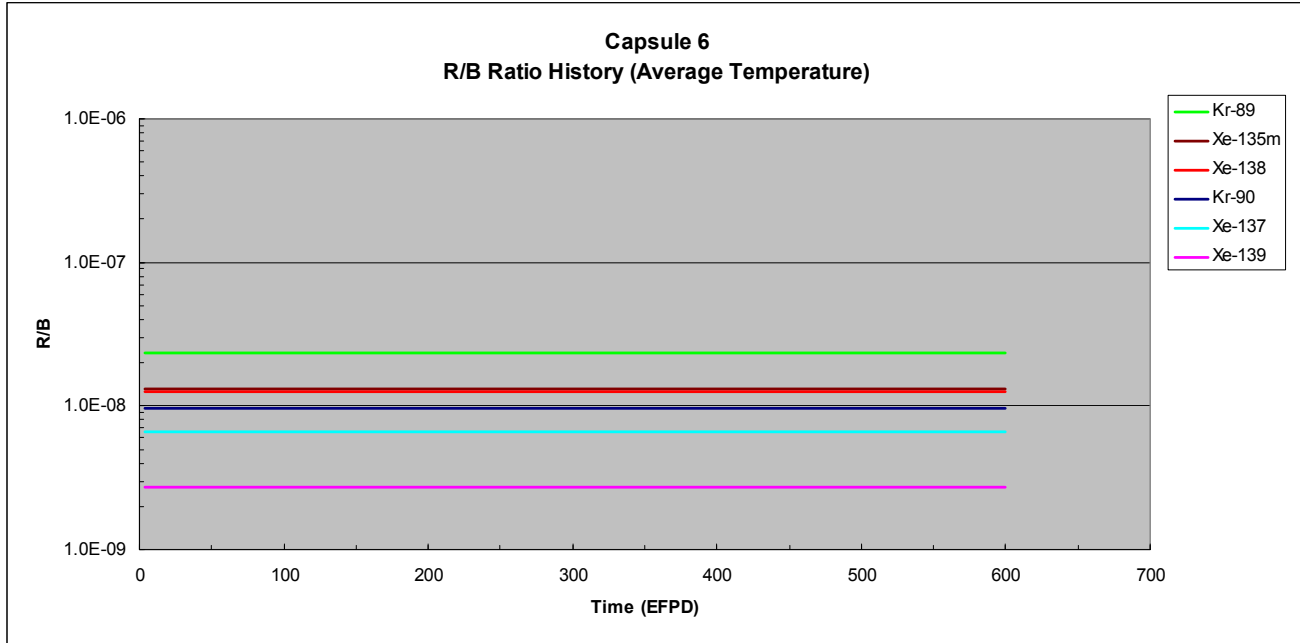


Figure B-45. Capsule 6 R/B for fission products with relatively short (<1000 s) half-lives.

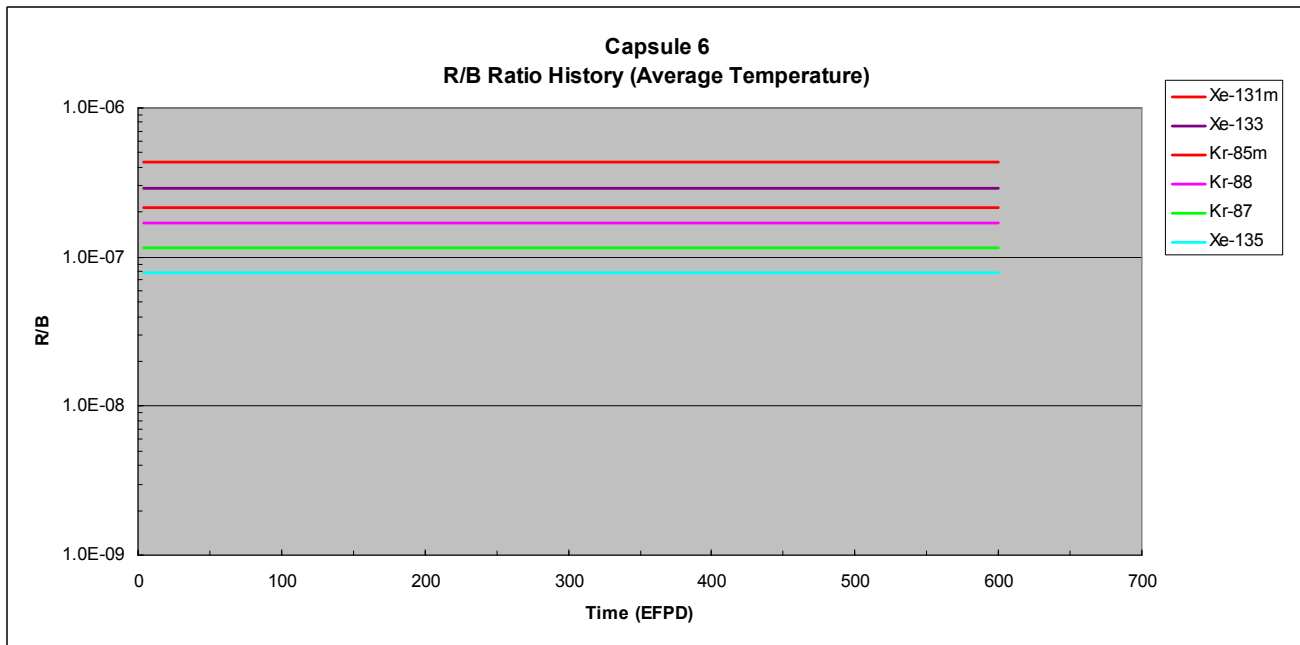


Figure B-46. Capsule 6 R/B for fission products with relatively long (>1000 s) half-lives.

Title: AGR-2 Pre-Test Prediction Analyses using the PARFUME Code for U.S. Fuel Particles

ECAR No.: 1020

ECAR Rev. No.: 2

Project File No.: 23841

Date: 05/29/2012

Appendix C – Input Data Decks

AGR-2 Capsule-2 UCO High Temperature Run

```
*
*PARFUME V2.18 Input Data Deck: ECAR-1020R1
* Note: default values in brackets [default]
*
#####
***** GENERAL OPTIONS (SOLVERS/MODELS) *****
* CARD 100001 (simulation name)
*   title
100001   'AGR-2 Capsule-2 UCO High Temp Run ECAR-1020R1'
*
* CARD 101001 (run parameters)
*   pfss      ncases      nburp      sample      dtf [0]      iseed [305]
101001      2          100          100          1
*
* CARD 101002 (models)
*   idebondp   ifacet   rbvalue   comodel   fgmodel   idebug
101002      1          1          12          3          2          0
*
***** MATERIAL PROPERTIES *****
* CARD 102001 (fuel characteristics)
*   u235enr(wt%)  ourat  curat
102001      14.03    1.43   0.39
*
* CARD 103001 (kernel properties)
*   kernd(g/cm^3)  kernt(g/cm^3) [11.030]
103001      10.97
*
* CARD 103002 (buffer properties)
*   buffd(g/cm^3)  bufft(g/cm^3) [2.250]
103002      1.04
*
* CARD 103003 (IPyC properties)
*   ipycdn(g/cm^3)  ipycdvar(g/cm^3)
103003      1.89      0.010
*
* CARD 103005 (OPyC properties)
*   opycdn(g/cm^3)  opycdvar(g/cm^3)
103005      1.91      0.010
*
* CARD 103013 (IPyC Bacon anisotropic factor)
*   ibafn  ibafvar
103013   1.047  0.005
*
* CARD 103015 (OPyC Bacon anisotropic factor)
*   obafn  obafvar
103015   1.043  0.002
*
* CARD 103023 (IPyC Weibull modulus)
*   ipycm [9.50]
*103023
*
* CARD 103024 (SiC Weibull modulus)
*   sigm [6.00]
*103024
*
* CARD 103025 (OPyC Weibull modulus)
*   opycm [9.50]
*103025
*
* CARD 103033 (Poisson's ratio)
*   cnu [0.500]  cnub [0.500]
*103033
*
* CARD 103043 (creep amplification factor)
*   creepampn [2.0]  creepvar [0.00]
*103043
*
* CARD 103054 (Enable ZrC)
```


Title: AGR-2 Pre-Test Prediction Analyses using the PARFUME Code for U.S. Fuel Particles

ECAR No.: 1020

ECAR Rev. No.: 2

Project File No.: 23841

Date: 05/29/2012

```
*          zrc [0]          zrcp [1]
*103054
*
* CARD 103061 (defective SiC layers)
*          fdef [0.00]
*103061
*
***** FUEL PARTICLE GEOMETRY *****
* CARD 104001 (kernel geometry)
*          kerndia(e-6 m) kernvar(e-6 m)
104001          426.7          8.8
* CARD 104002 (buffer geometry)
*          buffthk(e-6 m) buffvar(e-6 m)
104002          98.9          8.4
* CARD 104003 (IPyC geometry)
*          ipycthk(e-6 m) ipycvar(e-6 m)
104003          40.4          2.5
* CARD 104004 (SiC geometry)
*          sicthk(e-6 m) sicvar(e-6 m)
104004          35.2          1.2
* CARD 104005 (OPyC geometry)
*          opycthk(e-6 m) opycvar(e-6 m)
104005          43.4          2.9
*
***** FUEL ELEMENT DESCRIPTION *****
* CARD 105001 (Plane Geometry w/modified Inputs for a Capsule)
105001          PLANEGEOM
* CARD 105011 (Planegeom)
*          partnum(particles/capsule) ngnfm ngn
105011          38052.          3          6
* CARD 105021 (Planegeom)
*          fmthk(m) cldthk(m)
105021          1.          1.
* CARD 105031 (Planegeom)
*          fmden(g/cm^3) [1.70]
*105031
* CARD 105041 (Planegeom)
*          ucontam
105041          9.74E-6
*
***** FUEL ELEMENT ENVIRONMENT *****
* CARD 106001 (fuel temperature option)
*          rtmpopt
106001          VOLAVGTMP
* CARD 106021 (global node temperatures)
*          tgi(k) ntgi {not required with VOLAVGTMP option}
*106021
* CARD 201001 (fission product transport description)
*          fpspecie {diffusion not modeled}
*201001
*
* CARD SERIES 301XXX (fluence v- time input)
*          timeirr(days) flu(e25 n/m^2)
301001          0.          0.0000
301002          50.          0.2933
301003          100.          0.5913
301004          150.          0.8975
301005          200.          1.2117
301006          250.          1.5300
301007          300.          1.8525
301008          350.          2.1717
301009          400.          2.4854
301010          450.          2.7971
301011          500.          3.1021
301012          550.          3.4021
```

Title: AGR-2 Pre-Test Prediction Analyses using the PARFUME Code for U.S. Fuel Particles

ECAR No.: 1020

ECAR Rev. No.: 2

Project File No.: 23841

Date: 05/29/2012

```
301013      600.      3.6988
*
*
* CARD SERIES 302XXX (burnup v- fluence input)
*      flu(e25 n/m^2)  bup(%fima)
302001      0.0000      0.000
302002      0.2933      0.710
302003      0.5913      1.548
302004      0.8975      2.543
302005      1.2117      3.710
302006      1.5300      5.024
302007      1.8525      6.399
302008      2.1717      7.718
302009      2.4854      8.912
302010      2.7971      9.965
302011      3.1021      10.892
302012      3.4021      11.707
302013      3.6988      12.434
*
* CARD SERIES 303XXX (external pressure v- fluence input)
*      external pressure v- fluence input
*      flu(e25 n/m^2)  pamb(MPa)
303001      0.      .1
*
* CARD SERIES 304XXX (boundary temperature v- fluence input)
*      flu(e25 n/m^2)  btemp(k)
304001      0.0000      1663.
304002      0.2933      1663.
304003      0.5913      1663.
304004      0.8975      1663.
304005      1.2117      1663.
304006      1.5300      1663.
304007      1.8525      1663.
304008      2.1717      1663.
304009      2.4854      1663.
304010      2.7971      1663.
304011      3.1021      1663.
304012      3.4021      1663.
304013      3.6988      1663.
*
* CARD SERIES 306XXX (time heatup starts and irradiation ends)
*      thus(days) [1xe6] {casualty condition not modeled}
*306001
*
***** CORRELATION COEFFICIENTS *****
* CARD SERIES 401XXX (correlation coefficients for ipyc cracking)
*      sigcr0 (MPa)  umc (MPa)
401001      1084.964  106.400
*      c1c      c2c
401002      0.0000      0.0000      * for fuel particle radial posit
401003      0.0000      0.0000      * for kernel diameter
401004      0.0000      0.0000      * for buffer thickness
401005      1.863080E-02  8.647889E-05  * for ipyc thickness
401006      8.116068E-03  5.312641E-04  * for sic thickness
401007      -1.758922E-02  3.639176E-04  * for opyc thickness
401008      0.0000      0.0000      * for ipyc density
401009      0.0000      0.0000      * for opyc density
401010      0.0000      0.0000      * for ipyc baf
401011      0.0000      0.0000      * for opyc baf
401012      0.0000      0.0000      * for creep coeff amplication
*
* CARD SERIES 402XXX (correlation coefficients for ipyc asphericity)
*      siga0 (MPa)  um (MPa)  delum (MPa)  aration  aratvar
402001      1384.023  267.500  413.900  1.052  0.013
*      c1a      c2a      d1a      d2a
```

Title: AGR-2 Pre-Test Prediction Analyses using the PARFUME Code for U.S. Fuel Particles

ECAR No.: 1020

ECAR Rev. No.: 2

Project File No.: 23841

Date: 05/29/2012

402002	0.0000	0.0000	0.0000	0.0000	* fuel part rad pos
402003	0.0000	0.0000	0.0000	0.0000	* for kernel diamet
402004	0.0000	0.0000	0.0000	0.0000	* for buffer thickn
402005	3.707684E-03	2.446398E-05	-2.307772E-03	2.801605E-05	*i thickn
402006	-2.981942E-03	-9.092333E-05	-1.075004E-02	1.284585E-04	*s thickn
402007	2.971356E-03	-1.221197E-05	1.035991E-03	1.043966E-05	*o thickn
402008	0.0000	0.0000	0.0000	0.0000	* for ipyc density
402009	0.0000	0.0000	0.0000	0.0000	* for opyc density
402010	0.0000	0.0000	0.0000	0.0000	* for ipyc baf
402011	0.0000	0.0000	0.0000	0.0000	* for opyc baf
402012	0.0000	0.0000	0.0000	0.0000	* for creep coef
402013	4.051038E+00	-6.338829E+01	8.902414E+00	-6.460501E+01	* aspheri

*
* CARD SERIES 403XXX (correlation coefficients for ipyc debonding)
* sigd0 (MPa) umd(MPa) bond0(MPa) bond0var(MPa)
403001 1000. 100. 100. 0.
* c1d c2d
403002 0.0000 0.0000 * for fuel particle radial posit
403003 0.0000 0.0000 * for kernel diameter
403004 0.0000 0.0000 * for buffer thickness
403005 0.0000 0.0000 * for ipyc thickness
403006 0.0000 0.0000 * for sic thickness
403007 0.0000 0.0000 * for opyc thickness
403008 0.0000 0.0000 * for ipyc density
403009 0.0000 0.0000 * for opyc density
403010 0.0000 0.0000 * for ipyc baf
403011 0.0000 0.0000 * for opyc baf
403012 0.0000 0.0000 * for creep coeff amplication
403013 0.0000 0.0000 * for asphericity effects
*
*
.

