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PARFUME – Modeling Update

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ART
ADVANCED REACTOR TECHNOLOGIES

ADVANCED REACTOR TECHNOLOGIES

Outline

- PARFUME Objective
- PARFUME Code Description and Modeling Capabilities
- AGR-5/6/7 Pre-test Predictions
- Accident Conditions Benchmark
- PARFUME Theory and Model Basis Report Update
- Material Properties
- CO Production Model

ADVANCED REACTOR TECHNOLOGIES

PARFUME Objective

- Develop first-principle based fuel performance models of coated particle fuel that can be used to:
  - Guide current and future particle designs
  - Assist in irradiation and safety experiment planning
  - Predict observed fuel failures
  - Interpolate fuel performance for core design assessments

PARFUME

- Advanced high temperature gas-cooled reactor fuel performance modeling code
- PARFUME (PARticle FUel ModEl) is currently under development at the Idaho National Laboratory
  - An integrated mechanistic code that evaluates the thermal, mechanical, and physico-chemical behavior of tristructural isotropic (TRISO) fuel particles
  - Capable of evaluating fuel particle failure under both irradiation and accident conditions
  - Tracks the probability of fuel particle failure given the particle-to-particle statistical variations in physical dimensions and material properties

PARFUME Modeling Capabilities

- Solution schemes
  - Monte Carlo
  - Direct numerical integration (fast and full)
- Reactor fuel geometry
  - Pebble Bed
  - Prismatic
  - Slab
  - Cylinder
- UCO and UO_2 fuel particles
  - Intact fuel particles
  - Layer cracking
  - IPyC/SiC debonding
  - Faceted particles
  - ZrC as SiC layer replacement
  - Initially defective SiC

PARFUME Modeling Capabilities

- Physico-chemical Models
  - Booth equivalent sphere fission gas release using Turnbull diffusivities
  - Redlich-Kwon equation of state
  - HSC thermodynamic based analysis for CO production
  - Fission product transport across each layer
- Layer Interactions
  - Fission product SiC interactions (e.g. Pd)
  - Amoeba effect
  - Thermal decomposition

AGR-5/6/7 Irradiation Test Predictions

- Modeling Conditions
  - Duration 510 EFPD
  - Burnup: 7.42 – 18.58 %FIMA
  - Fluence (E_n > 0.18 MeV): 2.21 – 7.35 $\times 10^{25}$ n/m^2
  - Temperature 696 - 1421°C
- Failure Mechanisms Considered
  - Pressure vessel failure (considering an asphericity of 1.04 ± 0.02)
  - IPyC-SiC debonding (bond strength of 100 MPa)
  - Kernel migration (amoeba effect)
  - IPyC Cracking

ADVANCED REACTOR TECHNOLOGIES

AGR-5/6/7 Irradiation Test Predictions

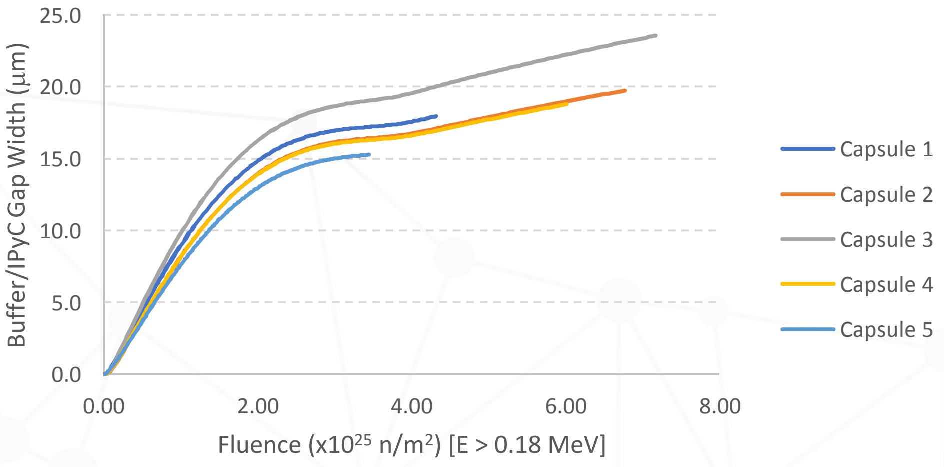
Capsule	Compact	Fluence ($\times 10^{25}$ n/m^2)	Burnup (%FIMA)	TAVA (°C)	Bounding Conditions
1	1-1-1	2.21	7.42	888	Low fast fluence, minimum TAVA
	1-8-6	5.74	13.96	1241	Maximum TAVA
	1-9-6	5.95	14.47	1146	Maximum fast fluence
	Average	4.32	11.49	1105	Average fast fluence, burnup, and TAVA
2	2-1-1	6.13	16.71	851	Low fast fluence, minimum TAVA
	2-7-3	7.21	18.58	935	Maximum TAVA
	2-8-3	7.24	18.56	923	Maximum fast fluence
	Average	6.77	17.97	910	Average fast fluence , burnup, and TAVA
3	3-1-1	7.13	17.70	1292	Low fast fluence, minimum TAVA
	3-3-2	7.35	18.33	1405	Maximum fast fluence
	3-6-2	7.18	18.19	1421	Maximum TAVA
	Average	7.17	18.03	1382	Average fast fluence, burnup, and TAVA
4	4-1-3	6.61	17.44	913	Maximum fast fluence
	4-4-4	6.07	16.77	933	Maximum TAVA
	4-6-2	5.31	15.47	881	Low fast fluence, minimum TAVA
	Average	6.01	16.63	916	Average fast fluence, burnup, and TAVA
5	5-1-3	4.54	12.67	803	Maximum fast fluence
	5-2-3	4.19	12.17	812	Maximum TAVA
	5-6-1	2.25	8.24	696	Low fast fluence, minimum TAVA
	Average	3.45	10.74	777	Average fast fluence, burnup, and TAVA

