APPENDIX F

PANEL MEMBER DETAILED PIRT SUBMITTALS FOR TRISO FUEL DEPRESSURIZATION ACCIDENT WITH AIR INGRESS

The INEEL submittal is provided in Appendix F.1 (pages F-2 through F-79).

The ORNL submittal is provided in Appendix F.2 (pages F-80 through F-160).

The SNL submittal is provided in Appendix F.3 (pages F-161 through F-239).

Appendix F.1

Detailed PIRT Submittal by the INEEL Panel Member

F. A. Petti

TRISO Fuel PIRT: Accident With Subsequent Air Intrusion

Life Cycle Phase	Factor, Characteristic or Phenomenon	Definition
Accident With Subsequent Air Intrusion	Fuel Element Irradiation history	The temperature, burnup and fast fluence history of the layer

Importance Rank and Rationale	Knowledge Level and Rationale	Remedy for Inadequate Knowledge/Issue Closure Criteria
Rank: M	7	Remedy:
Rationale: Irradiation history determines inventory at risk and initial conditions in particle relative to internal pressure in the particle and stress state.	Rationale:	Closure Criterion:

Additional Discussion

Life Cycle Phase	Factor, Characteristic or Phenomenon	Definition
Accident With Subsequent Air Intrusion	Fuel Element Condensed phase diffusion	Inter granular diffusion and/or intra-grannular solid-state diffusion

Importance Rank and Rationale	Knowledge Level and Rationale	Remedy for Inadequate Knowledge/Issue Closure Criteria
Rank: H	6	Remedy:
Rationale: Mechanism describing the transport of fission products in matrix of the fuel element. Important to understanding source term for the reactor.	Rationale: Air or water ingress can change the microstructure of the matrix, which can influence the surface diffusion of fission products by making transport easier. At very low partial pressures, air and water oxidation rates can be determined by the number of active sites in the matrix at which the oxidation can occur. In some cases oxidation can be catalyzed by impurity elements that are trapped at adsorption sites in the graphitic matrix. Thus there can be competition between fission product adsorption and the reaction between the air or steam and the matrix. The isotherms are fairly well known. The key issue is whether the internal surface area of the matrix has been changed by the air or water oxidation event and thus the amount of material available for release. Dislocations and/or defects can act as trapping sites for fission products as they transport through the matrix. If the number of dislocations is about the same as the number of fission products then the effect may be important. If the fission product concentration is much greater than the dislocation density then the effect is probably second order. Exact values have not been measured nor has any transport behavior been directly correlated with these parameters. The influence of the oxidation event may be to provide enough energy to the matrix to release fission products from the traps. Sensitivity analysis can be performed to scope this out.	Closure Criterion:

Additional Discussion

Life Cycle Phase	Factor, Characteristic or Phenomenon	Definition
Accident With Subsequent Air Intrusion	Fuel Element Gas phase diffusion	Diffusion of gaseous fission products through layer (Knudsen and bulk diffusion through pore structure, and pressure driven permeation through structure). Other factors include holdup, cracking, adsorption, site poisoning, permeability, sintering and annealing.

Importance Rank and Rationale	Knowledge Level and Rationale	Remedy for Inadequate Knowledge/Issue Closure Criteria
Rank: H	5	Remedy:
Rationale: Gas phase diffusion is thought to be the mechanism for gaseous fission product transport in the matrix.	Rationale: Air or water ingress can change the microstructure and porosity of the matrix, which can influence the gas diffusion of fission products by making transport easier. The interconnected porosity can be a transport path for the air or water intrusion. The reaction of air or water with the matrix can change the microstructure, porosity, tortuosity, and permeability, and hence affect gaseous fission product transport in the matrix.	Closure Criterion:

Additional Discussion

Life Cycle Phase	Factor, Characteristic or Phenomenon	Definition
Accident With Subsequent Air Intrusion	Fuel Element: Transport of metallic FPs through fuel element	Chemical stoichiometry of the chemical species that includes the radioisotope of interest
	Chemical form	

Importance Rank and Rationale	Knowledge Level and Rationale	Remedy for Inadequate Knowledge/Issue Closure Criteria
Rank: H	7	Remedy:
Rationale: Transport has been assumed to be elemental for the major fission products (Cs, Ag, I, Xe, Sr). Potential changes in chemical form due to the presence of air or water can be calculated.	Rationale:	Closure Criterion:

Additional Discussion

Life Cycle Phase	Factor, Characteristic or Phenomenon	Definition
Accident With Subsequent Air Intrusion	Fuel Element: Chemical attack by air Kinetics	Rate of reaction per unit surface area as a function of temperature and partial pressure of air

Importance Rank and Rationale	Knowledge Level and Rationale	Remedy for Inadequate Knowledge/Issue Closure Criteria
Rank: H	7	Remedy:
Rationale: Key parameter to describe thermal response and subsequent fission product release during the event.	Rationale: Kinetics are fairly well known for both air and steam as a function of temperature and partial pressure and flowrate.	Closure Criterion:

Additional Discussion

Life Cycle Phase	Factor, Characteristic or Phenomenon	Definition
Accident With Subsequent Air Intrusion	Fuel Element: Chemical attack by air	Modification of the reaction rate by fission products or impurities
	Catalysis	

Importance Rank and Rationale	Knowledge Level and Rationale	Remedy for Inadequate Knowledge/Issue Closure Criteria
Rank: M	5	Remedy:
Rationale: Impurities can affect reaction rate and thus impact overall behavior during the intrusion event.	Rationale: Oxidation rate data have been determined for actual pebbles and compacts and thus implicitly include the effects of impurities. The effects of fission products have not been included because oxidation testing has not been performed on irradiated material. In principle, sensitivity calculations can be performed with variations in the oxidation rate to bound this effect.	Closure Criterion:

Additional Discussion

Life Cycle Phase	Factor, Characteristic or Phenomenon	Definition
Accident With Subsequent Air Intrusion	Fuel Element: Chemical attack by air	Changes in chemical form resulting from oxidizing or reducing fission products
	Changes in chemical form of fission products	

Importance Rank and Rationale	Knowledge Level and Rationale	Remedy for Inadequate Knowledge/Issue Closure Criteria
Rank: H	6	Remedy:
Rationale: This can be important because the transport behavior is dependent on the chemical form.	Rationale: This can also be calculated for a range of oxygen potentials to determine if any of the key fission products change in chemical form during the air or water ingress accident.	Closure Criterion:

Additional Discussion

Life Cycle Phase	Factor, Characteristic or Phenomenon	Definition
Accident With Subsequent Air Intrusion	Fuel Element: Chemical attack by air Changes in graphite properties	Changes in diffusivity, porosity, adsorptivity, etc.

Importance Rank and Rationale	Knowledge Level and Rationale	Remedy for Inadequate Knowledge/Issue Closure Criteria
Rank: H	6	Remedy:
Rationale: The oxidation can change the microstructure of the graphite by creating tunnels or pathways in the matrix. Thus, because the microstructure changes, the porosity, adsorptivity, etc., can also change.	Rationale: No measurements have been made on this effect. Conservative assumptions on such changes may allow sensitivity studies in this area.	Closure Criterion:

Additional Discussion

Life Cycle Phase	Factor, Characteristic or Phenomenon	Definition
Accident With Subsequent Air Intrusion	Fuel Element: Chemical attack by air Holdup reversals	Release of graphite FP inventory

Importance Rank and Rationale	Knowledge Level and Rationale	Remedy for Inadequate Knowledge/Issue Closure Criteria
Rank: M	6	Remedy:
Rationale: As the oxidation process continues any fission products trapped at sites in the matrix may be released because of the thermal energy associated with the oxidation.	Rationale: This can be accounted for in a very simplistic yet conservative manner if details are not well known or more sophisticated models with detrapping can be used if the fundamental data needed for such models exist.	Closure Criterion:

Additional Discussion

Life Cycle Phase	Factor, Characteristic or Phenomenon	Definition
Accident With Subsequent Air Intrusion	Fuel Element: Chemical attack by air Temperature distributions	Impact of graphite oxidation on temperature distribution through material

Importance Rank and Rationale	Knowledge Level and Rationale	Remedy for Inadequate Knowledge/Issue Closure Criteria
Rank: H	8	Remedy:
Rationale: Very important in doing an oxidation calculation is to make sure the temperature response of the material as a result of the energy generation is properly calculated.	Rationale: This is well known and can be done in most of the safety codes used by NRC (e.g. MELCOR). The high conductivity of the PyC should make the gradient quite small in general. The degree of fine detail in the model may be an open question but can be handled with sensitivity studies.	Closure Criterion:

Additional Discussion

Life Cycle Phase	Factor, Characteristic or Phenomenon	Definition
Accident With Subsequent Air Intrusion	Outer PyC Layer Gas-phase diffusion	Diffusion of gaseous fission products through layer (Knudsen and bulk diffusion through pore structure, and pressure driven permeation through structure)

Importance Rank and Rationale	Knowledge Level and Rationale	Remedy for Inadequate Knowledge/Issue Closure Criteria
Rank: H	6	Remedy:
Rationale: OPyC can hold up gaseous fission products.	Rationale: Effective diffusion coefficients for noble gases through PyC exist for both German and U.S. PyC. The Knudsen diffusion formalism has not been historically used in the modeling. The effect of oxidation on changes in the transport behavior has not been studied. Sensitivity studies can be performed to bound potential changes to determine the impact on the overall source term.	Closure Criterion:

Life Cycle Phase	Factor, Characteristic or Phenomenon	Definition
Accident With Subsequent Air Intrusion	Outer PyC Layer Condensed-phase diffusion	Inter-granular diffusion an/or intra-grannular solid state diffusion

Importance Rank and Rationale	Knowledge Level and Rationale	Remedy for Inadequate Knowledge/Issue Closure Criteria
Rank: H	6	Remedy:
Rationale: PyC layers provide for some transport delay of metallic fission products.	Rationale: Data exist on the effective diffusivity of Cs, Ag, and Sr through the PyC layer. The mechanism responsible for the transport has not been definitively identified. The effect of oxidation on transport properties has not been studied. Sensitivity studies can be performed to bound potential changes to determine the impact on the overall source term.	Closure Criterion:

Life Cycle Phase	Factor, Characteristic or Phenomenon	Definition
Accident With Subsequent Air Intrusion	Outer PyC Layer Layer oxidation	Uptake of oxygen by the layer through a chemical reaction

Importance Rank and Rationale	Knowledge Level and Rationale	Remedy for Inadequate Knowledge/Issue Closure Criteria
Rank: H	7	Remedy:
Rationale: Oxidation of OPyC is needed to understand thermal response of the particles in the fuel element.	Rationale: Reaction rates for PyC are known at these temperatures.	Closure Criterion:

Additional Discussion

Life Cycle Phase	Factor, Characteristic or Phenomenon	Definition
Accident With Subsequent Air Intrusion	Outer PyC Layer Stress state (compression/tension)	The state of the forces induced by external forces that are acting across the layer to resist movement