Title: AGR-2 Pre-Test Prediction Analyses using the PARFUME Code for U.S. Fuel Particles

ECAR No.: 1020

ECAR Rev. No.: 2

Project File No.: 23841

Date: 05/29/2012

AGR-2 Capsule-2 UCO Volume Average Temperature Run

```
*
*PARFUME V2.18 Input Data Deck: ECAR-1020R1
*
* Note: default values in brackets [default]
*
#####
***** GENERAL OPTIONS (SOLVERS/MODELS) *****
* CARD 100001 (simulation name)
*      title
100001   'AGR-2 Capsule-2 UCO Volume Average Temp Run ECAR-1020R1'
*
* CARD 101001 (run parameters)
*      pfss      ncases      nburp      sample      dtf [0]      izeed [305]
101001      2      100      100      1
*
* CARD 101002 (models)
*      idebondp      ifacet      rbvalue      comodel      fgmodel      idebug
101002      1      1      12      3      2      0
*
***** MATERIAL PROPERTIES *****
* CARD 102001 (fuel characteristics)
*      u235enr(wt%)      ourat      curat
102001      14.03      1.43      0.39
*
* CARD 103001 (kernel properties)
*      kernd(g/cm^3)      kernt(g/cm^3) [11.030]
103001      10.97
*
* CARD 103002 (buffer properties)
*      buffd(g/cm^3)      bufft(g/cm^3) [2.250]
103002      1.04
*
* CARD 103003 (IPyC properties)
*      ipycdn(g/cm^3)      ipycdvar(g/cm^3)
103003      1.89      0.010
*
* CARD 103005 (OPyC properties)
*      opycdn(g/cm^3)      opycdvar(g/cm^3)
103005      1.91      0.010
*
* CARD 103013 (IPyC Bacon anisotropic factor)
*      ibafn      ibafvar
103013      1.047      0.005
*
* CARD 103015 (OPyC Bacon anisotropic factor)
*      obafn      obafvar
103015      1.043      0.002
*
* CARD 103023 (IPyC Weibull modulus)
*      ipycm [9.50]
*103023
*
* CARD 103024 (SiC Weibull modulus)
*      sigm [6.00]
*103024
*
* CARD 103025 (OPyC Weibull modulus)
*      opycm [9.50]
*103025
*
* CARD 103033 (Poisson's ratio)
*      cnu [0.500]      cnub [0.500]
*103033
*
* CARD 103043 (creep amplification factor)
*      creepampn [2.0]      creepvar [0.00]
*103043
*
* CARD 103054 (Enable ZrC)
*      zrc [0]      zrcp [1]
```

Title: AGR-2 Pre-Test Prediction Analyses using the PARFUME Code for U.S. Fuel Particles

ECAR No.: 1020

ECAR Rev. No.: 2

Project File No.: 23841

Date: 05/29/2012

```
*103054
*
* CARD 103061 (defective SiC layers)
*      fdef [0.00]
*103061
*
***** FUEL PARTICLE GEOMETRY *****
* CARD 104001 (kernel geometry)
*      kerndia(e-6 m)  kernvar(e-6 m)
104001      426.7      8.8
* CARD 104002 (buffer geometry)
*      buffthk(e-6 m)  buffvar(e-6 m)
104002      98.9      8.4
* CARD 104003 (IPyC geometry)
*      ipycthk(e-6 m)  ipycvar(e-6 m)
104003      40.4      2.5
* CARD 104004 (SiC geometry)
*      sicthk(e-6 m)   sicvar(e-6 m)
104004      35.2      1.2
* CARD 104005 (OPyC geometry)
*      opycthk(e-6 m)  opycvar(e-6 m)
104005      43.4      2.9
*
***** FUEL ELEMENT DESCRIPTION *****
* CARD 105001 (Plane Geometry w/modified Inputs for a Capsule)
105001  PLANEGEOM
* CARD 105011 (Planegeom)
*      partnum(particles/capsule)  ngngfm  ngngn
105011      38052.      3      6
* CARD 105021 (Planegeom)
*      fmthk(m)  cldthk(m)
105021      1.      1.
* CARD 105031 (Planegeom)
*      fmden(g/cm^3) [1.70]
*105031
* CARD 105041 (Planegeom)
*      ucontam
105041      9.74E-6
*
***** FUEL ELEMENT ENVIRONMENT *****
* CARD 106001 (fuel temperature option)
*      rtmpopt
106001  VOLAVGTMP
* CARD 106021 (global node temperatures)
*      tgi(k)  ntgi  {not required with VOLAVGTMP option}
*106021
* CARD 201001 (fission product transport description)
*      fpspecie  {diffusion not modeled}
*201001
*
* CARD SERIES 301XXX (fluence v- time input)
*      timeirr(days)  flu(e25 n/m^2)
301001      0.      0.0000
301002      50.     0.2933
301003      100.    0.5913
301004      150.    0.8975
301005      200.    1.2117
301006      250.    1.5300
301007      300.    1.8525
301008      350.    2.1717
301009      400.    2.4854
301010      450.    2.7971
301011      500.    3.1021
301012      550.    3.4021
301013      600.    3.6988
```

Title: AGR-2 Pre-Test Prediction Analyses using the PARFUME Code for U.S. Fuel Particles

ECAR No.: 1020

ECAR Rev. No.: 2

Project File No.: 23841

Date: 05/29/2012

```
*
*
* CARD SERIES 302XXX (burnup v- fluence input)
*      flu(e25 n/m^2)  bup(%fima)
302001      0.0000      0.000
302002      0.2933      0.710
302003      0.5913      1.548
302004      0.8975      2.543
302005      1.2117      3.710
302006      1.5300      5.024
302007      1.8525      6.399
302008      2.1717      7.718
302009      2.4854      8.912
302010      2.7971      9.965
302011      3.1021      10.892
302012      3.4021      11.707
302013      3.6988      12.434
*
*
* CARD SERIES 303XXX (external pressure v- fluence input)
*      external pressure v- fluence input
*      flu(e25 n/m^2)  pamb(MPa)
303001      0.          .1
*
* CARD SERIES 304XXX (boundary temperature v- fluence input)
*      flu(e25 n/m^2)  btemp(k)
304001      0.0000      1498.
304002      0.2933      1498.
304003      0.5913      1498.
304004      0.8975      1498.
304005      1.2117      1498.
304006      1.5300      1498.
304007      1.8525      1498.
304008      2.1717      1498.
304009      2.4854      1498.
304010      2.7971      1498.
304011      3.1021      1498.
304012      3.4021      1498.
304013      3.6988      1498.
*
* CARD SERIES 306XXX (time heatup starts and irradiation ends)
*      thus(days) [1xe6] {casualty condition not modeled}
*306001
*
***** CORRELATION COEFFICIENTS *****
* CARD SERIES 401XXX (correlation coefficients for ipyc cracking)
*      sigcr0(MPa)  umc(MPa)
401001      1084.571  137.700
*      c1c          c2c
401002      0.0000      0.0000      * for fuel particle radial posit
401003      0.0000      0.0000      * for kernel diameter
401004      0.0000      0.0000      * for buffer thickness
401005      1.822837E-02  7.449184E-05  * for ipyc thickness
401006      9.046776E-03  4.510922E-04  * for sic thickness
401007      -1.726981E-02  3.548404E-04  * for opyc thickness
401008      0.0000      0.0000      * for ipyc density
401009      0.0000      0.0000      * for opyc density
401010      0.0000      0.0000      * for ipyc baf
401011      0.0000      0.0000      * for opyc baf
401012      0.0000      0.0000      * for creep coeff amplication
*
* CARD SERIES 402XXX (correlation coefficients for ipyc asphericity)
*      siga0(MPa)  um(MPa)  delum(MPa)  aration  aratvar
402001      1848.872  352.200  376.320  1.052  0.013
```

Title: AGR-2 Pre-Test Prediction Analyses using the PARFUME Code for U.S. Fuel Particles

ECAR No.: 1020

ECAR Rev. No.: 2

Project File No.: 23841

Date: 05/29/2012

*	c1a	c2a	d1a	d2a	
402002	0.0000	0.0000	0.0000	0.0000	* fuel part rad pos
402003	0.0000	0.0000	0.0000	0.0000	* for kernel diamet
402004	0.0000	0.0000	0.0000	0.0000	* for buffer thickn
402005	3.537697E-03	1.875963E-05	-1.721269E-03	-2.748799E-05	*i thickn
402006	-3.479152E-03	-7.354489E-05	-7.323945E-03	-1.420497E-05	*s thickn
402007	2.908329E-03	-1.739757E-05	8.959330E-04	-7.362291E-05	*o thickn
402008	0.0000	0.0000	0.0000	0.0000	* for ipyc density
402009	0.0000	0.0000	0.0000	0.0000	* for opyc density
402010	0.0000	0.0000	0.0000	0.0000	* for ipyc baf
402011	0.0000	0.0000	0.0000	0.0000	* for opyc baf
402012	0.0000	0.0000	0.0000	0.0000	* for creep coef
402013	4.258940E+00	-6.436719E+01	7.597099E+00	-6.982822E+01	* aspheri

*
* CARD SERIES 403XXX (correlation coefficients for ipyc debonding)
* sigd0 (MPa) umd(MPa) bond0 (MPa) bond0var (MPa)
403001 100. 100. 100. 0.
* c1d c2d
403002 0.0000 0.0000 * for fuel particle radial posit
403003 0.0000 0.0000 * for kernel diameter
403004 0.0000 0.0000 * for buffer thickness
403005 0.0000 0.0000 * for ipyc thickness
403006 0.0000 0.0000 * for sic thickness
403007 0.0000 0.0000 * for opyc thickness
403008 0.0000 0.0000 * for ipyc density
403009 0.0000 0.0000 * for opyc density
403010 0.0000 0.0000 * for ipyc baf
403011 0.0000 0.0000 * for opyc baf
403012 0.0000 0.0000 * for creep coeff amplication
403013 0.0000 0.0000 * for asphericity effects

*
*
.

Title: AGR-2 Pre-Test Prediction Analyses using the PARFUME Code for U.S. Fuel Particles

ECAR No.: 1020

ECAR Rev. No.: 2

Project File No.: 23841

Date: 05/29/2012

AGR-2 Capsule-2 UCO Low Temperature Run

```
*
*PARFUME V2.18 Input Data Deck: ECAR-1020R1
*
* Note: default values in brackets [default]
*
#####
***** GENERAL OPTIONS (SOLVERS/MODELS) *****
* CARD 100001 (simulation name)
*      title
100001   'AGR-2 Capsule-2 UCO Low Temp Run ECAR-1020R1'
*
* CARD 101001 (run parameters)
*      pfss      ncases      nburp      sample      dtf [0]      izeed [305]
101001      2        100        100        1
*
* CARD 101002 (models)
*      idebondp      ifacet      rbvalue      comodel      fgmodel      idebug
101002      1        1        12        3        2        0
*
***** MATERIAL PROPERTIES *****
* CARD 102001 (fuel characteristics)
*      u235enr(wt%)      ourat      curat
102001      14.03      1.43      0.39
*
* CARD 103001 (kernel properties)
*      kernd(g/cm^3)      kernt(g/cm^3) [11.030]
103001      10.97
*
* CARD 103002 (buffer properties)
*      buffd(g/cm^3)      bufft(g/cm^3) [2.250]
103002      1.04
*
* CARD 103003 (IPyC properties)
*      ipycdn(g/cm^3)      ipycdvar(g/cm^3)
103003      1.89      0.010
*
* CARD 103005 (OPyC properties)
*      opycdn(g/cm^3)      opycdvar(g/cm^3)
103005      1.91      0.010
*
* CARD 103013 (IPyC Bacon anisotropic factor)
*      ibafn      ibafvar
103013      1.047      0.005
*
* CARD 103015 (OPyC Bacon anisotropic factor)
*      obafn      obafvar
103015      1.043      0.002
*
* CARD 103023 (IPyC Weibull modulus)
*      ipycm [9.50]
*103023
*
* CARD 103024 (SiC Weibull modulus)
*      sigm [6.00]
*103024
*
* CARD 103025 (OPyC Weibull modulus)
*      opycm [9.50]
*103025
*
* CARD 103033 (Poisson's ratio)
*      cnu [0.500]      cnub [0.500]
*103033
*
* CARD 103043 (creep amplification factor)
*      creepampn [2.0]      creepvar [0.00]
*103043
*
* CARD 103054 (Enable ZrC)
*      zrc [0]      zrcp [1]
```


Title: AGR-2 Pre-Test Prediction Analyses using the PARFUME Code for U.S. Fuel Particles

ECAR No.: 1020

ECAR Rev. No.: 2

Project File No.: 23841

Date: 05/29/2012

```
*103054
*
* CARD 103061 (defective SiC layers)
*      fdef [0.00]
*103061
*
***** FUEL PARTICLE GEOMETRY *****
* CARD 104001 (kernel geometry)
*      kerndia(e-6 m)  kernvar(e-6 m)
104001      426.7      8.8
* CARD 104002 (buffer geometry)
*      buffthk(e-6 m)  buffvar(e-6 m)
104002      98.9      8.4
* CARD 104003 (IPyC geometry)
*      ipycthk(e-6 m)  ipycvar(e-6 m)
104003      40.4      2.5
* CARD 104004 (SiC geometry)
*      sicthk(e-6 m)   sicvar(e-6 m)
104004      35.2      1.2
* CARD 104005 (OPyC geometry)
*      opycthk(e-6 m)  opycvar(e-6 m)
104005      43.4      2.9
*
***** FUEL ELEMENT DESCRIPTION *****
* CARD 105001 (Plane Geometry w/modified Inputs for a Capsule)
105001  PLANEGEOM
* CARD 105011 (Planegeom)
*      partnum(particles/capsule)  ngngfm  ngngn
105011      38052.      3      6
* CARD 105021 (Planegeom)
*      fmthk(m)  cldthk(m)
105021      1.      1.
* CARD 105031 (Planegeom)
*      fmden(g/cm^3) [1.70]
*105031
* CARD 105041 (Planegeom)
*      ucontam
105041      9.74E-6
*
***** FUEL ELEMENT ENVIRONMENT *****
* CARD 106001 (fuel temperature option)
*      rtmpopt
106001  VOLAVGTMP
* CARD 106021 (global node temperatures)
*      tgi(k)  ntgi  {not required with VOLAVGTMP option}
*106021
* CARD 201001 (fission product transport description)
*      fpspecie  {diffusion not modeled}
*201001
*
* CARD SERIES 301XXX (fluence v- time input)
*      timeirr(days)  flu(e25 n/m^2)
301001      0.      0.0000
301002      50.     0.2933
301003      100.    0.5913
301004      150.    0.8975
301005      200.    1.2117
301006      250.    1.5300
301007      300.    1.8525
301008      350.    2.1717
301009      400.    2.4854
301010      450.    2.7971
301011      500.    3.1021
301012      550.    3.4021
301013      600.    3.6988
```

Title: AGR-2 Pre-Test Prediction Analyses using the PARFUME Code for U.S. Fuel Particles