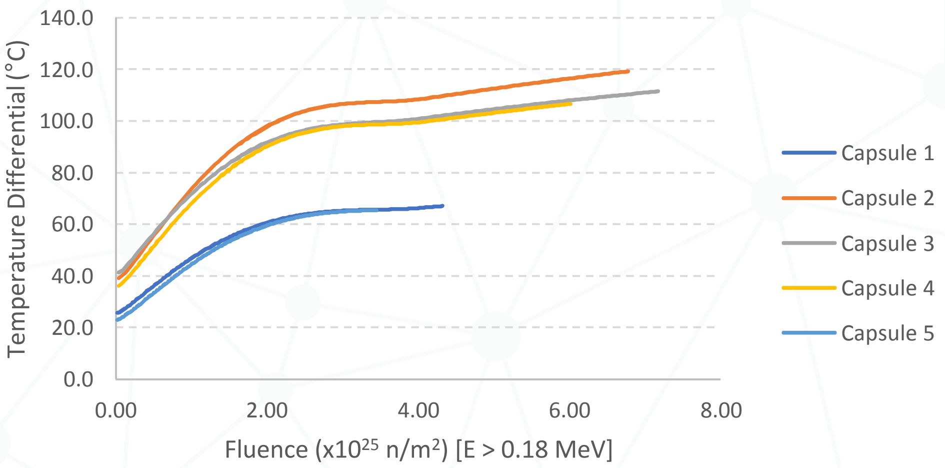
AGR-5/6/7 Irradiation Test Predictions

Capsule	Compact	Fluence (×10^{25} n/m^2) [E > 0.18 MeV]	Burnup (%FIMA)	Temperature (°C)	Probability of Failure due to SiC Failure	Probability of Failure due to IPyC Cracking	Probability of Failure due to Pressure	Probability of IPyC Cracking	Estimated Number of Particle Failures per Compact
1	1-1-1	2.21	7.42	888	5.0E-05	5.0E-05	0.0E+00	2.74E-01	0
	1-8-6	5.74	13.96	1241	1.4E-07	1.0E-08	1.3E-07	2.16E-03	0
	1-9-6	5.95	14.47	1146	9.7E-08	9.2E-08	4.8E-09	7.02E-03	0
	Average	4.32	11.49	1105	2.5E-07	2.5E-07	0.0E+00	1.20E-02	0
2	2-1-1	6.13	16.71	851	9.9E-05	9.9E-05	0.0E+00	4.06E-01	0
	2-7-3	7.21	18.58	935	1.7E-05	1.7E-05	0.0E+00	1.45E-01	0
	2-8-3	7.24	18.56	923	2.3E-05	2.3E-05	0.0E+00	1.71E-01	0
	Average	6.77	17.97	910	3.0E-05	3.0E-05	0.0E+00	2.04E-01	0
3	3-1-1	7.13	17.70	1292	2.5E-05	3.3E-09	2.5E-05	1.18E-03	0
	3-3-2	7.35	18.33	1405	3.2E-04	5.0E-10	3.2E-04	5.89E-04	1
	3-6-2	7.18	18.19	1421	3.7E-04	4.2E-10	3.7E-04	5.75E-04	1
	Average	7.17	18.03	1382	1.9E-04	6.7E-10	1.9E-04	6.04E-04	0
4	4-1-3	6.61	17.44	913	2.8E-05	2.8E-05	0.0E+00	1.97E-01	0
	4-4-4	6.07	16.77	933	1.8E-05	1.8E-05	0.0E+00	1.49E-01	0
	4-6-2	5.31	15.47	881	5.7E-05	5.7E-05	0.0E+00	2.95E-01	0
	Average	6.01	16.63	916	2.6E-05	2.6E-05	0.0E+00	1.89E-01	0
5	5-1-3	4.54	12.67	803	2.0E-04	2.0E-04	0.0E+00	5.98E-01	1
	5-2-3	4.19	12.17	812	1.8E-04	1.8E-04	0.0E+00	5.63E-01	1
	5-6-1	2.25	8.24	696	4.8E-04	4.8E-04	0.0E+00	8.55E-01	2
	Average	3.45	10.74	777	2.8E-04	2.8E-04	0.0E+00	6.88E-01	1