Importance Rank and Rationale	Knowledge Level and Rationale	Remedy for Inadequate Knowledge/Issue Closure Criteria
Rank: L	8	Remedy:
Rationale: The stress state is judged to be of low importance for a chemical oxidation event.	Rationale: Stress state is easily calculated using current finite element models for coated particles.	Closure Criterion:

Additional Discussion

Life Cycle Phase	Factor, Characteristic or Phenomenon	Definition
Accident With Subsequent Air Intrusion	Outer PyC Layer Intercalation	Trapping of species between crystallite planes of the graphite structure

Importance Rank and Rationale	Knowledge Level and Rationale	Remedy for Inadequate Knowledge/Issue Closure Criteria
Rank: M	4	Remedy:
Rationale: In an intact particle, little diffusion of fission products is expected. If the level of adsorption or defect sites is high in the OPyC due to neutron irradiation for example, then these sites may be effective in holding up fission products if they are not annealed out during the oxidation event. In a failed particle, the number of fission product atoms is so large that such a mechanism is very small. This is based on diffusion and trapping modeling performed for tritium under the NPR program in the early 1990s. The oxidation event if severe enough could probably liberate any adsorbed or trapped fission products. Sensitivity studies with a diffusion and trapping model can study this in more detail to determine overall significance in the core for the oxidation event.	Rationale:	Closure Criterion:

Additional Discussion

Life Cycle Phase	Factor, Characteristic or Phenomenon	Definition
Accident With Subsequent Air Intrusion	Outer PyC Layer Trapping	Adsorption of fission products on defects

Importance Rank and Rationale	Knowledge Level and Rationale	Remedy for Inadequate Knowledge/Issue Closure Criteria
Rank: M	4	Remedy:
Rationale: In an intact particle, little diffusion of fission products is expected. If the level of adsorption or defect sites is high in the OPyC due to neutron irradiation for example, then these sites may be effective in holding up fission products if they are not annealed out during the oxidation event. In a failed particle the number of fission product atoms is so large that such a mechanism is very small. This is based on diffusion and trapping modeling performed for tritium under the NPR program in the early 1990s. The oxidation event if severe enough could probably liberate any adsorbed or trapped fission products. Sensitivity studies with a diffusion and trapping model can study this in more detail to determine overall significance in the core for the oxidation event.	Rationale:	Closure Criterion:

Additional Discussion

Life Cycle Phase	Factor, Characteristic or Phenomenon	Definition
Accident With Subsequent Air Intrusion	Outer PyC Layer Cracking	Lengths, widths and numbers of cracks produced in layer during operation or an accident

Importance Rank and Rationale	Knowledge Level and Rationale	Remedy for Inadequate Knowledge/Issue Closure Criteria
Rank: M	6	Remedy:
Rationale: A cracked OPyC will not retain fission gases and would act as a fast transport path for oxidation of the SiC.	Rationale: Models can be used to calculate the stress state in the OPyC layer.	Closure Criterion:

Additional Discussion

Life Cycle Phase	Factor, Characteristic or Phenomenon	Definition
Accident With Subsequent Air Intrusion	Outer PyC Layer: Chemical attack by air Kinetics	Rate of reaction per unit surface area as a function of temperature and partial pressure of air

Importance Rank and Rationale	Knowledge Level and Rationale	Remedy for Inadequate Knowledge/Issue Closure Criteria
Rank: H	7	Remedy:
Rationale: Oxidation of OPyC is needed to understand thermal response of the particles in the fuel element.	Rationale: Reaction rates for PyC are known at these temperatures.	Closure Criterion:

Additional Discussion

Life Cycle Phase	Factor, Characteristic or Phenomenon	Definition
Accident With Subsequent Air Intrusion	Outer PyC Layer: Chemical attack by air Catalysis	Modification of the reaction rate by fission products or impurities

Importance Rank and Rationale	Knowledge Level and Rationale	Remedy for Inadequate Knowledge/Issue Closure Criteria
Rank: M	4	Remedy:
Rationale: Impurities can alter reaction rates and change nature of the event.	Rationale: Reaction rate testing of PyC would implicitly include the effects of any impurities on the overall oxidation. No chemical reaction rate measurements have been performed using irradiated PyC where fission products may be in the layer. In principle sensitivity calculations can be performed with variations in the oxidation rate to bound this effect.	Closure Criterion:

Additional Discussion

Life Cycle Phase	Factor, Characteristic or Phenomenon	Definition
Accident With Subsequent Air Intrusion	Outer PyC Layer: Chemical attack by air	Changes in chemical form resulting from oxidizing or reducing fission products
	Changes in chemical form of fission products	

Importance Rank and Rationale	Knowledge Level and Rationale	Remedy for Inadequate Knowledge/Issue Closure Criteria
Rank: H	7	Remedy:
Rationale: This can be important because the transport behavior is dependent on the chemical form.	Rationale: This can also be calculated for a range of oxygen potentials to determine if any of the key fission products change in chemical form during the air or water ingress accident.	Closure Criterion:

Additional Discussion

Life Cycle Phase	Factor, Characteristic or Phenomenon	Definition
Accident With Subsequent Air Intrusion	Outer PyC Layer: Chemical attack by air Changes in graphite properties	Changes in diffusivity, porosity, adsorptivity, etc.