ECAR No.: 1020

ECAR Rev. No.: 2

Project File No.: 23841

Date: 05/29/2012

```
*
*
* CARD SERIES 302XXX (burnup v- fluence input)
*      flu(e25 n/m^2)  bup(%fima)
302001      0.0000      0.000
302002      0.2933      0.710
302003      0.5913      1.548
302004      0.8975      2.543
302005      1.2117      3.710
302006      1.5300      5.024
302007      1.8525      6.399
302008      2.1717      7.718
302009      2.4854      8.912
302010      2.7971      9.965
302011      3.1021      10.892
302012      3.4021      11.707
302013      3.6988      12.434
*
*
* CARD SERIES 303XXX (external pressure v- fluence input)
*      external pressure v- fluence input
*      flu(e25 n/m^2)  pamb(MPa)
303001      0.          .1
*
* CARD SERIES 304XXX (boundary temperature v- fluence input)
*      flu(e25 n/m^2)  btemp(k)
304001      0.0000      1333.
304002      0.2933      1333.
304003      0.5913      1333.
304004      0.8975      1333.
304005      1.2117      1333.
304006      1.5300      1333.
304007      1.8525      1333.
304008      2.1717      1333.
304009      2.4854      1333.
304010      2.7971      1333.
304011      3.1021      1333.
304012      3.4021      1333.
304013      3.6988      1333.
*
* CARD SERIES 306XXX (time heatup starts and irradiation ends)
*      thus(days) [1xe6] {casualty condition not modeled}
*306001
*
***** CORRELATION COEFFICIENTS *****
* CARD SERIES 401XXX (correlation coefficients for ipyc cracking)
*      sigcr0(MPa)  umc(MPa)
401001      1084.599  176.800
*      c1c          c2c
401002      0.0000      0.0000      * for fuel particle radial posit
401003      0.0000      0.0000      * for kernel diameter
401004      0.0000      0.0000      * for buffer thickness
401005      1.775306E-02  6.682239E-05 * for ipyc thickness
401006      9.875041E-03  3.891481E-04 * for sic thickness
401007      -1.709696E-02  3.501242E-04 * for opyc thickness
401008      0.0000      0.0000      * for ipyc density
401009      0.0000      0.0000      * for opyc density
401010      0.0000      0.0000      * for ipyc baf
401011      0.0000      0.0000      * for opyc baf
401012      0.0000      0.0000      * for creep coeff amplication
*
* CARD SERIES 402XXX (correlation coefficients for ipyc asphericity)
*      siga0(MPa)  um(MPa)  delum(MPa)  aration  aratvar
402001      1038.101  450.500  394.590  1.052  0.013
```

Title: AGR-2 Pre-Test Prediction Analyses using the PARFUME Code for U.S. Fuel Particles

ECAR No.: 1020

ECAR Rev. No.: 2

Project File No.: 23841

Date: 05/29/2012

*	c1a	c2a	d1a	d2a	
402002	0.0000	0.0000	0.0000	0.0000	* fuel part rad pos
402003	0.0000	0.0000	0.0000	0.0000	* for kernel diamet
402004	0.0000	0.0000	0.0000	0.0000	* for buffer thickn
402005	3.198554E-03	1.860503E-05	4.357605E-04	2.458878E-05	*i thickn
402006	-3.145595E-03	-8.978341E-05	-3.078888E-03	-2.047198E-04	*s thickn
402007	2.771442E-03	-1.405273E-05	1.812438E-03	-9.556301E-06	*o thickn
402008	0.0000	0.0000	0.0000	0.0000	* for ipyc density
402009	0.0000	0.0000	0.0000	0.0000	* for opyc density
402010	0.0000	0.0000	0.0000	0.0000	* for ipyc baf
402011	0.0000	0.0000	0.0000	0.0000	* for opyc baf
402012	0.0000	0.0000	0.0000	0.0000	* for creep coef
402013	4.292235E+00	-6.431873E+01	5.924841E+00	-7.142645E+01	* aspheri

*
* CARD SERIES 403XXX (correlation coefficients for ipyc debonding)
* sigd0 (MPa) umd(MPa) bond0 (MPa) bond0var (MPa)
403001 1000. 100. 100. 0.
* c1d c2d
403002 0.0000 0.0000 * for fuel particle radial posit
403003 0.0000 0.0000 * for kernel diameter
403004 0.0000 0.0000 * for buffer thickness
403005 0.0000 0.0000 * for ipyc thickness
403006 0.0000 0.0000 * for sic thickness
403007 0.0000 0.0000 * for opyc thickness
403008 0.0000 0.0000 * for ipyc density
403009 0.0000 0.0000 * for opyc density
403010 0.0000 0.0000 * for ipyc baf
403011 0.0000 0.0000 * for opyc baf
403012 0.0000 0.0000 * for creep coeff amplication
403013 0.0000 0.0000 * for asphericity effects

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*
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Title: AGR-2 Pre-Test Prediction Analyses using the PARFUME Code for U.S. Fuel Particles

ECAR No.: 1020

ECAR Rev. No.: 2

Project File No.: 23841

Date: 05/29/2012

AGR-2 Capsule-3 UO2 High Temperature Run

```
*
*PARFUME V2.18 Input Data Deck: ECAR-1020R1
*
* Note: default values in brackets [default]
*
#####
***** GENERAL OPTIONS (SOLVERS/MODELS) *****
* CARD 100001 (simulation name)
*      title
100001   'AGR-2 Capsule-3 UO2 High Temp Run ECAR-1020R1'
*
* CARD 101001 (run parameters)
*      pfss      ncases      nburp      sample      dtf [0]      izeed [305]
101001      2        100        100        1
*
* CARD 101002 (models)
*      idebondp      ifacet      rbvalue      comodel      fgmodel      idebug
101002      1        1        12        3        2        0
*
***** MATERIAL PROPERTIES *****
* CARD 102001 (fuel characteristics)
*      u235enr(wt%)      ourat      curat
102001      9.60        2.00      0.00
*
* CARD 103001 (kernel properties)
*      kernd(g/cm^3)      kernt(g/cm^3) [11.030]
103001      10.86
*
* CARD 103002 (buffer properties)
*      buffd(g/cm^3)      bufft(g/cm^3) [2.250]
103002      0.99
*
* CARD 103003 (IPyC properties)
*      ipycdn(g/cm^3)      ipycdvar(g/cm^3)
103003      1.89        0.020
*
* CARD 103005 (OPyC properties)
*      opycdn(g/cm^3)      opycdvar(g/cm^3)
103005      1.88        0.010
*
* CARD 103013 (IPyC Bacon anisotropic factor)
*      ibafn      ibafvar
103013      1.047      0.004
*
* CARD 103015 (OPyC Bacon anisotropic factor)
*      obafn      obafvar
103015      1.037      0.002
*
* CARD 103023 (IPyC Weibull modulus)
*      ipycm [9.50]
*103023
*
* CARD 103024 (SiC Weibull modulus)
*      sigm [6.00]
*103024
*
* CARD 103025 (OPyC Weibull modulus)
*      opycm [9.50]
*103025
*
* CARD 103033 (Poisson's ratio)
*      cnu [0.500]      cnub [0.500]
*103033
*
* CARD 103043 (creep amplification factor)
*      creepampn [2.0]      creepvar [0.00]
*103043
*
* CARD 103054 (Enable ZrC)
*      zrc [0]      zrcp [1]
```

Title: AGR-2 Pre-Test Prediction Analyses using the PARFUME Code for U.S. Fuel Particles

ECAR No.: 1020

ECAR Rev. No.: 2

Project File No.: 23841

Date: 05/29/2012

```
*103054
*
* CARD 103061 (defective SiC layers)
*      fdef [0.00]
*103061
*
***** FUEL PARTICLE GEOMETRY *****
* CARD 104001 (kernel geometry)
*      kerndia(e-6 m)  kernvar(e-6 m)
104001      507.7      11.9
* CARD 104002 (buffer geometry)
*      buffthk(e-6 m)  buffvar(e-6 m)
104002      97.7      9.9
* CARD 104003 (IPyC geometry)
*      ipycthk(e-6 m)  ipycvar(e-6 m)
104003      41.9      3.2
* CARD 104004 (SiC geometry)
*      sicthk(e-6 m)   sicvar(e-6 m)
104004      37.5      1.2
* CARD 104005 (OPyC geometry)
*      opycthk(e-6 m)  opycvar(e-6 m)
104005      45.6      2.4
*
***** FUEL ELEMENT DESCRIPTION *****
* CARD 105001 (Plane Geometry w/modified Inputs for a Capsule)
105001  PLANEGEOM
* CARD 105011 (Planegeom)
*      partnum(particles/capsule)  ngngfm  ngngn
105011      18660.      3      6
* CARD 105021 (Planegeom)
*      fmthk(m)  cldthk(m)
105021      1.      1.
* CARD 105031 (Planegeom)
*      fmden(g/cm^3) [1.70]
*105031
* CARD 105041 (Planegeom)
*      ucontam
105041      8.55E-6
*
***** FUEL ELEMENT ENVIRONMENT *****
* CARD 106001 (fuel temperature option)
*      rtmpopt
106001  VOLAVGTMP
* CARD 106021 (global node temperatures)
*      tgi(k)  ntgi  {not required with VOLAVGTMP option}
*106021
* CARD 201001 (fission product transport description)
*      fpspecie  {diffusion not modeled}
*201001
*
* CARD SERIES 301XXX (fluence v- time input)
*      timeirr(days)  flu(e25 n/m^2)
301001      0.      0.0000
301002      50.      0.3083
301003      100.     0.6208
301004      150.     0.9388
301005      200.     1.2625
301006      250.     1.5892
301007      300.     1.9154
301008      350.     2.2383
301009      400.     2.5588
301010      450.     2.8758
301011      500.     3.1888
301012      550.     3.5017
301013      600.     3.8117
```

Title: AGR-2 Pre-Test Prediction Analyses using the PARFUME Code for U.S. Fuel Particles

ECAR No.: 1020

ECAR Rev. No.: 2

Project File No.: 23841

Date: 05/29/2012

```
*
*
* CARD SERIES 302XXX (burnup v- fluence input)
*      flu(e25 n/m^2)  bup(%fima)
302001      0.0000      0.000
302002      0.3083      0.595
302003      0.6208      1.334
302004      0.9388      2.237
302005      1.2625      3.309
302006      1.5892      4.472
302007      1.9154      5.609
302008      2.2383      6.641
302009      2.5588      7.556
302010      2.8758      8.365
302011      3.1888      9.087
302012      3.5017      9.743
302013      3.8117      10.344
*
*
* CARD SERIES 303XXX (external pressure v- fluence input)
*      external pressure v- fluence input
*      flu(e25 n/m^2)  pamb(MPa)
303001      0.          .1
*
* CARD SERIES 304XXX (boundary temperature v- fluence input)
*      flu(e25 n/m^2)  btemp(k)
304001      0.0000      1413.
304002      0.3083      1413.
304003      0.6208      1413.
304004      0.9388      1413.
304005      1.2625      1413.
304006      1.5892      1413.
304007      1.9154      1413.
304008      2.2383      1413.
304009      2.5588      1413.
304010      2.8758      1413.
304011      3.1888      1413.
304012      3.5017      1413.
304013      3.8117      1413.
*
* CARD SERIES 306XXX (time heatup starts and irradiation ends)
*      thus(days) [1xe6] {casualty condition not modeled}
*306001
*
***** CORRELATION COEFFICIENTS *****
* CARD SERIES 401XXX (correlation coefficients for ipyc cracking)
*      sigcr0(MPa)  umc(MPa)
401001      1034.501  147.800
*      c1c          c2c
401002      0.0000      0.0000      * for fuel particle radial posit
401003      0.0000      0.0000      * for kernel diameter
401004      0.0000      0.0000      * for buffer thickness
401005      1.867732E-02  1.009260E-04  * for ipyc thickness
401006      7.532756E-03  5.346951E-04  * for sic thickness
401007      -1.609670E-02  4.366692E-04  * for opyc thickness
401008      0.0000      0.0000      * for ipyc density
401009      0.0000      0.0000      * for opyc density
401010      0.0000      0.0000      * for ipyc baf
401011      0.0000      0.0000      * for opyc baf
401012      0.0000      0.0000      * for creep coeff amplication
*
* CARD SERIES 402XXX (correlation coefficients for ipyc asphericity)
*      sigma0(MPa)  um(MPa)  delum(MPa)  aration  aratvar
402001      1183.359  376.300  951.000  1.052  0.013
```

Title: AGR-2 Pre-Test Prediction Analyses using the PARFUME Code for U.S. Fuel Particles

ECAR No.: 1020

ECAR Rev. No.: 2

Project File No.: 23841

Date: 05/29/2012

*	c1a	c2a	d1a	d2a	
402002	0.0000	0.0000	0.0000	0.0000	* fuel part rad pos
402003	0.0000	0.0000	0.0000	0.0000	* for kernel diamet
402004	0.0000	0.0000	0.0000	0.0000	* for buffer thickn
402005	2.832693E-03	2.152240E-05	-1.494475E-03	6.664079E-06	*i thickn
402006	-2.067733E-03	-1.445600E-04	-1.091079E-02	1.139076E-04	*s thickn
402007	2.947812E-03	-2.134667E-05	3.039007E-04	3.015641E-06	*o thickn
402008	0.0000	0.0000	0.0000	0.0000	* for ipyc density
402009	0.0000	0.0000	0.0000	0.0000	* for opyc density
402010	0.0000	0.0000	0.0000	0.0000	* for ipyc baf
402011	0.0000	0.0000	0.0000	0.0000	* for opyc baf
402012	0.0000	0.0000	0.0000	0.0000	* for creep coef
402013	3.917186E+00	-6.412679E+01	9.524989E+00	-6.262098E+01	*aspheric

*
* CARD SERIES 403XXX (correlation coefficients for ipyc debonding)
* sigd0 (MPa) umd(MPa) bond0 (MPa) bond0var (MPa)
403001 100. 100. 100. 0.
* c1d c2d
403002 0.0000 0.0000 * for fuel particle radial posit
403003 0.0000 0.0000 * for kernel diameter
403004 0.0000 0.0000 * for buffer thickness
403005 0.0000 0.0000 * for ipyc thickness
403006 0.0000 0.0000 * for sic thickness
403007 0.0000 0.0000 * for opyc thickness
403008 0.0000 0.0000 * for ipyc density
403009 0.0000 0.0000 * for opyc density
403010 0.0000 0.0000 * for ipyc baf
403011 0.0000 0.0000 * for opyc baf
403012 0.0000 0.0000 * for creep coeff amplication
403013 0.0000 0.0000 * for asphericity effects

*
*
.