AGR-5/6/7 Irradiation Test Predictions

- Buffer-IPyC Gap
  - Gap width is closely correlated with fluence and temperature
  - Largest buffer-IPyC gap in Capsule 3
  - Temperature differentials are higher across particles with large gaps
- Release Fractions
  - Vary depending on capsule location and temperature
  - Maximum in Capsule 3 (Ag 85%, Cs 10%, and Sr 19%)
  - Cs and Sr in other capsules <1%
- Complete results in INL/EXT-17-43189, “AGR-5/6/7 Irradiation Test Predictions using PARFUME”





Accident Conditions Benchmark

- Part of the IAEA Coordinated Research Program on coated particle fuel technology (CRP-6)
- INL, JAEA, and KAERI participated in a benchmark on TRISO fuel performance modeling under accident conditions in the frame of the Generation IV International Forum
  - INL – PARFUME
  - JAEA – B-2 and FORNAX-A
  - KAERI – COPA
- Codes were compared on calculations of safety tests
  - AGR-1 and AGR-2 compacts
  - HFR-EU1bis spheres
- Benchmark divided into three parts
  - Modeling of a simplified benchmark problem to assess potential numerical calculation issues at low levels of FP release
  - Modeling of FP release during the AGR-1, AGR-2, and HFR-EU1bis safety testing experiments
  - Comparison of all the AGR-1, AGR-2, and HFR-EU1bis modeling results with experimental data

Accident Conditions Benchmark

- The code-to-code comparison showed very good agreement for Ag results, good agreement for Cs and Sr results, but some rather large discrepancy for Kr results
  - Ag: very good agreement between the three codes, the discrepancy is limited to less than 20%
  - Cs: good agreement between the codes with a discrepancy factor of ~4 at most
  - Sr: good agreement between the codes with a discrepancy factor of ~3 at most
  - Kr: large discrepancy between INL and KAERI; INL results were consistently over KAERI results but some of the large discrepancies were observed at low Kr release; JAEA did not predict any Kr release
- Agreement became better for compacts/spheres at higher safety testing temperatures, i.e., higher release fractions
- Comparison to experimental data did not yield such good agreement, with large over-predictions from the fuel performance modeling codes
  - Two orders of magnitude for Ag
  - Four orders of magnitude for Cs, Sr and Kr
- The large over-prediction of calculated release fractions signals a large over-estimation of some of the diffusion coefficients used in modeling and shared by all participants
  - Recommended IAEA diffusivities that are the basis of fission product transport in TRISO fuel in most current fuel performance modeling codes do not seem adequate for calculations under accident conditions

PARFUME Theory and Model Basis Report

- Revision – Level 2 Milestone, due 9/15/2018
- Cross-checking between the manual and source code for consistency and accuracy and correcting the manuals according to the source code
- Additional description of some physics models and equations
  - Amoeba effect
  - Pd-SiC penetration
  - Fission gas release
  - CO production models
  - Buffer-IPyC gap formation model
  - R/B release fraction
  - Cylindrical geometry
- PARFUME Theory and Model Basis Report, INL/EXT-08-14497

PARFUME Material Properties

- Level 3 Milestone, due 8/3/2018
- Purpose – to identify the material properties that have the largest impact on the failure probabilities of TRISO fuel particles under irradiation
- Current material properties obtained from historical experimental data
  - Incompleteness or uncertainty require assumptions and approximations
  - Obtained from strip samples (i.e., flat geometry) and were assumed representative for coating layers with spherical geometry
- Determine whether there is a need or requirement to re-evaluate their values for use in fuel performance modeling codes
- Assessed by parametric variations of each property on the calculated stress in the particle layers and on the resultant failure probability of a TRISO-coated fuel particle under representative irradiation conditions

PARFUME Material Properties

- Irradiation conditions correspond to the average values for the AGR-5/6 irradiation
  - 700 to 1300°C were chosen to fall within the range of applicability of the material properties
- Fuel parameters based on the AGR-5/6/7 fuel specification
- Properties varied around their nominal values by applying sensitivity multiplication factors