Importance Rank and Rationale	Knowledge Level and Rationale	Remedy for Inadequate Knowledge/Issue Closure Criteria
Rank: M	6	Remedy:
Rationale: The oxidation can change the microstructure of the PyC by creating tunnels or pathways in the matrix. Thus, because the microstructure changes, the porosity, adsorptivity, etc. can also change.	Rationale: No measurements have been made on this effect. Conservative assumptions on such changes may allow sensitivity studies in this area.	Closure Criterion:

Additional Discussion

Life Cycle Phase	Factor, Characteristic or Phenomenon	Definition
Accident With Subsequent Air Intrusion	Outer PyC Layer: Chemical attack by air	Release of graphite FP inventory
	Holdup reversal	

Importance Rank and Rationale	Knowledge Level and Rationale	Remedy for Inadequate Knowledge/Issue Closure Criteria
Rank: M	6	Remedy:
Rationale: As the oxidation process continues, any fission products trapped at sites in the PyC may be released because of the thermal energy associated with the oxidation and thus increase the source term.	Rationale: This can be accounted for in a very simplistic, yet conservative manner if details are not well known or more sophisticated models with detrapping can be used if the fundamental data needed for such models exist.	Closure Criterion:

Additional Discussion

Life Cycle Phase	Factor, Characteristic or Phenomenon	Definition
Accident With Subsequent Air Intrusion	Outer PyC Layer: Chemical attack by air Temperature distribution	Impact of graphite oxidation on temperature distribution through material

Importance Rank and Rationale	Knowledge Level and Rationale	Remedy for Inadequate Knowledge/Issue Closure Criteria
Rank: H	8	Remedy:
Rationale: Very important in doing an oxidation calculation is to make sure the temperature response of the material as a result of the energy generation is properly calculated.	Rationale: This is well known and can be done in most of the safety codes used by NRC (e.g. MELCOR). The high conductivity of the PyC should make the gradient quite small in general. The degree of fine detail in the model may be an open question but can be handled with sensitivity studies.	Closure Criterion:

Additional Discussion

Life Cycle Phase	Factor, Characteristic or Phenomenon	Definition
Accident With Subsequent Air Intrusion	SiC Layer Gas-phase diffusion	Diffusion of gaseous fission products through layer (Knudsen and bulk diffusion through pore structure, and pressure driven permeation through structure)

Importance Rank and Rationale	Knowledge Level and Rationale	Remedy for Inadequate Knowledge/Issue Closure Criteria
Rank: H	7	Remedy:
Rationale: As the primary fission product barrier, understanding the transport is very important.	Rationale: Effective diffusion coefficients exist in both the U.S. and Germany for the fission gases through the SiC. They are probably a combination of bulk diffusion and Knudsen diffusion at these high temperatures but the two mechanisms have never been individually sorted out in any experiment. The parameters needed for such detailed models and the changes in microstructure of the SiC particle to particle and/or across the layer and/or as a result of the oxidation make such an effort very expensive and time consuming. The use of effective diffusion coefficients although less scientifically satisfying is more pragmatic and may be completely acceptable in system safety analysis when accompanied by proper sensitivity studies.	Closure Criterion:

Additional Discussion

Life Cycle Phase	Factor, Characteristic or Phenomenon	Definition
Accident With Subsequent Air Intrusion	SiC Layer Condensed-phase diffusion	Inter-granular diffusion and/or intra-grannular solid-state diffusion

Importance Rank and Rationale	Knowledge Level and Rationale	Remedy for Inadequate Knowledge/Issue Closure Criteria
Rank: H	7	Remedy:
Rationale: As the primary fission product barrier, understanding the transport is very important.	Rationale: Effective diffusion coefficients exist in both the U.S. and Germany for the metallic fission products through the SiC. They are probably a combination of bulk diffusion and grain boundary diffusion at these high temperatures but the two mechanisms have never been individually sorted out in any experiment. The parameters needed for such detailed models and the changes in microstructure of the SiC particle to particle and/or across the layer and/or as a result of the oxidation process make such an effort very expensive and time consuming. The use of effective diffusion coefficients although less scientifically satisfying is more pragmatic and may be completely acceptable in system safety analysis when accompanied by proper sensitivity studies.	Closure Criterion:

Additional Discussion

Life Cycle Phase	Factor, Characteristic or Phenomenon	Definition
Accident With Subsequent Air Intrusion	SiC Layer Thermal deterioration/decomposition	Decline in the quality of the layer due to thermal loading

Importance Rank and Rationale	Knowledge Level and Rationale	Remedy for Inadequate Knowledge/Issue Closure Criteria
Rank: M	8	Remedy:
Rationale: Less important in oxidation events than in the longer term traditional heatup event. (See similar factor in heatup PIRT table for more information).	Rationale:	Closure Criterion:

Additional Discussion

Life Cycle Phase	Factor, Characteristic or Phenomenon	Definition
Accident With Subsequent Air Intrusion	SiC Layer Fission product corrosion	Attack of layer by fission products, e.g., Pd

Importance Rank and Rationale	Knowledge Level and Rationale	Remedy for Inadequate Knowledge/Issue Closure Criteria
Rank: M	7	Remedy:
Rationale: The deterioration of the SiC layer via Pd attack has been postulated as a key failure mechanism because Pd forms silicides based on phase diagram and experimental measurements. This is very important for the high burnup fuel being proposed in new reactor designs since the Pd yield from Pu fission is much greater (~ 25 x) that from U fission. Overall, it is judged to be of less importance in the oxidation event since it is assumed that the chemical energy associated with the oxidation event would dominate the subsequent fission product behavior in the particle.	Rationale: Various research institutions have performed many measurements. The kinetics of this mechanism is not known with enough certainty since extrapolations from the database are required. More testing would help develop a better understanding of the phenomena and its impact above 1600°C. Synergistic effects between oxidation and Pd attack (e.g., increase in temperature due to oxidation and its impact on greater Pd corrosion) have never been studied experimentally but can be examined use computer models with appropriate sensitivity studies.	Closure Criterion:

Additional Discussion

Life Cycle Phase	Factor, Characteristic or Phenomenon	Definition
Accident With Subsequent Air Intrusion	SiC Layer Heavy metal diffusion	Diffusion of heavy metals through the intact layer

Importance Rank and Rationale	Knowledge Level and Rationale	Remedy for Inadequate Knowledge/Issue Closure Criteria
Rank: L	3	Remedy:
Rationale: Although higher oxides of uranium (UO_{2+x}) can be volatile, this factor is judged to be of low importance in air or water ingress events since the ability of air or water to get to the kernel to mobilize the uranium is quite small given the large amount of carbon in the system available to react with air or steam.	Rationale: Heavy metal diffusion has never been observed in German accident heating tests.	Closure Criterion:

Additional Discussion

Life Cycle Phase	Factor, Characteristic or Phenomenon	Definition
Accident With Subsequent Air Intrusion	SiC Layer Layer oxidation	Uptake of oxygen by the layer through a chemical reaction

Importance Rank and Rationale	Knowledge Level and Rationale	Remedy for Inadequate Knowledge/Issue Closure Criteria
Rank: H	5	Remedy:
Rationale: Oxidation by air or water is important to understand the response of the fuel.	Rationale: At high partial pressures of air a protective layer of SiO_2 is expected. But at lower partial pressures of air, volatile SiO is predicted to form.	Closure Criterion:

Additional Discussion

Life Cycle Phase	Factor, Characteristic or Phenomenon	Definition
Accident With Subsequent Air Intrusion	SiC Layer Fission product release through undetected defects	Passage of fission products from the buffer region through defects in the SiC layer

Importance Rank and Rationale	Knowledge Level and Rationale	Remedy for Inadequate Knowledge/Issue Closure Criteria
Rank: M	5	Remedy:
Rationale: As the primary fission product barrier, understanding the transport is very important.	Rationale: Effective diffusion coefficients exist in both the U.S. and Germany for the fission gases through the SiC. Release via defects has never been individually sorted out from the other transport mechanisms in any experiment. The parameters needed to model release via defects and the presence or absence of defects in the SiC layer particle to particle, and/or across the layer, and/or changes in the defect structure as a result of oxidation makes such an effort very expensive and time consuming. The use of effective diffusion coefficients although less scientifically satisfying is more pragmatic and may be completely acceptable in system safety analysis when accompanied by proper sensitivity studies that assume some percentage of defective SiC layers present in the core.	Closure Criterion:

Additional Discussion

Life Cycle Phase	Factor, Characteristic or Phenomenon	Definition
Accident With Subsequent Air Intrusion	SiC Layer Fission product release through failures, e.g., cracking	Passage of fission products from the buffer region through regions in the SiC layer that fail during operation or an accident

Importance Rank and Rationale	Knowledge Level and Rationale	Remedy for Inadequate Knowledge/Issue Closure Criteria
Rank: H	7	Remedy:
Rationale: A particle with a failed SiC layer but intact PyC layers will not release fission gas. The PyC layers must fail in order to have fission gas release. A failed layer sometimes is modeled as having no fission product retention characteristics in fuel performance models. This conservative assumption is reasonable assuming that the code can adequately calculate when an SiC layer can fail. The oxidation event may cause failure of the layer, which would then result in fission product release.	Rationale: Such a causal relationship can be modeled and sensitivity studies performed to determine the overall impact in an oxidation event.	Closure Criterion:

Additional Discussion

Life Cycle Phase	Factor, Characteristic or Phenomenon	Definition
Accident With Subsequent Air Intrusion	SiC Layer Thermodynamics of the SiC-fission product system	Chemical form of fission products including the effects of solubility, intermetallics, and chemical activity

Importance Rank and Rationale	Knowledge Level and Rationale	Remedy for Inadequate Knowledge/Issue Closure Criteria
Rank: H	7	Remedy:
Rationale: Critical to understanding transport behavior of fission products	Rationale: Thermodynamic calculations have been performed for both the UO_2 and UCO systems over a broad temperature, burnup and enrichment range to establish the chemical forms of the fission products. Similar calculations can be performed in the presence of steam or air to determine the changes in chemical form of the fission products.	Closure Criterion:

Additional Discussion

Life Cycle Phase	Factor, Characteristic or Phenomenon	Definition
Accident With Subsequent Air Intrusion	SiC Layer Sintering	Change of SiC microstructure as a function of temperature

Importance Rank and Rationale	Knowledge Level and Rationale	Remedy for Inadequate Knowledge/Issue Closure Criteria
Rank: L	2	Remedy:
Rationale: The CVD SiC is very high density,almost theoretical, so it is difficult to see that there would be much of a role for sintering to change the microstructure. Chemical effects from the oxidation event are much more important.	Rationale:	Closure Criterion:

Additional Discussion

Life Cycle Phase	Factor, Characteristic or Phenomenon	Definition
Accident With Subsequent Air Intrusion	SiC Layer: Chemical attack by air Kinetics	Rate of reaction per unit surface area as a function of temperature and partial pressure of air