Title: AGR-2 Pre-Test Prediction Analyses using the PARFUME Code for U.S. Fuel Particles

ECAR No.: 1020

ECAR Rev. No.: 2

Project File No.: 23841

Date: 05/29/2012

AGR-2 Capsule-3 UO2 Volume Average Temperature Run

```
*
*PARFUME V2.18 Input Data Deck: ECAR-1020R1
*
* Note: default values in brackets [default]
*
#####
***** GENERAL OPTIONS (SOLVERS/MODELS) *****
* CARD 100001 (simulation name)
*      title
100001   'AGR-2 Capsule-3 UO2 Volume Average Temp Run ECAR-1020R1'
*
* CARD 101001 (run parameters)
*      pfss      ncases      nburp      sample      dtf [0]      izeed [305]
101001      2      100      100      1
*
* CARD 101002 (models)
*      idebondp      ifacet      rbvalue      comodel      fgmodel      idebug
101002      1      1      12      3      2      0
*
***** MATERIAL PROPERTIES *****
* CARD 102001 (fuel characteristics)
*      u235enr(wt%)      ourat      curat
102001      9.60      2.00      0.00
*
* CARD 103001 (kernel properties)
*      kernd(g/cm^3)      kernt(g/cm^3) [11.030]
103001      10.86
*
* CARD 103002 (buffer properties)
*      buffd(g/cm^3)      bufft(g/cm^3) [2.250]
103002      0.99
*
* CARD 103003 (IPyC properties)
*      ipycdn(g/cm^3)      ipycdvar(g/cm^3)
103003      1.89      0.020
*
* CARD 103005 (OPyC properties)
*      opycdn(g/cm^3)      opycdvar(g/cm^3)
103005      1.88      0.010
*
* CARD 103013 (IPyC Bacon anisotropic factor)
*      ibafn      ibafvar
103013      1.047      0.004
*
* CARD 103015 (OPyC Bacon anisotropic factor)
*      obafn      obafvar
103015      1.037      0.002
*
* CARD 103023 (IPyC Weibull modulus)
*      ipycm [9.50]
*103023
*
* CARD 103024 (SiC Weibull modulus)
*      sigm [6.00]
*103024
*
* CARD 103025 (OPyC Weibull modulus)
*      opycm [9.50]
*103025
*
* CARD 103033 (Poisson's ratio)
*      cnu [0.500]      cnub [0.500]
*103033
*
* CARD 103043 (creep amplification factor)
*      creepampn [2.0]      creepvar [0.00]
*103043
*
* CARD 103054 (Enable ZrC)
*      zrc [0]      zrcp [1]
```


Title: AGR-2 Pre-Test Prediction Analyses using the PARFUME Code for U.S. Fuel Particles

ECAR No.: 1020

ECAR Rev. No.: 2

Project File No.: 23841

Date: 05/29/2012

```
*103054
*
* CARD 103061 (defective SiC layers)
*      fdef [0.00]
*103061
*
***** FUEL PARTICLE GEOMETRY *****
* CARD 104001 (kernel geometry)
*      kerndia(e-6 m)  kernvar(e-6 m)
104001      507.7      11.9
* CARD 104002 (buffer geometry)
*      buffthk(e-6 m)  buffvar(e-6 m)
104002      97.7      9.9
* CARD 104003 (IPyC geometry)
*      ipycthk(e-6 m)  ipycvar(e-6 m)
104003      41.9      3.2
* CARD 104004 (SiC geometry)
*      sicthk(e-6 m)   sicvar(e-6 m)
104004      37.5      1.2
* CARD 104005 (OPyC geometry)
*      opycthk(e-6 m)  opycvar(e-6 m)
104005      45.6      2.4
*
***** FUEL ELEMENT DESCRIPTION *****
* CARD 105001 (Plane Geometry w/modified Inputs for a Capsule)
105001  PLANEGEOM
* CARD 105011 (Planegeom)
*      partnum(particles/capsule)  ngngfm  ngng
105011      18660.      3      6
* CARD 105021 (Planegeom)
*      fmthk(m)  cldthk(m)
105021      1.      1.
* CARD 105031 (Planegeom)
*      fmden(g/cm^3) [1.70]
*105031
* CARD 105041 (Planegeom)
*      ucontam
105041      8.55E-6
*
***** FUEL ELEMENT ENVIRONMENT *****
* CARD 106001 (fuel temperature option)
*      rtmpopt
106001  VOLAVGTMP
* CARD 106021 (global node temperatures)
*      tgi(k)  ntgi  {not required with VOLAVGTMP option}
*106021
* CARD 201001 (fission product transport description)
*      fpspecie  {diffusion not modeled}
*201001
*
* CARD SERIES 301XXX (fluence v- time input)
*      timeirr(days)  flu(e25 n/m^2)
301001      0.      0.0000
301002      50.      0.3083
301003      100.     0.6208
301004      150.     0.9388
301005      200.     1.2625
301006      250.     1.5892
301007      300.     1.9154
301008      350.     2.2383
301009      400.     2.5588
301010      450.     2.8758
301011      500.     3.1888
301012      550.     3.5017
301013      600.     3.8117
```

Title: AGR-2 Pre-Test Prediction Analyses using the PARFUME Code for U.S. Fuel Particles

ECAR No.: 1020

ECAR Rev. No.: 2

Project File No.: 23841

Date: 05/29/2012

```
*
*
* CARD SERIES 302XXX (burnup v- fluence input)
*      flu(e25 n/m^2)  bup(%fima)
302001      0.0000      0.000
302002      0.3083      0.595
302003      0.6208      1.334
302004      0.9388      2.237
302005      1.2625      3.309
302006      1.5892      4.472
302007      1.9154      5.609
302008      2.2383      6.641
302009      2.5588      7.556
302010      2.8758      8.365
302011      3.1888      9.087
302012      3.5017      9.743
302013      3.8117      10.344
*
* CARD SERIES 303XXX (external pressure v- fluence input)
*      external pressure v- fluence input
*      flu(e25 n/m^2)  pamb(MPa)
303001      0.          .1
*
* CARD SERIES 304XXX (boundary temperature v- fluence input)
*      flu(e25 n/m^2)  btemp(k)
304001      0.0000      1243.
304002      0.3083      1243.
304003      0.6208      1243.
304004      0.9388      1243.
304005      1.2625      1243.
304006      1.5892      1243.
304007      1.9154      1243.
304008      2.2383      1243.
304009      2.5588      1243.
304010      2.8758      1243.
304011      3.1888      1243.
304012      3.5017      1243.
304013      3.8117      1243.
*
* CARD SERIES 306XXX (time heatup starts and irradiation ends)
*      thus(days) [1xe6] {casualty condition not modeled}
*306001
*
***** CORRELATION COEFFICIENTS *****
* CARD SERIES 401XXX (correlation coefficients for ipyc cracking)
*      sigcr0(MPa)  umc(MPa)
401001      1034.949  193.600
*      c1c          c2c
401002      0.0000      0.0000      * for fuel particle radial posit
401003      0.0000      0.0000      * for kernel diameter
401004      0.0000      0.0000      * for buffer thickness
401005      1.822823E-02  1.051286E-04  * for ipyc thickness
401006      8.945395E-03  4.446288E-04  * for sic thickness
401007      -1.589262E-02  4.366515E-04  * for opyc thickness
401008      0.0000      0.0000      * for ipyc density
401009      0.0000      0.0000      * for opyc density
401010      0.0000      0.0000      * for ipyc baf
401011      0.0000      0.0000      * for opyc baf
401012      0.0000      0.0000      * for creep coeff amplication
*
* CARD SERIES 402XXX (correlation coefficients for ipyc asphericity)
*      siga0(MPa)  um(MPa)  delum(MPa)  aration  aratvar
402001      1245.891  495.000  804.400  1.052  0.013
```

Title: AGR-2 Pre-Test Prediction Analyses using the PARFUME Code for U.S. Fuel Particles

ECAR No.: 1020

ECAR Rev. No.: 2

Project File No.: 23841

Date: 05/29/2012

*	c1a	c2a	d1a	d2a	
402002	0.0000	0.0000	0.0000	0.0000	* fuel part rad pos
402003	0.0000	0.0000	0.0000	0.0000	* for kernel diamet
402004	0.0000	0.0000	0.0000	0.0000	* for buffer thickn
402005	2.732390E-03	2.154754E-05	-2.163655E-03	1.865719E-05	*i thickn
402006	-1.829884E-03	-1.200029E-04	-6.804187E-03	-7.336255E-05	*s thickn
402007	2.728837E-03	-1.109934E-05	-5.288199E-04	2.577869E-06	*o thickn
402008	0.0000	0.0000	0.0000	0.0000	* for ipyc density
402009	0.0000	0.0000	0.0000	0.0000	* for opyc density
402010	0.0000	0.0000	0.0000	0.0000	* for ipyc baf
402011	0.0000	0.0000	0.0000	0.0000	* for opyc baf
402012	0.0000	0.0000	0.0000	0.0000	* for creep coef
402013	3.923850E+00	-6.350488E+01	8.155022E+00	-6.483160E+01	* aspheri

*
* CARD SERIES 403XXX (correlation coefficients for ipyc debonding)
* sigd0 (MPa) umd(MPa) bond0 (MPa) bond0var (MPa)
403001 100. 100. 100. 0.
* c1d c2d
403002 0.0000 0.0000 * for fuel particle radial posit
403003 0.0000 0.0000 * for kernel diameter
403004 0.0000 0.0000 * for buffer thickness
403005 0.0000 0.0000 * for ipyc thickness
403006 0.0000 0.0000 * for sic thickness
403007 0.0000 0.0000 * for opyc thickness
403008 0.0000 0.0000 * for ipyc density
403009 0.0000 0.0000 * for opyc density
403010 0.0000 0.0000 * for ipyc baf
403011 0.0000 0.0000 * for opyc baf
403012 0.0000 0.0000 * for creep coeff amplication
403013 0.0000 0.0000 * for asphericity effects

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*
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Title: AGR-2 Pre-Test Prediction Analyses using the PARFUME Code for U.S. Fuel Particles

ECAR No.: 1020

ECAR Rev. No.: 2

Project File No.: 23841

Date: 05/29/2012

AGR-2 Capsule-3 UO2 Low Temperature Run

```
*
*PARFUME V2.18 Input Data Deck: ECAR-1020R1
*
* Note: default values in brackets [default]
*
#####
***** GENERAL OPTIONS (SOLVERS/MODELS) *****
* CARD 100001 (simulation name)
*      title
100001  'AGR-2 Capsule-3 UO2 Low Temp Run ECAR-1020R1'
*
* CARD 101001 (run parameters)
*      pfss      ncases      nburp      sample      dtf [0]      izeed [305]
101001      2      100      100      1
*
* CARD 101002 (models)
*      idebondp      ifacet      rbvalue      comodel      fgmodel      idebug
101002      1      1      12      3      2      0
*
***** MATERIAL PROPERTIES *****
* CARD 102001 (fuel characteristics)
*      u235enr(wt%)      ourat      curat
102001      9.60      2.00      0.00
*
* CARD 103001 (kernel properties)
*      kernd(g/cm^3)      kernt(g/cm^3) [11.030]
103001      10.86
*
* CARD 103002 (buffer properties)
*      buffd(g/cm^3)      bufft(g/cm^3) [2.250]
103002      0.99
*
* CARD 103003 (IPyC properties)
*      ipycdn(g/cm^3)      ipycdvar(g/cm^3)
103003      1.89      0.020
*
* CARD 103005 (OPyC properties)
*      opycdn(g/cm^3)      opycdvar(g/cm^3)
103005      1.88      0.010
*
* CARD 103013 (IPyC Bacon anisotropic factor)
*      ibafn      ibafvar
103013      1.047      0.004
*
* CARD 103015 (OPyC Bacon anisotropic factor)
*      obafn      obafvar
103015      1.037      0.002
*
* CARD 103023 (IPyC Weibull modulus)
*      ipycm [9.50]
*103023
*
* CARD 103024 (SiC Weibull modulus)
*      sigm [6.00]
*103024
*
* CARD 103025 (OPyC Weibull modulus)
*      opycm [9.50]
*103025
*
* CARD 103033 (Poisson's ratio)
*      cnu [0.500]      cnuv [0.500]
*103033
*
* CARD 103043 (creep amplification factor)
*      creepampn [2.0]      creepvar [0.00]
*103043
*
* CARD 103054 (Enable ZrC)
*      zrc [0]      zrcp [1]
```

Title: AGR-2 Pre-Test Prediction Analyses using the PARFUME Code for U.S. Fuel Particles

ECAR No.: 1020

ECAR Rev. No.: 2

Project File No.: 23841

Date: 05/29/2012

```
*103054
*
* CARD 103061 (defective SiC layers)
*      fdef [0.00]
*103061
*
***** FUEL PARTICLE GEOMETRY *****
* CARD 104001 (kernel geometry)
*      kerndia(e-6 m)  kernvar(e-6 m)
104001      507.7      11.9
* CARD 104002 (buffer geometry)
*      buffthk(e-6 m)  buffvar(e-6 m)
104002      97.7      9.9
* CARD 104003 (IPyC geometry)
*      ipycthk(e-6 m)  ipycvar(e-6 m)
104003      41.9      3.2
* CARD 104004 (SiC geometry)
*      sicthk(e-6 m)   sicvar(e-6 m)
104004      37.5      1.2
* CARD 104005 (OPyC geometry)
*      opycthk(e-6 m)  opycvar(e-6 m)
104005      45.6      2.4
*
***** FUEL ELEMENT DESCRIPTION *****
* CARD 105001 (Plane Geometry w/modified Inputs for a Capsule)
105001  PLANEGEOM
* CARD 105011 (Planegeom)
*      partnum(particles/capsule)  ngnfm  ngn
105011      18660.      3      6
* CARD 105021 (Planegeom)
*      fmthk(m)  cldthk(m)
105021      1.      1.
* CARD 105031 (Planegeom)
*      fmden(g/cm^3) [1.70]
*105031
* CARD 105041 (Planegeom)
*      ucontam
105041      8.55E-6
*
***** FUEL ELEMENT ENVIRONMENT *****
* CARD 106001 (fuel temperature option)
*      rtmpopt
106001  VOLAVGTMP
* CARD 106021 (global node temperatures)
*      tgi(k)  ntgi  {not required with VOLAVGTMP option}
*106021
* CARD 201001 (fission product transport description)
*      fpspecie  {diffusion not modeled}
*201001
*
* CARD SERIES 301XXX (fluence v- time input)
*      timeirr(days)  flu(e25 n/m^2)
301001      0.      0.0000
301002      50.      0.3083
301003      100.     0.6208
301004      150.     0.9388
301005      200.     1.2625
301006      250.     1.5892
301007      300.     1.9154
301008      350.     2.2383
301009      400.     2.5588
301010      450.     2.8758
301011      500.     3.1888
301012      550.     3.5017
301013      600.     3.8117
```

Title: AGR-2 Pre-Test Prediction Analyses using the PARFUME Code for U.S. Fuel Particles

ECAR No.: 1020

ECAR Rev. No.: 2

Project File No.: 23841

Date: 05/29/2012

```
*
*
* CARD SERIES 302XXX (burnup v- fluence input)
*      flu(e25 n/m^2)  bup(%fima)
302001      0.0000      0.000
302002      0.3083      0.595
302003      0.6208      1.334
302004      0.9388      2.237
302005      1.2625      3.309
302006      1.5892      4.472
302007      1.9154      5.609
302008      2.2383      6.641
302009      2.5588      7.556
302010      2.8758      8.365
302011      3.1888      9.087
302012      3.5017      9.743
302013      3.8117      10.344
*
*
* CARD SERIES 303XXX (external pressure v- fluence input)
*      external pressure v- fluence input
*      flu(e25 n/m^2)  pamb(MPa)
303001      0.          .1
*
* CARD SERIES 304XXX (boundary temperature v- fluence input)
*      flu(e25 n/m^2)  btemp(k)
304001      0.0000      1073.
304002      0.3083      1073.
304003      0.6208      1073.
304004      0.9388      1073.
304005      1.2625      1073.
304006      1.5892      1073.
304007      1.9154      1073.
304008      2.2383      1073.
304009      2.5588      1073.
304010      2.8758      1073.
304011      3.1888      1073.
304012      3.5017      1073.
304013      3.8117      1073.
*
* CARD SERIES 306XXX (time heatup starts and irradiation ends)
*      thus(days) [1xe6] {casualty condition not modeled}
*306001
*
***** CORRELATION COEFFICIENTS *****
* CARD SERIES 401XXX (correlation coefficients for ipyc cracking)
*      sigcr0(MPa)  umc(MPa)
401001      1035.378  251.700
*      c1c          c2c
401002      0.0000      0.0000      * for fuel particle radial posit
401003      0.0000      0.0000      * for kernel diameter
401004      0.0000      0.0000      * for buffer thickness
401005      1.787135E-02  1.161038E-04  * for ipyc thickness
401006      1.005964E-02  4.100172E-04  * for sic thickness
401007      -1.575756E-02  4.430003E-04  * for opyc thickness
401008      0.0000      0.0000      * for ipyc density
401009      0.0000      0.0000      * for opyc density
401010      0.0000      0.0000      * for ipyc baf
401011      0.0000      0.0000      * for opyc baf
401012      0.0000      0.0000      * for creep coeff amplication
*
* CARD SERIES 402XXX (correlation coefficients for ipyc asphericity)
*      siga0(MPa)  um(MPa)  delum(MPa)  aration  aratvar
402001      1022.260  641.800  595.110  1.052  0.013
```