Condition	EFPD	Burnup (%FIMA)	Fast fluence ($\times 10^{25}$ n/m^2, E > 0.18 MeV)	Irradiation Temperature (°C)
1	500	13.5	5	700
2	500	13.5	5	1000
3	500	13.5	5	1300

- Multi-dimensional coefficients obtained using Abaqus
- Failure probabilities compared to the nominal material property value

PARFUME Material Properties

Layer	Property	Sensitivity Multiplication Factor (or values)	
		Nominal	Variation
Kernel	Swelling	1	0.33, 0.5, 2, 3
	Thermal Conductivity	1	0.33, 0.5, 2, 3
Buffer	Elastic Modulus	1	0.2, 0.5, 2, 5
	Poisson's Ratio	0.33	0, 0.25, 0.4, 0.5
	Irradiation Induced Creep	1	0.05, 0.2, 5, 20
	Poisson's Ratio in Creep	0.5	0, 0.25, 0.4
	Strain Rates	1	0.1, 0.33, 3, 10
	Thermal Conductivity	1	0.1, 0.33, 3, 10
	Thermal Expansion	1	0.5, 0.66, 1.5, 2
PyC	Elastic Moduli	1	0.33, 0.5, 2, 3
	Poisson's Ratio	0.33	0, 0.25, 0.4, 0.5
	Irradiation Induced Creep	1	0.2, 0.33, 0.5, 2, 3, 5
	Strain Rates	1	0.2, 0.33, 0.5, 2, 3, 5
	Poisson's Ratio in Creep	0.5	0, 0.25, 0.4
	Weibull (m/s_0)	9.5/16.8	8/10, 11/24.5
	Thermal Conductivity	1	0.33, 0.5, 2, 3
	Thermal Expansion	1	0.5, 0.66, 1.5, 2
SiC	Elastic Moduli	1	0.2, 0.5, 2, 5
	Poisson's Ratio	0.13	0, 0.25, 0.5
	Weibull (m/s_0)	6/9.64	9/37.58
	Thermal Conductivity	1	0.1, 0.33, 3, 10
	Thermal Expansion	1	0.5, 0.66, 1.5, 2

PARFUME Material Properties

Material Property	Sensitivity Multiplication Factor or Material Property Value	Irradiation Temperature (°C)	Increase in SiC failure probability	SiC failure probability
PyC elastic moduli	×3	700	1.6	6.54×10^{-4}
		1000	2.7	6.84×10^{-6}
		1300	2.0	4.47×10^{-9}
PyC Poisson's ratio	0.5	700	1.3	5.04×10^{-4}
		1000	1.6	3.96×10^{-6}
		1300	1.37	3.03×10^{-9}
PyC irradiation-induced creep	×0.2	700	1.12	2.48×10^{-1}
		1000	2.2×10^{4}	5.57×10^{-2}
		1300	3.4×10^{6}	7.50×10^{-3}
PyC Poisson's ratio in creep	Failure probability is maximum at nominal Poisson's ratio in creep			
PyC irradiation-induced dimensional change	×5	700	2.4×10^{3}	9.68×10^{-1}
		1000	1.7×10^{5}	4.21×10^{-1}
		1300	1.1×10^{7}	2.48×10^{-2}
PyC Weibull parameters (m / σ_0)	8 / 10.0	700	1.04	4.20×10^{-4}
		1000	2.1	5.37×10^{-5}
		1300	4.1	9.02×10^{-9}
SiC elastic modulus	×5	700	1.6	6.45×10^{-4}
		1000	1.7	4.21×10^{-6}
		1300	1.36	3.01×10^{-9}
SiC Poisson's ratio	0.5	700	2.6	1.03×10^{-3}
		1000	2.7	6.79×10^{-6}
		1300	2.6	5.67×10^{-9}
SiC Weibull parameters	Failure probability is maximum at nominal Weibull parameters			

CO Production Model

- Purpose – estimate the net production of CO and fission gas during the irradiation of TRISO fuel
- Inventory of FP varies depending on:
  - Initial O/U and C/U density fractions
  - ^{235}U enrichment
  - Burnup
  - Temperature
- Two-step approach
  - Calculation of FP inventory
  - Calculation of the formation of FP oxides – net excess of free oxygen to form CO
- Parametric model
  - 1% enrichment steps from 8 to 16%
  - 2% FIMA steps from 0 to 20% FIMA
  - O/U and C/U fractions
  - Irradiation temperature

Future Activities

- Continue code development
- On-going support of AGR irradiations
- AGR safety testing and PIE support
- CO production model
- Possible transition to BISON

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