Importance Rank and Rationale	Knowledge Level and Rationale	Remedy for Inadequate Knowledge/Issue Closure Criteria
Rank: H	5	Remedy:
Rationale: Oxidation by air or water is important to understand the response of the fuel.	Rationale: At high partial pressures of air a protective layer of SiO_2 is expected. But at lower partial pressures of air, volatile SiO is predicted to form.	Closure Criterion:

Additional Discussion

Life Cycle Phase	Factor, Characteristic or Phenomenon	Definition
Accident With Subsequent Air Intrusion	SiC Layer: Chemical attack by air Catalysis	Modification of the reaction rate by fission products or impurities

Importance Rank and Rationale	Knowledge Level and Rationale	Remedy for Inadequate Knowledge/Issue Closure Criteria
Rank: M	5	Remedy:
Rationale: Impurities can change the reaction rate	Rationale: Some air oxidation rate data have been determined for SiC and thus implicitly include the effects of impurities. The effects of fission products have not been included because oxidation testing has not been performed on irradiated SiC material with fission products. In principle, sensitivity calculations can be performed with variations in the oxidation rate to bound this effect.	Closure Criterion:

Additional Discussion

Life Cycle Phase	Factor, Characteristic or Phenomenon	Definition
Accident With Subsequent Air Intrusion	SiC Layer: Chemical attack by air	Changes in chemical form resulting from oxidizing or reducing fission products
	Changes in chemical form of fission products	

Importance Rank and Rationale	Knowledge Level and Rationale	Remedy for Inadequate Knowledge/Issue Closure Criteria
Rank: H	7	Remedy:
Rationale: This can be important because the transport behavior is dependent on the chemical form.	Rationale: This can also be calculated for a range of oxygen potentials to determine if any of the key fission products change in chemical form during the air or water ingress accident.	Closure Criterion:

Additional Discussion

Life Cycle Phase	Factor, Characteristic or Phenomenon	Definition
Accident With Subsequent Air Intrusion	SiC Layer: Chemical attack by air Changes in SiC properties	Changes in diffusivity, porosity, adsorptivity, etc.

Importance Rank and Rationale	Knowledge Level and Rationale	Remedy for Inadequate Knowledge/Issue Closure Criteria
Rank: M	4	Remedy:
Rationale: The oxidation can change the microstructure of the SiC by creating tunnels or pathways in the matrix. Thus, because the microstructure changes, the porosity, adsorptivity, etc. can also change.	Rationale: No measurements have been made on this effect. Conservative assumptions on such changes may allow sensitivity studies in this area.	Closure Criterion:

Additional Discussion

Life Cycle Phase	Factor, Characteristic or Phenomenon	Definition
Accident With Subsequent Air Intrusion	SiC Layer: Chemical attack by air	Release of SiC FP inventory
	Holdup reversal	

Importance Rank and Rationale	Knowledge Level and Rationale	Remedy for Inadequate Knowledge/Issue Closure Criteria
Rank: M	4	Remedy:
Rationale: As the oxidation process continues any fission products trapped at sites in the SiC may be released because of the thermal energy associated with the oxidation.	Rationale: This can be accounted for in a very simplistic, yet conservative manner if details are not well known or more sophisticated models with detrapping can be used if the fundamental data needed for such models exist.	Closure Criterion:

Additional Discussion

Life Cycle Phase	Factor, Characteristic or Phenomenon	Definition
Accident With Subsequent Air Intrusion	SiC Layer: Chemical attack by air Temperature distribution	Impact of SiC oxidation on temperature distribution through material

Importance Rank and Rationale	Knowledge Level and Rationale	Remedy for Inadequate Knowledge/Issue Closure Criteria
Rank: H	8	Remedy:
Rationale: Very important in doing an oxidation calculation is to make sure the temperature response of the material as a result of the chemical reaction is properly calculated.	Rationale: This is well known and can be done in most of the safety codes used by NRC (e.g. MELCOR). The degree of fine detail in the model may be an open question but can be handled with sensitivity studies.	Closure Criterion:

Additional Discussion

Life Cycle Phase	Factor, Characteristic or Phenomenon	Definition
Accident With Subsequent Air Intrusion	Inner PyC Layer Gas-phase diffusion	Diffusion of gaseous fission products through layer (Knudsen and bulk diffusion through pore structure, and pressure driven permeation through structure)

Importance Rank and Rationale	Knowledge Level and Rationale	Remedy for Inadequate Knowledge/Issue Closure Criteria
Rank: H	6	Remedy:
Rationale: PyC can hold up gaseous fission products.	Rationale: PyC effectively retain fission gases. Effective diffusion coefficients for noble gases through PyC exist for both German and U.S. PyC. The Knudsen diffusion formalism has not been historically used in the modeling. The effect of oxidation on changes in the transport behavior has not been studied. Sensitivity studies can be performed to bound potential changes to determine the impact on the overall source term.	Closure Criterion:

Additional Discussion

Life Cycle Phase	Factor, Characteristic or Phenomenon	Definition
Accident With Subsequent Air Intrusion	Inner PyC Layer Condensed phase diffusion	Inter-granular diffusion and/or intra-grannular solid-state diffusion

Importance Rank and Rationale	Knowledge Level and Rationale	Remedy for Inadequate Knowledge/Issue Closure Criteria
Rank: M	6	Remedy:
Rationale: Transport through intact particles is less important than those with exposed kernels in ingress events	Rationale: Data exist on the effective diffusivity of Cs, Ag, and Sr through the PyC layer. The mechanism responsible for the transport has not been definitively identified. The effect of oxidation on transport properties has not been studied. Sensitivity studies can be performed to bound potential changes to determine the impact on the overall source term.	Closure Criterion:

Additional Discussion

Life Cycle Phase	Factor, Characteristic or Phenomenon	Definition
Accident With Subsequent Air Intrusion	Inner PyC Layer Pressure loading (Fission products)	Stress loading of the layer by increased pressure from fission products

Importance Rank and Rationale	Knowledge Level and Rationale	Remedy for Inadequate Knowledge/Issue Closure Criteria
Rank: H	8	Remedy:
Rationale: A key parameter to determine stress in coating layer.	Rationale: Noble gases contribute to the pressure loading in the particle. The effect of temperature due to the oxidation event on the pressure is easily calculated.	Closure Criterion:

Additional Discussion

Life Cycle Phase	Factor, Characteristic or Phenomenon	Definition
Accident With Subsequent Air Intrusion	Inner PyC Layer Pressure loading (Carbon monoxide)	Stress loading of the layer by carbon monoxide by increased pressure

Importance Rank and Rationale	Knowledge Level and Rationale	Remedy for Inadequate Knowledge/Issue Closure Criteria
Rank: H for UO_2 and L for UCO	8	Remedy:
Rationale: A key parameter to determine stress in coating layer.	Rationale: Co (for UO_2 only) contributes to the pressure loading in the particle. The effect of temperature due to the oxidation event on the pressure is easily calculated.	Closure Criterion:

Additional Discussion

Life Cycle Phase	Factor, Characteristic or Phenomenon	Definition
Accident With Subsequent Air Intrusion	Inner PyC Layer Layer oxidation	Reaction of pyrolytic graphite with oxygen released from the kernel

Importance Rank and Rationale	Knowledge Level and Rationale	Remedy for Inadequate Knowledge/Issue Closure Criteria
Rank: H	3	Remedy:
Rationale: At high temperatures, oxygen release from kernel increases over that in normal operations because of instability of some oxidic fission products at high temperatures.	Rationale: Known at these temperatures	Closure Criterion:

Additional Discussion

Life Cycle Phase	Factor, Characteristic or Phenomenon	Definition
Accident With Subsequent Air Intrusion	Inner PyC Layer Stress state (compression/tension)	The state of the forces induced by external forces that are acting across the layer to resist movement

Importance Rank and Rationale	Knowledge Level and Rationale	Remedy for Inadequate Knowledge/Issue Closure Criteria
Rank: L	8	Remedy:
Rationale: The stress state is judged to be of low importance for a chemical oxidation event.	Rationale: Stress state is easily calculated using current finite element models for coated particles.	Closure Criterion:

Additional Discussion

Life Cycle Phase	Factor, Characteristic or Phenomenon	Definition
Accident With Subsequent Air Intrusion	Inner PyC Layer Cracking	Lengths, widths and numbers of cracks produced in layer during accident

Importance Rank and Rationale	Knowledge Level and Rationale	Remedy for Inadequate Knowledge/Issue Closure Criteria
Rank: H	5	Remedy:
Rationale: A cracked IPyC will not retain fission gases and would act as a fast transport path for metallic fission products to the SiC layer. Furthermore, a cracked IPyC will allow CO to attack the SiC layer.	Rationale:	Closure Criterion:

Additional Discussion

Life Cycle Phase	Factor, Characteristic or Phenomenon	Definition
Accident With Subsequent Air Intrusion	Inner PyC Layer Intercalation	Trapping of species between sheets of the graphite structure

Importance Rank and Rationale	Knowledge Level and Rationale	Remedy for Inadequate Knowledge/Issue Closure Criteria
Rank: M	6	Remedy:
Rationale: Surface and bulk diffusion with intercalation of Cs and Sr (trapping) is probably the underlying mechanism of transport through the PyC. Given the large number of Cs atoms, the trapping may be somewhat less important in the IPyC than in the OPyC where fewer Cs atoms are expected and their concentration may be more on the order of the number of trapping sites.	Rationale: Transport models do not consider intercalation. Effective diffusion coefficients exist in both the U.S. and Germany for the Cs and Sr through IPyC. The data are probably a combination of diffusion and trapping via intercalation at these high temperatures but the two mechanisms have never been individually sorted out in any experiment. Furthermore, the models do not consider effects that oxidation could have on changing the microstucture and the intercalation behavior. The parameters needed for such detailed models and the changes in microstructure of the IPyC particle to particle and/or sometimes across the layer and/or as a result of oxidation make such an effort very expensive and time consuming. The use of effective diffusion coefficients although less scientifically satisfying is more pragmatic and may be completely acceptable in system safety analysis when accompanied by proper sensitivity studies.	Closure Criterion:

Additional Discussion

Life Cycle Phase	Factor, Characteristic or Phenomenon	Definition
Accident With Subsequent Air Intrusion	Inner PyC Layer: Chemical attack by air Kinetics	Rate of reaction per unit surface area as a function of temperature and partial pressure of air

Importance Rank and Rationale	Knowledge Level and Rationale	Remedy for Inadequate Knowledge/Issue Closure Criteria
Rank: H	7	Remedy:
Rationale: Oxidation of IPyC is needed to understand thermal response of the particles in the fuel element.	Rationale: Reaction rates for PyC are known at these temperatures.	Closure Criterion:

Additional Discussion

Life Cycle Phase	Factor, Characteristic or Phenomenon	Definition
Accident With Subsequent Air Intrusion	Inner PyC Layer: Chemical attack by air Catalysis	Modification of the reaction rate by fission products or impurities