Title: AGR-2 Pre-Test Prediction Analyses using the PARFUME Code for U.S. Fuel Particles

ECAR No.: 1020

ECAR Rev. No.: 2

Project File No.: 23841

Date: 05/29/2012

*	c1a	c2a	d1a	d2a	
402002	0.0000	0.0000	0.0000	0.0000	* fuel part rad pos
402003	0.0000	0.0000	0.0000	0.0000	* for kernel diamet
402004	0.0000	0.0000	0.0000	0.0000	* for buffer thickn
402005	2.540589E-03	2.210913E-05	-1.862403E-03	3.422378E-05	*i thickn
402006	-1.378254E-03	-1.334027E-04	-2.545496E-05	-3.375448E-04	*s thickn
402007	2.424594E-03	-1.143743E-05	-8.310304E-04	-1.073864E-06	*o thickn
402008	0.0000	0.0000	0.0000	0.0000	* for ipyc density
402009	0.0000	0.0000	0.0000	0.0000	* for opyc density
402010	0.0000	0.0000	0.0000	0.0000	* for ipyc baf
402011	0.0000	0.0000	0.0000	0.0000	* for opyc baf
402012	0.0000	0.0000	0.0000	0.0000	* for creep coef
402013	3.835364E+00	-6.182916E+01	5.823095E+00	-6.247914E+01	* aspheri

*
* CARD SERIES 403XXX (correlation coefficients for ipyc debonding)
* sigd0 (MPa) umd(MPa) bond0 (MPa) bond0var (MPa)
403001 100. 100. 100. 0.
* c1d c2d
403002 0.0000 0.0000 * for fuel particle radial posit
403003 0.0000 0.0000 * for kernel diameter
403004 0.0000 0.0000 * for buffer thickness
403005 0.0000 0.0000 * for ipyc thickness
403006 0.0000 0.0000 * for sic thickness
403007 0.0000 0.0000 * for opyc thickness
403008 0.0000 0.0000 * for ipyc density
403009 0.0000 0.0000 * for opyc density
403010 0.0000 0.0000 * for ipyc baf
403011 0.0000 0.0000 * for opyc baf
403012 0.0000 0.0000 * for creep coeff amplication
403013 0.0000 0.0000 * for asphericity effects

*
*
.

Title: AGR-2 Pre-Test Prediction Analyses using the PARFUME Code for U.S. Fuel Particles

ECAR No.: 1020

ECAR Rev. No.: 2

Project File No.: 23841

Date: 05/29/2012

AGR-2 Capsule-5 UCO High Temperature Run

```
*
*PARFUME V2.18 Input Data Deck: ECAR-1020R1
*
* Note: default values in brackets [default]
*
#####
***** GENERAL OPTIONS (SOLVERS/MODELS) *****
* CARD 100001 (simulation name)
*   title
100001   'AGR-2 Capsule-5 UCO High Temp Run ECAR-1020R1'
*
* CARD 101001 (run parameters)
*   pfss      ncases      nburp      sample      dtf [0]      izeed [305]
101001      2          100          100          1
*
* CARD 101002 (models)
*   idebondp   ifacet   rbvalue   comodel   fgmodel   idebug
101002      1          1          12          3          2          0
*
***** MATERIAL PROPERTIES *****
* CARD 102001 (fuel characteristics)
*   u235enr(wt%)  ourat  curat
102001      14.03    1.43  0.39
*
* CARD 103001 (kernel properties)
*   kernd(g/cm^3) kernt(g/cm^3) [11.030]
103001      10.97
*
* CARD 103002 (buffer properties)
*   buffd(g/cm^3) bufft(g/cm^3) [2.250]
103002      1.04
*
* CARD 103003 (IPyC properties)
*   ipycdn(g/cm^3) ipycdvar(g/cm^3)
103003      1.89      0.010
*
* CARD 103005 (OPyC properties)
*   opycdn(g/cm^3) opycdvar(g/cm^3)
103005      1.91      0.010
*
* CARD 103013 (IPyC Bacon anisotropic factor)
*   ibafn  ibafvar
103013    1.047  0.005
*
* CARD 103015 (OPyC Bacon anisotropic factor)
*   obafn  obafvar
103015    1.043  0.002
*
* CARD 103023 (IPyC Weibull modulus)
*   ipycm [9.50]
*103023
*
* CARD 103024 (SiC Weibull modulus)
*   sigm [6.00]
*103024
*
* CARD 103025 (OPyC Weibull modulus)
*   opycm [9.50]
*103025
*
* CARD 103033 (Poisson's ratio)
*   cnu [0.500]  cnub [0.500]
*103033
*
* CARD 103043 (creep amplification factor)
*   creepampn [2.0]  creepvar [0.00]
*103043
*
* CARD 103054 (Enable ZrC)
*   zrc [0]  zrcp [1]
```


Title: AGR-2 Pre-Test Prediction Analyses using the PARFUME Code for U.S. Fuel Particles

ECAR No.: 1020

ECAR Rev. No.: 2

Project File No.: 23841

Date: 05/29/2012

```
*103054
*
* CARD 103061 (defective SiC layers)
*      fdef [0.00]
*103061
*
***** FUEL PARTICLE GEOMETRY *****
* CARD 104001 (kernel geometry)
*      kerndia(e-6 m)  kernvar(e-6 m)
104001      426.7      8.8
* CARD 104002 (buffer geometry)
*      buffthk(e-6 m)  buffvar(e-6 m)
104002      98.9      8.4
* CARD 104003 (IPyC geometry)
*      ipycthk(e-6 m)  ipycvar(e-6 m)
104003      40.4      2.5
* CARD 104004 (SiC geometry)
*      sicthk(e-6 m)   sicvar(e-6 m)
104004      35.2      1.2
* CARD 104005 (OPyC geometry)
*      opycthk(e-6 m)  opycvar(e-6 m)
104005      43.4      2.9
*
***** FUEL ELEMENT DESCRIPTION *****
* CARD 105001 (Plane Geometry w/modified Inputs for a Capsule)
105001      PLANEGEOM
* CARD 105011 (Planegeom)
*      partnum(particles/capsule)  ngngfm  ngngn
105011      38052.      3      6
* CARD 105021 (Planegeom)
*      fmthk(m)  cldthk(m)
105021      1.      1.
* CARD 105031 (Planegeom)
*      fmden(g/cm^3) [1.70]
*105031
* CARD 105041 (Planegeom)
*      ucontam
105041      9.74E-6
*
***** FUEL ELEMENT ENVIRONMENT *****
* CARD 106001 (fuel temperature option)
*      rtmpopt
106001      VOLAVGTMP
* CARD 106021 (global node temperatures)
*      tgi(k)  ntgi  {not required with VOLAVGTMP option}
*106021
* CARD 201001 (fission product transport description)
*      fpspecie  {diffusion not modeled}
*201001
*
* CARD SERIES 301XXX (fluence v- time input)
*      timeirr(days)  flu(e25 n/m^2)
301001      0.      0.0000
301002      50.      0.2788
301003      100.      0.5629
301004      150.      0.8529
301005      200.      1.1471
301006      250.      1.4483
301007      300.      1.7538
301008      350.      2.0596
301009      400.      2.3596
301010      450.      2.6575
301011      500.      2.9483
301012      550.      3.2375
301013      600.      3.5217
```

Title: AGR-2 Pre-Test Prediction Analyses using the PARFUME Code for U.S. Fuel Particles

ECAR No.: 1020

ECAR Rev. No.: 2

Project File No.: 23841

Date: 05/29/2012

```
*
*
* CARD SERIES 302XXX (burnup v- fluence input)
*      flu(e25 n/m^2)  bup(%fima)
302001      0.0000      0.000
302002      0.2788      0.660
302003      0.5629      1.434
302004      0.8529      2.344
302005      1.1471      3.398
302006      1.4483      4.583
302007      1.7538      5.845
302008      2.0596      7.084
302009      2.3596      8.230
302010      2.6575      9.260
302011      2.9483      10.175
302012      3.2375      10.985
302013      3.5217      11.707
*
*
* CARD SERIES 303XXX (external pressure v- fluence input)
*      external pressure v- fluence input
*      flu(e25 n/m^2)  pamb(MPa)
303001      0.          .1
*
* CARD SERIES 304XXX (boundary temperature v- fluence input)
*      flu(e25 n/m^2)  btemp(k)
304001      0.0000      1513.
304002      0.2788      1513.
304003      0.5629      1513.
304004      0.8529      1513.
304005      1.1471      1513.
304006      1.4483      1513.
304007      1.7538      1513.
304008      2.0596      1513.
304009      2.3596      1513.
304010      2.6575      1513.
304011      2.9483      1513.
304012      3.2375      1513.
304013      3.5217      1513.
*
* CARD SERIES 306XXX (time heatup starts and irradiation ends)
*      thus(days) [1xe6] {casualty condition not modeled}
*306001
*
***** CORRELATION COEFFICIENTS *****
* CARD SERIES 401XXX (correlation coefficients for ipyc cracking)
*      sigcr0 (MPa)  umc (MPa)
401001      1084.828  134.700
*      c1c          c2c
401002      0.0000      0.0000      * for fuel particle radial posit
401003      0.0000      0.0000      * for kernel diameter
401004      0.0000      0.0000      * for buffer thickness
401005      1.824388E-02  7.280707E-05 * for ipyc thickness
401006      9.013128E-03  4.533721E-04 * for sic thickness
401007      -1.729392E-02  3.506499E-04 * for opyc thickness
401008      0.0000      0.0000      * for ipyc density
401009      0.0000      0.0000      * for opyc density
401010      0.0000      0.0000      * for ipyc baf
401011      0.0000      0.0000      * for opyc baf
401012      0.0000      0.0000      * for creep coeff amplication
*
* CARD SERIES 402XXX (correlation coefficients for ipyc asphericity)
*      siga0 (MPa)  um (MPa)  delum (MPa)  aration  aratvar
402001      1936.247  344.100  362.570  1.052  0.013
```

Title: AGR-2 Pre-Test Prediction Analyses using the PARFUME Code for U.S. Fuel Particles

ECAR No.: 1020

ECAR Rev. No.: 2

Project File No.: 23841

Date: 05/29/2012

*	c1a	c2a	d1a	d2a	
402002	0.0000	0.0000	0.0000	0.0000	* fuel part rad pos
402003	0.0000	0.0000	0.0000	0.0000	* for kernel diamet
402004	0.0000	0.0000	0.0000	0.0000	* for buffer thickn
402005	3.537402E-03	2.075732E-05	-1.545765E-03	1.187809E-05	*i thickn
402006	-3.486931E-03	-7.022193E-05	-7.081619E-03	-2.665115E-05	*s thickn
402007	2.928835E-03	-1.279172E-05	1.358251E-03	-1.522899E-05	*o thickn
402008	0.0000	0.0000	0.0000	0.0000	* for ipyc density
402009	0.0000	0.0000	0.0000	0.0000	* for opyc density
402010	0.0000	0.0000	0.0000	0.0000	* for ipyc baf
402011	0.0000	0.0000	0.0000	0.0000	* for opyc baf
402012	0.0000	0.0000	0.0000	0.0000	* for creep coef
402013	4.253008E+00	-6.416275E+01	7.554505E+00	-6.892159E+01	* aspheri

*
* CARD SERIES 403XXX (correlation coefficients for ipyc debonding)
* sigd0 (MPa) umd(MPa) bond0 (MPa) bond0var (MPa)
403001 100. 100. 100. 0.
* c1d c2d
403002 0.0000 0.0000 * for fuel particle radial posit
403003 0.0000 0.0000 * for kernel diameter
403004 0.0000 0.0000 * for buffer thickness
403005 0.0000 0.0000 * for ipyc thickness
403006 0.0000 0.0000 * for sic thickness
403007 0.0000 0.0000 * for opyc thickness
403008 0.0000 0.0000 * for ipyc density
403009 0.0000 0.0000 * for opyc density
403010 0.0000 0.0000 * for ipyc baf
403011 0.0000 0.0000 * for opyc baf
403012 0.0000 0.0000 * for creep coeff amplication
403013 0.0000 0.0000 * for asphericity effects

*
*
.

Title: AGR-2 Pre-Test Prediction Analyses using the PARFUME Code for U.S. Fuel Particles

ECAR No.: 1020

ECAR Rev. No.: 2

Project File No.: 23841

Date: 05/29/2012

AGR-2 Capsule-5 UCO Volume Average Temperature Run

```
*
*PARFUME V2.18 Input Data Deck: ECAR-1020R1
*
* Note: default values in brackets [default]
*
#####
***** GENERAL OPTIONS (SOLVERS/MODELS) *****
* CARD 100001 (simulation name)
*      title
100001  'AGR-2 Capsule-5 UCO Volume Average Temp Run ECAR-1020R1'
*
* CARD 101001 (run parameters)
*      pfss      ncases      nburp      sample      dtf [0]      izeed [305]
101001      2      100      100      1
*
* CARD 101002 (models)
*      idebondp      ifacet      rbvalue      comodel      fgmodel      idebug
101002      1      1      12      3      2      0
*
***** MATERIAL PROPERTIES *****
* CARD 102001 (fuel characteristics)
*      u235enr(wt%)      ourat      curat
102001      14.03      1.43      0.39
*
* CARD 103001 (kernel properties)
*      kernd(g/cm^3)      kernt(g/cm^3) [11.030]
103001      10.97
* CARD 103002 (buffer properties)
*      buffd(g/cm^3)      bufft(g/cm^3) [2.250]
103002      1.04
* CARD 103003 (IPyC properties)
*      ipycdn(g/cm^3)      ipycdvar(g/cm^3)
103003      1.89      0.010
* CARD 103005 (OPyC properties)
*      opycdn(g/cm^3)      opycdvar(g/cm^3)
103005      1.91      0.010
*
* CARD 103013 (IPyC Bacon anisotropic factor)
*      ibafn      ibafvar
103013      1.047      0.005
* CARD 103015 (OPyC Bacon anisotropic factor)
*      obafn      obafvar
103015      1.043      0.002
*
* CARD 103023 (IPyC Weibull modulus)
*      ipycm [9.50]
*103023
* CARD 103024 (SiC Weibull modulus)
*      sigm [6.00]
*103024
* CARD 103025 (OPyC Weibull modulus)
*      opycm [9.50]
*103025
*
* CARD 103033 (Poisson's ratio)
*      cnu [0.500]      cnub [0.500]
*103033
* CARD 103043 (creep amplification factor)
*      creepampn [2.0]      creepvar [0.00]
*103043
*
* CARD 103054 (Enable ZrC)
*      zrc [0]      zrcp [1]
```

Title: AGR-2 Pre-Test Prediction Analyses using the PARFUME Code for U.S. Fuel Particles

ECAR No.: 1020

ECAR Rev. No.: 2

Project File No.: 23841

Date: 05/29/2012

```
*103054
*
* CARD 103061 (defective SiC layers)
*      fdef [0.00]
*103061
*
***** FUEL PARTICLE GEOMETRY *****
* CARD 104001 (kernel geometry)
*      kerndia(e-6 m)  kernvar(e-6 m)
104001      426.7      8.8
* CARD 104002 (buffer geometry)
*      buffthk(e-6 m) buffvar(e-6 m)
104002      98.9      8.4
* CARD 104003 (IPyC geometry)
*      ipycthk(e-6 m)  ipycvar(e-6 m)
104003      40.4      2.5
* CARD 104004 (SiC geometry)
*      sicthk(e-6 m)   sicvar(e-6 m)
104004      35.2      1.2
* CARD 104005 (OPyC geometry)
*      opycthk(e-6 m)  opycvar(e-6 m)
104005      43.4      2.9
*
***** FUEL ELEMENT DESCRIPTION *****
* CARD 105001 (Plane Geometry w/modified Inputs for a Capsule)
105001  PLANEGEOM
* CARD 105011 (Planegeom)
*      partnum(particles/capsule)  ngngfm  ngng
105011      38052.      3      6
* CARD 105021 (Planegeom)
*      fmthk(m)  cldthk(m)
105021      1.      1.
* CARD 105031 (Planegeom)
*      fmden(g/cm^3) [1.70]
*105031
* CARD 105041 (Planegeom)
*      ucontam
105041      9.74E-6
*
***** FUEL ELEMENT ENVIRONMENT *****
* CARD 106001 (fuel temperature option)
*      rtmpopt
106001  VOLAVGTMP
* CARD 106021 (global node temperatures)
*      tgi(k)  ntgi  {not required with VOLAVGTMP option}
*106021
* CARD 201001 (fission product transport description)
*      fpspecie  {diffusion not modeled}
*201001
*
* CARD SERIES 301XXX (fluence v- time input)
*      timeirr(days)  flu(e25 n/m^2)
301001      0.      0.0000
301002      50.     0.2788
301003      100.    0.5629
301004      150.    0.8529
301005      200.    1.1471
301006      250.    1.4483
301007      300.    1.7538
301008      350.    2.0596
301009      400.    2.3596
301010      450.    2.6575
301011      500.    2.9483
301012      550.    3.2375
301013      600.    3.5217
```

Title: AGR-2 Pre-Test Prediction Analyses using the PARFUME Code for U.S. Fuel Particles

ECAR No.: 1020

ECAR Rev. No.: 2

Project File No.: 23841

Date: 05/29/2012

```
*
*
* CARD SERIES 302XXX (burnup v- fluence input)
*      flu(e25 n/m^2)  bup(%fima)
302001      0.0000      0.000
302002      0.2788      0.660
302003      0.5629      1.434
302004      0.8529      2.344
302005      1.1471      3.398
302006      1.4483      4.583
302007      1.7538      5.845
302008      2.0596      7.084
302009      2.3596      8.230
302010      2.6575      9.260
302011      2.9483      10.175
302012      3.2375      10.985
302013      3.5217      11.707
*
*
* CARD SERIES 303XXX (external pressure v- fluence input)
*      external pressure v- fluence input
*      flu(e25 n/m^2)  pamb(MPa)
303001      0.          .1
*
* CARD SERIES 304XXX (boundary temperature v- fluence input)
*      flu(e25 n/m^2)  btemp(k)
304001      0.0000      1348.
304002      0.2788      1348.
304003      0.5629      1348.
304004      0.8529      1348.
304005      1.1471      1348.
304006      1.4483      1348.
304007      1.7538      1348.
304008      2.0596      1348.
304009      2.3596      1348.
304010      2.6575      1348.
304011      2.9483      1348.
304012      3.2375      1348.
304013      3.5217      1348.
*
* CARD SERIES 306XXX (time heatup starts and irradiation ends)
*      thus(days) [1xe6] {casualty condition not modeled}
*306001
*
***** CORRELATION COEFFICIENTS *****
* CARD SERIES 401XXX (correlation coefficients for ipyc cracking)
*      sigcr0(MPa)  umc(MPa)
401001      1084.657  163.600
*      c1c          c2c
401002      0.0000      0.0000      * for fuel particle radial posit
401003      0.0000      0.0000      * for kernel diameter
401004      0.0000      0.0000      * for buffer thickness
401005      1.792787E-02  6.839354E-05 * for ipyc thickness
401006      9.592446E-03  4.173933E-04 * for sic thickness
401007      -1.713905E-02  3.496627E-04 * for opyc thickness
401008      0.0000      0.0000      * for ipyc density
401009      0.0000      0.0000      * for opyc density
401010      0.0000      0.0000      * for ipyc baf
401011      0.0000      0.0000      * for opyc baf
401012      0.0000      0.0000      * for creep coeff amplication
*
* CARD SERIES 402XXX (correlation coefficients for ipyc asphericity)
*      sigma0(MPa)  um(MPa)  delum(MPa)  aration  aratvar
402001      1045.565  417.700  368.520  1.052  0.013
```

Title: AGR-2 Pre-Test Prediction Analyses using the PARFUME Code for U.S. Fuel Particles

ECAR No.: 1020

ECAR Rev. No.: 2

Project File No.: 23841

Date: 05/29/2012

*	c1a	c2a	d1a	d2a	
402002	0.0000	0.0000	0.0000	0.0000	* fuel part rad pos
402003	0.0000	0.0000	0.0000	0.0000	* for kernel diamet
402004	0.0000	0.0000	0.0000	0.0000	* for buffer thickn
402005	3.313294E-03	1.822319E-05	-2.092338E-04	2.635363E-05	*i thickn
402006	-3.290799E-03	-8.735825E-05	-3.518463E-03	-1.847821E-04	*s thickn
402007	2.840243E-03	-1.508929E-05	1.843376E-03	-7.729046E-06	*o thickn
402008	0.0000	0.0000	0.0000	0.0000	* for ipyc density
402009	0.0000	0.0000	0.0000	0.0000	* for opyc density
402010	0.0000	0.0000	0.0000	0.0000	* for ipyc baf
402011	0.0000	0.0000	0.0000	0.0000	* for opyc baf
402012	0.0000	0.0000	0.0000	0.0000	* for creep coef
402013	4.297799E+00	-6.432275E+01	6.208822E+00	-7.134126E+01	* aspheri

*
* CARD SERIES 403XXX (correlation coefficients for ipyc debonding)
* sigd0 (MPa) umd(MPa) bond0 (MPa) bond0var (MPa)
403001 100. 100. 100. 0.
* c1d c2d
403002 0.0000 0.0000 * for fuel particle radial posit
403003 0.0000 0.0000 * for kernel diameter
403004 0.0000 0.0000 * for buffer thickness
403005 0.0000 0.0000 * for ipyc thickness
403006 0.0000 0.0000 * for sic thickness
403007 0.0000 0.0000 * for opyc thickness
403008 0.0000 0.0000 * for ipyc density
403009 0.0000 0.0000 * for opyc density
403010 0.0000 0.0000 * for ipyc baf
403011 0.0000 0.0000 * for opyc baf
403012 0.0000 0.0000 * for creep coeff amplication
403013 0.0000 0.0000 * for asphericity effects

*
*
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Title: AGR-2 Pre-Test Prediction Analyses using the PARFUME Code for U.S. Fuel Particles

ECAR No.: 1020

ECAR Rev. No.: 2

Project File No.: 23841

Date: 05/29/2012

AGR-2 Capsule-5 UCO Low Temperature Run

```
*
*PARFUME V2.18 Input Data Deck: ECAR-1020R1
*
* Note: default values in brackets [default]
*
#####
***** GENERAL OPTIONS (SOLVERS/MODELS) *****
* CARD 100001 (simulation name)
*   title
100001   'AGR-2 Capsule-5 UCO Low Temp Run ECAR-1020R1'
*
* CARD 101001 (run parameters)
*   pfss      ncases      nburp      sample      dtf [0]      izeed [305]
101001      2          100          100          1
*
* CARD 101002 (models)
*   idebondp   ifacet   rbvalue   comodel   fgmodel   idebug
101002      1          1          12          3          2          0
*
***** MATERIAL PROPERTIES *****
* CARD 102001 (fuel characteristics)
*   u235enr(wt%)  ourat  curat
102001      14.03    1.43  0.39
*
* CARD 103001 (kernel properties)
*   kernd(g/cm^3) kernt(g/cm^3) [11.030]
103001      10.97
*
* CARD 103002 (buffer properties)
*   buffd(g/cm^3) bufft(g/cm^3) [2.250]
103002      1.04
*
* CARD 103003 (IPyC properties)
*   ipycdn(g/cm^3) ipycdvar(g/cm^3)
103003      1.89      0.010
*
* CARD 103005 (OPyC properties)
*   opycdn(g/cm^3) opycdvar(g/cm^3)
103005      1.91      0.010
*
* CARD 103013 (IPyC Bacon anisotropic factor)
*   ibafn  ibafvar
103013   1.047  0.005
*
* CARD 103015 (OPyC Bacon anisotropic factor)
*   obafn  obafvar
103015   1.043  0.002
*
* CARD 103023 (IPyC Weibull modulus)
*   ipycm [9.50]
*103023
*
* CARD 103024 (SiC Weibull modulus)
*   sigm [6.00]
*103024
*
* CARD 103025 (OPyC Weibull modulus)
*   opycm [9.50]
*103025
*
* CARD 103033 (Poisson's ratio)
*   cnu [0.500]  cnub [0.500]
*103033
*
* CARD 103043 (creep amplification factor)
*   creepampn [2.0]  creepvar [0.00]
*103043
*
* CARD 103054 (Enable ZrC)
*   zrc [0]  zrcp [1]
```


Title: AGR-2 Pre-Test Prediction Analyses using the PARFUME Code for U.S. Fuel Particles

ECAR No.: 1020

ECAR Rev. No.: 2

Project File No.: 23841

Date: 05/29/2012

```
*103054
*
* CARD 103061 (defective SiC layers)
*      fdef [0.00]
*103061
*
***** FUEL PARTICLE GEOMETRY *****
* CARD 104001 (kernel geometry)
*      kerndia(e-6 m)  kernvar(e-6 m)
104001      426.7      8.8
* CARD 104002 (buffer geometry)
*      buffthk(e-6 m) buffvar(e-6 m)
104002      98.9      8.4
* CARD 104003 (IPyC geometry)
*      ipycthk(e-6 m)  ipycvar(e-6 m)
104003      40.4      2.5
* CARD 104004 (SiC geometry)
*      sicthk(e-6 m)   sicvar(e-6 m)
104004      35.2      1.2
* CARD 104005 (OPyC geometry)
*      opycthk(e-6 m)  opycvar(e-6 m)
104005      43.4      2.9
*
***** FUEL ELEMENT DESCRIPTION *****
* CARD 105001 (Plane Geometry w/modified Inputs for a Capsule)
105001  PLANEGEOM
* CARD 105011 (Planegeom)
*      partnum(particles/capsule)  ngngfm  ngngn
105011      38052.      3      6
* CARD 105021 (Planegeom)
*      fmthk(m)  cldthk(m)
105021      1.      1.
* CARD 105031 (Planegeom)
*      fmden(g/cm^3) [1.70]
*105031
* CARD 105041 (Planegeom)
*      ucontam
105041      9.74E-6
*
***** FUEL ELEMENT ENVIRONMENT *****
* CARD 106001 (fuel temperature option)
*      rtmpopt
106001  VOLAVGTMP
* CARD 106021 (global node temperatures)
*      tgi(k)  ntgi  {not required with VOLAVGTMP option}
*106021
* CARD 201001 (fission product transport description)
*      fpspecie  {diffusion not modeled}
*201001
*
* CARD SERIES 301XXX (fluence v- time input)
*      timeirr(days)  flu(e25 n/m^2)
301001      0.      0.0000
301002      50.      0.2788
301003      100.     0.5629
301004      150.     0.8529
301005      200.     1.1471
301006      250.     1.4483
301007      300.     1.7538
301008      350.     2.0596
301009      400.     2.3596
301010      450.     2.6575
301011      500.     2.9483
301012      550.     3.2375
301013      600.     3.5217
```

Title: AGR-2 Pre-Test Prediction Analyses using the PARFUME Code for U.S. Fuel Particles

ECAR No.: 1020

ECAR Rev. No.: 2

Project File No.: 23841

Date: 05/29/2012

```
*
*
* CARD SERIES 302XXX (burnup v- fluence input)
*      flu(e25 n/m^2)  bup(%fima)
302001      0.0000      0.000
302002      0.2788      0.660
302003      0.5629      1.434
302004      0.8529      2.344
302005      1.1471      3.398
302006      1.4483      4.583
302007      1.7538      5.845
302008      2.0596      7.084
302009      2.3596      8.230
302010      2.6575      9.260
302011      2.9483      10.175
302012      3.2375      10.985
302013      3.5217      11.707
*
*
* CARD SERIES 303XXX (external pressure v- fluence input)
*      external pressure v- fluence input
*      flu(e25 n/m^2)  pamb(MPa)
303001      0.          .1
*
* CARD SERIES 304XXX (boundary temperature v- fluence input)
*      flu(e25 n/m^2)  btemp(k)
304001      0.0000      1183.
304002      0.2788      1183.
304003      0.5629      1183.
304004      0.8529      1183.
304005      1.1471      1183.
304006      1.4483      1183.
304007      1.7538      1183.
304008      2.0596      1183.
304009      2.3596      1183.
304010      2.6575      1183.
304011      2.9483      1183.
304012      3.2375      1183.
304013      3.5217      1183.
*
* CARD SERIES 306XXX (time heatup starts and irradiation ends)
*      thus(days) [1xe6] {casualty condition not modeled}
*306001
*
***** CORRELATION COEFFICIENTS *****
* CARD SERIES 401XXX (correlation coefficients for ipyc cracking)
*      sigcr0 (MPa)  umc (MPa)
401001      1084.836  227.800
*      c1c          c2c
401002      0.0000      0.0000      * for fuel particle radial posit
401003      0.0000      0.0000      * for kernel diameter
401004      0.0000      0.0000      * for buffer thickness
401005      1.748115E-02  7.905532E-05  * for ipyc thickness
401006      1.056436E-02  3.787174E-04  * for sic thickness
401007      -1.705455E-02  3.599254E-04  * for opyc thickness
401008      0.0000      0.0000      * for ipyc density
401009      0.0000      0.0000      * for opyc density
401010      0.0000      0.0000      * for ipyc baf
401011      0.0000      0.0000      * for opyc baf
401012      0.0000      0.0000      * for creep coeff amplication
*
* CARD SERIES 402XXX (correlation coefficients for ipyc asphericity)
*      siga0 (MPa)  um (MPa)  delum (MPa)  aration  aratvar
402001      893.755  577.200  426.000  1.052  0.013
```

Title: AGR-2 Pre-Test Prediction Analyses using the PARFUME Code for U.S. Fuel Particles

ECAR No.: 1020

ECAR Rev. No.: 2

Project File No.: 23841

Date: 05/29/2012

*	c1a	c2a	d1a	d2a	
402002	0.0000	0.0000	0.0000	0.0000	* fuel part rad pos
402003	0.0000	0.0000	0.0000	0.0000	* for kernel diamet
402004	0.0000	0.0000	0.0000	0.0000	* for buffer thickn
402005	2.982834E-03	1.820084E-05	3.821455E-05	5.454756E-06	*i thickn
402006	-2.504567E-03	-1.220444E-04	2.383922E-03	-4.571265E-04	*s thickn
402007	2.487598E-03	-1.533423E-05	1.095189E-03	-2.047932E-05	*o thickn
402008	0.0000	0.0000	0.0000	0.0000	* for ipyc density
402009	0.0000	0.0000	0.0000	0.0000	* for opyc density
402010	0.0000	0.0000	0.0000	0.0000	* for ipyc baf
402011	0.0000	0.0000	0.0000	0.0000	* for opyc baf
402012	0.0000	0.0000	0.0000	0.0000	* for creep coef
402013	4.179657E+00	-6.320683E+01	4.579717E+00	-6.923318E+01	* aspheri

*
* CARD SERIES 403XXX (correlation coefficients for ipyc debonding)
* sigd0 (MPa) umd(MPa) bond0 (MPa) bond0var (MPa)
403001 100. 100. 100. 0.
* c1d c2d
403002 0.0000 0.0000 * for fuel particle radial posit
403003 0.0000 0.0000 * for kernel diameter
403004 0.0000 0.0000 * for buffer thickness
403005 0.0000 0.0000 * for ipyc thickness
403006 0.0000 0.0000 * for sic thickness
403007 0.0000 0.0000 * for opyc thickness
403008 0.0000 0.0000 * for ipyc density
403009 0.0000 0.0000 * for opyc density
403010 0.0000 0.0000 * for ipyc baf
403011 0.0000 0.0000 * for opyc baf
403012 0.0000 0.0000 * for creep coeff amplication
403013 0.0000 0.0000 * for asphericity effects

*
*
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Title: AGR-2 Pre-Test Prediction Analyses using the PARFUME Code for U.S. Fuel Particles

ECAR No.: 1020

ECAR Rev. No.: 2

Project File No.: 23841

Date: 05/29/2012

AGR-2 Capsule-6 UCO High Temperature Run

```
*
*PARFUME V2.18 Input Data Deck: ECAR-1020R1
*
* Note: default values in brackets [default]
*
#####
***** GENERAL OPTIONS (SOLVERS/MODELS) *****
* CARD 100001 (simulation name)
*      title
100001  'AGR-2 Capsule-6 UCO High Temp Run ECAR-1020R1'
*
* CARD 101001 (run parameters)
*      pfss      ncases      nburp      sample      dtf [0]      izeed [305]
101001      2        100        100        1
*
* CARD 101002 (models)
*      idebondp      ifacet      rbvalue      comodel      fgmodel      idebug
101002      1        1        12        3        2        0
*
***** MATERIAL PROPERTIES *****
* CARD 102001 (fuel characteristics)
*      u235enr(wt%)      ourat      curat
102001      14.03      1.43      0.39
*
* CARD 103001 (kernel properties)
*      kernd(g/cm^3)      kernt(g/cm^3) [11.030]
103001      10.97
*
* CARD 103002 (buffer properties)
*      buffd(g/cm^3)      bufft(g/cm^3) [2.250]
103002      1.04
*
* CARD 103003 (IPyC properties)
*      ipycdn(g/cm^3)      ipycdvar(g/cm^3)
103003      1.89      0.010
*
* CARD 103005 (OPyC properties)
*      opycdn(g/cm^3)      opycdvar(g/cm^3)
103005      1.91      0.010
*
* CARD 103013 (IPyC Bacon anisotropic factor)
*      ibafn      ibafvar
103013      1.047      0.005
*
* CARD 103015 (OPyC Bacon anisotropic factor)
*      obafn      obafvar
103015      1.043      0.002
*
* CARD 103023 (IPyC Weibull modulus)
*      ipycm [9.50]
*103023
*
* CARD 103024 (SiC Weibull modulus)
*      sigm [6.00]
*103024
*
* CARD 103025 (OPyC Weibull modulus)
*      opycm [9.50]
*103025
*
* CARD 103033 (Poisson's ratio)
*      cnu [0.500]      cnub [0.500]
*103033
*
* CARD 103043 (creep amplification factor)
*      creepampn [2.0]      creepvar [0.00]
*103043
*
* CARD 103054 (Enable ZrC)
*      zrc [0]      zrcp [1]
```

Title: AGR-2 Pre-Test Prediction Analyses using the PARFUME Code for U.S. Fuel Particles

ECAR No.: 1020

ECAR Rev. No.: 2

Project File No.: 23841

Date: 05/29/2012

```
*103054
*
* CARD 103061 (defective SiC layers)
*      fdef [0.00]
*103061
*
***** FUEL PARTICLE GEOMETRY *****
* CARD 104001 (kernel geometry)
*      kerndia(e-6 m)  kernvar(e-6 m)
104001      426.7      8.8
* CARD 104002 (buffer geometry)
*      buffthk(e-6 m)  buffvar(e-6 m)
104002      98.9      8.4
* CARD 104003 (IPyC geometry)
*      ipycthk(e-6 m)  ipycvar(e-6 m)
104003      40.4      2.5
* CARD 104004 (SiC geometry)
*      sicthk(e-6 m)   sicvar(e-6 m)
104004      35.2      1.2
* CARD 104005 (OPyC geometry)
*      opycthk(e-6 m)  opycvar(e-6 m)
104005      43.4      2.9
*
***** FUEL ELEMENT DESCRIPTION *****
* CARD 105001 (Plane Geometry w/modified Inputs for a Capsule)
105001  PLANEGEOM
* CARD 105011 (Planegeom)
*      partnum(particles/capsule)  ngngfm  ngngn
105011      38052.      3      6
* CARD 105021 (Planegeom)
*      fmthk(m)  cldthk(m)
105021      1.      1.
* CARD 105031 (Planegeom)
*      fmden(g/cm^3) [1.70]
*105031
* CARD 105041 (Planegeom)
*      ucontam
105041      9.74E-6
*
***** FUEL ELEMENT ENVIRONMENT *****
* CARD 106001 (fuel temperature option)
*      rtmpopt
106001  VOLAVGTMP
* CARD 106021 (global node temperatures)
*      tgi(k)  ntgi  {not required with VOLAVGTMP option}
*106021
* CARD 201001 (fission product transport description)
*      fpspecie  {diffusion not modeled}
*201001
*
* CARD SERIES 301XXX (fluence v- time input)
*      timeirr(days)  flu(e25 n/m^2)
301001      0.      0.0000
301002      50.     0.2088
301003      100.    0.4188
301004      150.    0.6317
301005      200.    0.8508
301006      250.    1.0717
301007      300.    1.2975
301008      350.    1.5238
301009      400.    1.7488
301010      450.    1.9725
301011      500.    2.1938
301012      550.    2.4121
301013      600.    2.6279
```

Title: AGR-2 Pre-Test Prediction Analyses using the PARFUME Code for U.S. Fuel Particles

ECAR No.: 1020

ECAR Rev. No.: 2

Project File No.: 23841

Date: 05/29/2012

```
*
*
* CARD SERIES 302XXX (burnup v- fluence input)
*      flu(e25 n/m^2)  bup(%fima)
302001      0.0000      0.000
302002      0.2088      0.543
302003      0.4188      1.157
302004      0.6317      1.846
302005      0.8508      2.621
302006      1.0717      3.475
302007      1.2975      4.392
302008      1.5238      5.338
302009      1.7488      6.273
302010      1.9725      7.163
302011      2.1938      7.991
302012      2.4121      8.751
302013      2.6279      9.448
*
*
* CARD SERIES 303XXX (external pressure v- fluence input)
*      external pressure v- fluence input
*      flu(e25 n/m^2)  pamb(MPa)
303001      0.          .1
*
* CARD SERIES 304XXX (boundary temperature v- fluence input)
*      flu(e25 n/m^2)  btemp(k)
304001      0.0000      1513.
304002      0.2088      1513.
304003      0.4188      1513.
304004      0.6317      1513.
304005      0.8508      1513.
304006      1.0717      1513.
304007      1.2975      1513.
304008      1.5238      1513.
304009      1.7488      1513.
304010      1.9725      1513.
304011      2.1938      1513.
304012      2.4121      1513.
304013      2.6279      1513.
*
* CARD SERIES 306XXX (time heatup starts and irradiation ends)
*      thus(days) [1xe6] {casualty condition not modeled}
*306001
*
***** CORRELATION COEFFICIENTS *****
* CARD SERIES 401XXX (correlation coefficients for ipyc cracking)
*      sigcr0(MPa)  umc(MPa)
401001      1084.497  134.700
*      c1c          c2c
401002      0.0000      0.0000      * for fuel particle radial posit
401003      0.0000      0.0000      * for kernel diameter
401004      0.0000      0.0000      * for buffer thickness
401005      1.831418E-02  7.728953E-05  * for ipyc thickness
401006      8.879602E-03  4.834873E-04  * for sic thickness
401007      -1.738158E-02  3.570677E-04  * for opyc thickness
401008      0.0000      0.0000      * for ipyc density
401009      0.0000      0.0000      * for opyc density
401010      0.0000      0.0000      * for ipyc baf
401011      0.0000      0.0000      * for opyc baf
401012      0.0000      0.0000      * for creep coeff amplication
*
* CARD SERIES 402XXX (correlation coefficients for ipyc asphericity)
*      siga0(MPa)  um(MPa)  delum(MPa)  aration  aratvar
402001      1036.626  342.500  283.810  1.052  0.013
```

Title: AGR-2 Pre-Test Prediction Analyses using the PARFUME Code for U.S. Fuel Particles

ECAR No.: 1020

ECAR Rev. No.: 2

Project File No.: 23841

Date: 05/29/2012

*	c1a	c2a	d1a	d2a	
402002	0.0000	0.0000	0.0000	0.0000	* fuel part rad pos
402003	0.0000	0.0000	0.0000	0.0000	* for kernel diamet
402004	0.0000	0.0000	0.0000	0.0000	* for buffer thickn
402005	3.561257E-03	2.092030E-05	-2.147374E-03	2.422649E-05	*i thickn
402006	-3.329320E-03	-7.303824E-05	-3.775883E-03	-1.898783E-04	*s thickn
402007	2.952390E-03	-1.217471E-05	7.647073E-04	2.386514E-06	*o thickn
402008	0.0000	0.0000	0.0000	0.0000	* for ipyc density
402009	0.0000	0.0000	0.0000	0.0000	* for opyc density
402010	0.0000	0.0000	0.0000	0.0000	* for ipyc baf
402011	0.0000	0.0000	0.0000	0.0000	* for opyc baf
402012	0.0000	0.0000	0.0000	0.0000	* for creep coef
402013	4.219536E+00	-6.408457E+01	6.782702E+00	-6.635200E+01	* aspheri

*
* CARD SERIES 403XXX (correlation coefficients for ipyc debonding)
* sigd0 (MPa) umd(MPa) bond0 (MPa) bond0var (MPa)
403001 100. 100. 100. 0.
* c1d c2d
403002 0.0000 0.0000 * for fuel particle radial posit
403003 0.0000 0.0000 * for kernel diameter
403004 0.0000 0.0000 * for buffer thickness
403005 0.0000 0.0000 * for ipyc thickness
403006 0.0000 0.0000 * for sic thickness
403007 0.0000 0.0000 * for opyc thickness
403008 0.0000 0.0000 * for ipyc density
403009 0.0000 0.0000 * for opyc density
403010 0.0000 0.0000 * for ipyc baf
403011 0.0000 0.0000 * for opyc baf
403012 0.0000 0.0000 * for creep coeff amplication
403013 0.0000 0.0000 * for asphericity effects
*
*
.

Title: AGR-2 Pre-Test Prediction Analyses using the PARFUME Code for U.S. Fuel Particles

ECAR No.: 1020

ECAR Rev. No.: 2

Project File No.: 23841

Date: 05/29/2012

AGR-2 Capsule-6 UCO Volume Average Temperature Run

```
*
*PARFUME V2.18 Input Data Deck: ECAR-1020R1
*
* Note: default values in brackets [default]
*
#####
***** GENERAL OPTIONS (SOLVERS/MODELS) *****
* CARD 100001 (simulation name)
*      title
100001   'AGR-2 Capsule-6 UCO Volume Average Temp Run ECAR-1020R1'
*
* CARD 101001 (run parameters)
*      pfss      ncases      nburp      sample      dtf [0]      izeed [305]
101001      2      100      100      1
*
* CARD 101002 (models)
*      idebondp      ifacet      rbvalue      comodel      fgmodel      idebug
101002      1      1      12      3      2      0
*
***** MATERIAL PROPERTIES *****
* CARD 102001 (fuel characteristics)
*      u235enr(wt%)      ourat      curat
102001      14.03      1.43      0.39
*
* CARD 103001 (kernel properties)
*      kernd(g/cm^3)      kernt(g/cm^3) [11.030]
103001      10.97
*
* CARD 103002 (buffer properties)
*      buffd(g/cm^3)      bufft(g/cm^3) [2.250]
103002      1.04
*
* CARD 103003 (IPyC properties)
*      ipycdn(g/cm^3)      ipycdvar(g/cm^3)
103003      1.89      0.010
*
* CARD 103005 (OPyC properties)
*      opycdn(g/cm^3)      opycdvar(g/cm^3)
103005      1.91      0.010
*
* CARD 103013 (IPyC Bacon anisotropic factor)
*      ibafn      ibafvar
103013      1.047      0.005
*
* CARD 103015 (OPyC Bacon anisotropic factor)
*      obafn      obafvar
103015      1.043      0.002
*
* CARD 103023 (IPyC Weibull modulus)
*      ipycm [9.50]
*103023
*
* CARD 103024 (SiC Weibull modulus)
*      sigm [6.00]
*103024
*
* CARD 103025 (OPyC Weibull modulus)
*      opycm [9.50]
*103025
*
* CARD 103033 (Poisson's ratio)
*      cnu [0.500]      cnuv [0.500]
*103033
*
* CARD 103043 (creep amplification factor)
*      creepampn [2.0]      creepvar [0.00]
*103043
*
* CARD 103054 (Enable ZrC)
*      zrc [0]      zrcp [1]
```


Title: AGR-2 Pre-Test Prediction Analyses using the PARFUME Code for U.S. Fuel Particles

ECAR No.: 1020

ECAR Rev. No.: 2

Project File No.: 23841

Date: 05/29/2012

```
*103054
*
* CARD 103061 (defective SiC layers)
*      fdef [0.00]
*103061
*
***** FUEL PARTICLE GEOMETRY *****
* CARD 104001 (kernel geometry)
*      kerndia(e-6 m)  kernvar(e-6 m)
104001      426.7      8.8
* CARD 104002 (buffer geometry)
*      buffthk(e-6 m)  buffvar(e-6 m)
104002      98.9      8.4
* CARD 104003 (IPyC geometry)
*      ipycthk(e-6 m)  ipycvar(e-6 m)
104003      40.4      2.5
* CARD 104004 (SiC geometry)
*      sicthk(e-6 m)   sicvar(e-6 m)
104004      35.2      1.2
* CARD 104005 (OPyC geometry)
*      opycthk(e-6 m)  opycvar(e-6 m)
104005      43.4      2.9
*
***** FUEL ELEMENT DESCRIPTION *****
* CARD 105001 (Plane Geometry w/modified Inputs for a Capsule)
105001  PLANEGEOM
* CARD 105011 (Planegeom)
*      partnum(particles/capsule)  ngngfm  ngngn
105011      38052.      3      6
* CARD 105021 (Planegeom)
*      fmthk(m)  cldthk(m)
105021      1.      1.
* CARD 105031 (Planegeom)
*      fmden(g/cm^3) [1.70]
*105031
* CARD 105041 (Planegeom)
*      ucontam
105041      9.74E-6
*
***** FUEL ELEMENT ENVIRONMENT *****
* CARD 106001 (fuel temperature option)
*      rtmpopt
106001  VOLAVGTMP
* CARD 106021 (global node temperatures)
*      tgi(k)  ntgi {not required with VOLAVGTMP option}
*106021
* CARD 201001 (fission product transport description)
*      fpspecie {diffusion not modeled}
*201001
*
* CARD SERIES 301XXX (fluence v- time input)
*      timeirr(days)  flu(e25 n/m^2)
301001      0.      0.0000
301002      50.     0.2088
301003     100.     0.4188
301004     150.     0.6317
301005     200.     0.8508
301006     250.     1.0717
301007     300.     1.2975
301008     350.     1.5238
301009     400.     1.7488
301010     450.     1.9725
301011     500.     2.1938
301012     550.     2.4121
301013     600.     2.6279
```

Title: AGR-2 Pre-Test Prediction Analyses using the PARFUME Code for U.S. Fuel Particles

ECAR No.: 1020

ECAR Rev. No.: 2

Project File No.: 23841

Date: 05/29/2012

```
*
*
* CARD SERIES 302XXX (burnup v- fluence input)
*      flu(e25 n/m^2)  bup(%fima)
302001      0.0000      0.000
302002      0.2088      0.543
302003      0.4188      1.157
302004      0.6317      1.846
302005      0.8508      2.621
302006      1.0717      3.475
302007      1.2975      4.392
302008      1.5238      5.338
302009      1.7488      6.273
302010      1.9725      7.163
302011      2.1938      7.991
302012      2.4121      8.751
302013      2.6279      9.448
*
*
* CARD SERIES 303XXX (external pressure v- fluence input)
*      external pressure v- fluence input
*      flu(e25 n/m^2)  pamb(MPa)
303001      0.          .1
*
* CARD SERIES 304XXX (boundary temperature v- fluence input)
*      flu(e25 n/m^2)  btemp(k)
304001      0.0000      1348.
304002      0.2088      1348.
304003      0.4188      1348.
304004      0.6317      1348.
304005      0.8508      1348.
304006      1.0717      1348.
304007      1.2975      1348.
304008      1.5238      1348.
304009      1.7488      1348.
304010      1.9725      1348.
304011      2.1938      1348.
304012      2.4121      1348.
304013      2.6279      1348.
*
* CARD SERIES 306XXX (time heatup starts and irradiation ends)
*      thus(days) [1xe6] {casualty condition not modeled}
*306001
*
***** CORRELATION COEFFICIENTS *****
* CARD SERIES 401XXX (correlation coefficients for ipyc cracking)
*      sigcr0 (MPa)  umc (MPa)
401001      1084.442  172.800
*      c1c          c2c
401002      0.0000      0.0000      * for fuel particle radial posit
401003      0.0000      0.0000      * for kernel diameter
401004      0.0000      0.0000      * for buffer thickness
401005      1.781578E-02  6.692670E-05  * for ipyc thickness
401006      9.678373E-03  4.192522E-04  * for sic thickness
401007      -1.710510E-02  3.508637E-04  * for opyc thickness
401008      0.0000      0.0000      * for ipyc density
401009      0.0000      0.0000      * for opyc density
401010      0.0000      0.0000      * for ipyc baf
401011      0.0000      0.0000      * for opyc baf
401012      0.0000      0.0000      * for creep coeff amplication
*
* CARD SERIES 402XXX (correlation coefficients for ipyc asphericity)
*      siga0 (MPa)  um (MPa)  delum (MPa)  aration  aratvar
402001      890.769  439.800  280.400  1.052  0.013
```

Title: AGR-2 Pre-Test Prediction Analyses using the PARFUME Code for U.S. Fuel Particles

ECAR No.: 1020

ECAR Rev. No.: 2

Project File No.: 23841

Date: 05/29/2012

*	c1a	c2a	d1a	d2a	
402002	0.0000	0.0000	0.0000	0.0000	* fuel part rad pos
402003	0.0000	0.0000	0.0000	0.0000	* for kernel diamet
402004	0.0000	0.0000	0.0000	0.0000	* for buffer thickn
402005	3.238029E-03	1.688674E-05	-1.955256E-03	1.050904E-05	*i thickn
402006	-3.128481E-03	-9.770710E-05	2.321729E-03	-4.616192E-04	*s thickn
402007	2.795386E-03	-1.585297E-05	4.777418E-04	-1.277588E-05	*o thickn
402008	0.0000	0.0000	0.0000	0.0000	* for ipyc density
402009	0.0000	0.0000	0.0000	0.0000	* for opyc density
402010	0.0000	0.0000	0.0000	0.0000	* for ipyc baf
402011	0.0000	0.0000	0.0000	0.0000	* for opyc baf
402012	0.0000	0.0000	0.0000	0.0000	* for creep coef
402013	4.280787E+00	-6.449609E+01	4.989434E+00	-6.627525E+01	* aspheri

*
* CARD SERIES 403XXX (correlation coefficients for ipyc debonding)
* sigd0 (MPa) umd(MPa) bond0 (MPa) bond0var (MPa)
403001 100. 100. 100. 0.
* c1d c2d
403002 0.0000 0.0000 * for fuel particle radial posit
403003 0.0000 0.0000 * for kernel diameter
403004 0.0000 0.0000 * for buffer thickness
403005 0.0000 0.0000 * for ipyc thickness
403006 0.0000 0.0000 * for sic thickness
403007 0.0000 0.0000 * for opyc thickness
403008 0.0000 0.0000 * for ipyc density
403009 0.0000 0.0000 * for opyc density
403010 0.0000 0.0000 * for ipyc baf
403011 0.0000 0.0000 * for opyc baf
403012 0.0000 0.0000 * for creep coeff amplication
403013 0.0000 0.0000 * for asphericity effects

*
*
.

Title: AGR-2 Pre-Test Prediction Analyses using the PARFUME Code for U.S. Fuel Particles

ECAR No.: 1020

ECAR Rev. No.: 2

Project File No.: 23841

Date: 05/29/2012

AGR-2 Capsule-6 UCO Low Temperature Run

```
*
*PARFUME V2.18 Input Data Deck: ECAR-1020R1
*
* Note: default values in brackets [default]
*
#####
***** GENERAL OPTIONS (SOLVERS/MODELS) *****
* CARD 100001 (simulation name)
*   title
100001   'AGR-2 Capsule-6 UCO Low Temp Run ECAR-1020R1'
*
* CARD 101001 (run parameters)
*   pfss      ncases      nburp      sample      dtf [0]      izeed [305]
101001      2          100          100          1
*
* CARD 101002 (models)
*   idebondp   ifacet   rbvalue   comodel   fgmodel   idebug
101002      1          1          12          3          2          0
*
***** MATERIAL PROPERTIES *****
* CARD 102001 (fuel characteristics)
*   u235enr(wt%)  ourat  curat
102001      14.03    1.43   0.39
*
* CARD 103001 (kernel properties)
*   kernd(g/cm^3) kernt(g/cm^3) [11.030]
103001      10.97
*
* CARD 103002 (buffer properties)
*   buffd(g/cm^3) bufft(g/cm^3) [2.250]
103002      1.04
*
* CARD 103003 (IPyC properties)
*   ipycdn(g/cm^3) ipycdvar(g/cm^3)
103003      1.89      0.010
*
* CARD 103005 (OPyC properties)
*   opycdn(g/cm^3) opycdvar(g/cm^3)
103005      1.91      0.010
*
* CARD 103013 (IPyC Bacon anisotropic factor)
*   ibafn  ibafvar
103013   1.047  0.005
*
* CARD 103015 (OPyC Bacon anisotropic factor)
*   obafn  obafvar
103015   1.043  0.002
*
* CARD 103023 (IPyC Weibull modulus)
*   ipycm [9.50]
*103023
*
* CARD 103024 (SiC Weibull modulus)
*   sigm [6.00]
*103024
*
* CARD 103025 (OPyC Weibull modulus)
*   opycm [9.50]
*103025
*
* CARD 103033 (Poisson's ratio)
*   cnu [0.500]  cnub [0.500]
*103033
*
* CARD 103043 (creep amplification factor)
*   creepampn [2.0]  creepvar [0.00]
*103043
*
* CARD 103054 (Enable ZrC)
*   zrc [0]  zrcp [1]
```

Title: AGR-2 Pre-Test Prediction Analyses using the PARFUME Code for U.S. Fuel Particles

ECAR No.: 1020

ECAR Rev. No.: 2

Project File No.: 23841

Date: 05/29/2012

```
*103054
*
* CARD 103061 (defective SiC layers)
*      fdef [0.00]
*103061
*
***** FUEL PARTICLE GEOMETRY *****
* CARD 104001 (kernel geometry)
*      kerndia(e-6 m)  kernvar(e-6 m)
104001      426.7      8.8
* CARD 104002 (buffer geometry)
*      buffthk(e-6 m)  buffvar(e-6 m)
104002      98.9      8.4
* CARD 104003 (IPyC geometry)
*      ipycthk(e-6 m)  ipycvar(e-6 m)
104003      40.4      2.5
* CARD 104004 (SiC geometry)
*      sicthk(e-6 m)   sicvar(e-6 m)
104004      35.2      1.2
* CARD 104005 (OPyC geometry)
*      opycthk(e-6 m)  opycvar(e-6 m)
104005      43.4      2.9
*
***** FUEL ELEMENT DESCRIPTION *****
* CARD 105001 (Plane Geometry w/modified Inputs for a Capsule)
105001  PLANEGEOM
* CARD 105011 (Planegeom)
*      partnum(particles/capsule)  ngngfm  ngngn
105011      38052.      3      6
* CARD 105021 (Planegeom)
*      fmthk(m)  cldthk(m)
105021      1.      1.
* CARD 105031 (Planegeom)
*      fmden(g/cm^3) [1.70]
*105031
* CARD 105041 (Planegeom)
*      ucontam
105041      9.74E-6
*
***** FUEL ELEMENT ENVIRONMENT *****
* CARD 106001 (fuel temperature option)
*      rtmpopt
106001  VOLAVGTMP
* CARD 106021 (global node temperatures)
*      tgi(k)  ntgi  {not required with VOLAVGTMP option}
*106021
* CARD 201001 (fission product transport description)
*      fpspecie  {diffusion not modeled}
*201001
*
* CARD SERIES 301XXX (fluence v- time input)
*      timeirr(days)  flu(e25 n/m^2)
301001      0.      0.0000
301002      50.     0.2088
301003      100.    0.4188
301004      150.    0.6317
301005      200.    0.8508
301006      250.    1.0717
301007      300.    1.2975
301008      350.    1.5238
301009      400.    1.7488
301010      450.    1.9725
301011      500.    2.1938
301012      550.    2.4121
301013      600.    2.6279
```

Title: AGR-2 Pre-Test Prediction Analyses using the PARFUME Code for U.S. Fuel Particles

ECAR No.: 1020

ECAR Rev. No.: 2

Project File No.: 23841

Date: 05/29/2012

```
*
*
* CARD SERIES 302XXX (burnup v- fluence input)
*      flu(e25 n/m^2)  bup(%fima)
302001      0.0000      0.000
302002      0.2088      0.543
302003      0.4188      1.157
302004      0.6317      1.846
302005      0.8508      2.621
302006      1.0717      3.475
302007      1.2975      4.392
302008      1.5238      5.338
302009      1.7488      6.273
302010      1.9725      7.163
302011      2.1938      7.991
302012      2.4121      8.751
302013      2.6279      9.448
*
*
* CARD SERIES 303XXX (external pressure v- fluence input)
*      external pressure v- fluence input
*      flu(e25 n/m^2)  pamb(MPa)
303001      0.          .1
*
* CARD SERIES 304XXX (boundary temperature v- fluence input)
*      flu(e25 n/m^2)  btemp(k)
304001      0.0000      1183.
304002      0.2088      1183.
304003      0.4188      1183.
304004      0.6317      1183.
304005      0.8508      1183.
304006      1.0717      1183.
304007      1.2975      1183.
304008      1.5238      1183.
304009      1.7488      1183.
304010      1.9725      1183.
304011      2.1938      1183.
304012      2.4121      1183.
304013      2.6279      1183.
*
* CARD SERIES 306XXX (time heatup starts and irradiation ends)
*      thus(days) [1xe6] {casualty condition not modeled}
*306001
*
***** CORRELATION COEFFICIENTS *****
* CARD SERIES 401XXX (correlation coefficients for ipyc cracking)
*      sigcr0(MPa)  umc(MPa)
401001      1084.947  227.800
*      c1c          c2c
401002      0.0000      0.0000      * for fuel particle radial posit
401003      0.0000      0.0000      * for kernel diameter
401004      0.0000      0.0000      * for buffer thickness
401005      1.747631E-02  7.917080E-05  * for ipyc thickness
401006      1.052414E-02  3.897331E-04  * for sic thickness
401007      -1.706111E-02  3.606882E-04  * for opyc thickness
401008      0.0000      0.0000      * for ipyc density
401009      0.0000      0.0000      * for opyc density
401010      0.0000      0.0000      * for ipyc baf
401011      0.0000      0.0000      * for opyc baf
401012      0.0000      0.0000      * for creep coeff amplication
*
* CARD SERIES 402XXX (correlation coefficients for ipyc asphericity)
*      siga0(MPa)  um(MPa)  delum(MPa)  aration  aratvar
402001      801.501  576.600  293.100  1.052  0.013
```

Title: AGR-2 Pre-Test Prediction Analyses using the PARFUME Code for U.S. Fuel Particles

ECAR No.: 1020

ECAR Rev. No.: 2

Project File No.: 23841

Date: 05/29/2012

*	c1a	c2a	d1a	d2a	
402002	0.0000	0.0000	0.0000	0.0000	* fuel part rad pos
402003	0.0000	0.0000	0.0000	0.0000	* for kernel diamet
402004	0.0000	0.0000	0.0000	0.0000	* for buffer thickn
402005	2.990631E-03	1.745205E-05	-3.066647E-03	-7.576309E-06	*i thickn
402006	-2.467996E-03	-1.250619E-04	9.440630E-03	-7.294783E-04	*s thickn
402007	2.502614E-03	-1.553586E-05	-8.270773E-04	-2.074195E-05	*o thickn
402008	0.0000	0.0000	0.0000	0.0000	* for ipyc density
402009	0.0000	0.0000	0.0000	0.0000	* for opyc density
402010	0.0000	0.0000	0.0000	0.0000	* for ipyc baf
402011	0.0000	0.0000	0.0000	0.0000	* for opyc baf
402012	0.0000	0.0000	0.0000	0.0000	* for creep coef
402013	4.172333E+00	-6.324054E+01	3.283858E+00	-5.999677E+01	* aspheri

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* CARD SERIES 403XXX (correlation coefficients for ipyc debonding)
* sigd0 (MPa) umd(MPa) bond0 (MPa) bond0var (MPa)
403001 100. 100. 100. 0.
* c1d c2d
403002 0.0000 0.0000 * for fuel particle radial posit
403003 0.0000 0.0000 * for kernel diameter
403004 0.0000 0.0000 * for buffer thickness
403005 0.0000 0.0000 * for ipyc thickness
403006 0.0000 0.0000 * for sic thickness
403007 0.0000 0.0000 * for opyc thickness
403008 0.0000 0.0000 * for ipyc density
403009 0.0000 0.0000 * for opyc density
403010 0.0000 0.0000 * for ipyc baf
403011 0.0000 0.0000 * for opyc baf
403012 0.0000 0.0000 * for creep coeff amplication
403013 0.0000 0.0000 * for asphericity effects

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