Importance Rank and Rationale	Knowledge Level and Rationale	Remedy for Inadequate Knowledge/Issue Closure Criteria
Rank: M	4	Remedy:
Rationale: Impurities can affect the reaction rate and thus the cause of the ingress event.	Rationale: Reaction rate testing of PyC would implicitly include the effects of any impurities on the overall oxidation. No chemical reaction rate measurements have been performed using irradiated PyC where fission products may be in the layer. In principle sensitivity calculations can be performed with variations in the oxidation rate to bound this effect.	Closure Criterion:

Additional Discussion

Life Cycle Phase	Factor, Characteristic or Phenomenon	Definition
Accident With Subsequent Air Intrusion	Inner PyC Layer: Chemical attack by air	Changes in chemical form resulting from oxidizing or reducing fission products
	Changes in chemical form of fission products	

Importance Rank and Rationale	Knowledge Level and Rationale	Remedy for Inadequate Knowledge/Issue Closure Criteria
Rank: H	7	Remedy:
Rationale: This can be important because the transport behavior is dependent on the chemical form.	Rationale: This can also be calculated for a range of oxygen potentials to determine if any of the key fission products change in chemical form during the air or water ingress accident.	Closure Criterion:

Additional Discussion

Life Cycle Phase	Factor, Characteristic or Phenomenon	Definition
Accident With Subsequent Air Intrusion	Inner PyC Layer: Chemical attack by air	Changes in diffusivity, porosity, adsorptivity, etc.
	Changes in graphite properties	

Importance Rank and Rationale	Knowledge Level and Rationale	Remedy for Inadequate Knowledge/Issue Closure Criteria
Rank: M	6	Remedy:
Rationale: The oxidation can change the microstructure of the PyC by creating tunnels or pathways in the matrix. Thus, because the microstructure changes, the porosity, adsorptivity, etc. can also change.	Rationale: No measurements have been made on this effect. Conservative assumptions on such changes may allow sensitivity studies in this area.	Closure Criterion:

Additional Discussion

Life Cycle Phase	Factor, Characteristic or Phenomenon	Definition
Accident With Subsequent Air Intrusion	Inner PyC Layer: Chemical attack by air	Release of graphite FP inventory
	Holdup reversal	

Importance Rank and Rationale	Knowledge Level and Rationale	Remedy for Inadequate Knowledge/Issue Closure Criteria
Rank: M	6	Remedy:
Rationale: As the oxidation process continues, any fission products trapped at sites in the PyC may be released because of the thermal energy associated with the oxidation.	Rationale: This can be accounted for in a very simplistic, yet conservative manner if details are not well known or more sophisticated models with detrapping can be used if the fundamental data needed for such models exist.	Closure Criterion:

Additional Discussion

Life Cycle Phase	Factor, Characteristic or Phenomenon	Definition
Accident With Subsequent Air Intrusion	Inner PyC Layer: Chemical attack by air Temperature distribution	Impact of graphite oxidation on temperature distribution through material

Importance Rank and Rationale	Knowledge Level and Rationale	Remedy for Inadequate Knowledge/Issue Closure Criteria
Rank: H	8	Remedy:
Rationale: Very important in doing an oxidation calculation is to make sure the temperature response of the material as a result of the energy generation is properly calculated.	Rationale: This is well known and can be done in most of the safety codes used by NRC (e.g. MELCOR). The high conductivity of the PyC should make the gradient quite small in general. The degree of fine detail in the model may be an open question but can be handled with sensitivity studies.	Closure Criterion:

Additional Discussion

Life Cycle Phase	Factor, Characteristic or Phenomenon	Definition
Accident With Subsequent Air Intrusion	Buffer Layer Gas-phase diffusion	Diffusion of gaseous fission products through layer (Knudsen and bulk diffusion through pore structure, and pressure driven permeation through structure)

Importance Rank and Rationale	Knowledge Level and Rationale	Remedy for Inadequate Knowledge/Issue Closure Criteria
Rank: L	7	Remedy:
Rationale: The transport is fairly rapid and thus oxidation is not expected to affect the transport in this layer significantly.	Rationale: Rapid diffusion through the porous structure of the buffer is assumed in both U.S. and German transport models. Knudsen diffusion calculations confirm rapid gas phase transport.	Closure Criterion:

Additional Discussion

Life Cycle Phase	Factor, Characteristic or Phenomenon	Definition
Accident With Subsequent Air Intrusion	Buffer Layer Condensed-phase diffusion	Inter-granular diffusion and/or intra-grannular solid-state diffusion

Importance Rank and Rationale	Knowledge Level and Rationale	Remedy for Inadequate Knowledge/Issue Closure Criteria
Rank: L	7	Remedy:
Rationale: The transport is fairly rapid and thus oxidation is not expected to affect the transport in this layer significantly.	Rationale: Rapid transport of metallic fission products through the buffer has also been historically assumed in U.S. and German models. Key measurements needed to develop grain boundary diffusion models along the edges of the crystallite plans have never been obtained. Instead, effective diffusion coefficients are used.	Closure Criterion:

Additional Discussion

Life Cycle Phase	Factor, Characteristic or Phenomenon	Definition
Accident With Subsequent Air Intrusion	Buffer Layer Response to kernel swelling	Mechanical reaction of the layer to the growth of the kernel via swelling

Importance Rank and Rationale	Knowledge Level and Rationale	Remedy for Inadequate Knowledge/Issue Closure Criteria
Rank: M	4	Remedy:
Rationale: Not expected to be important in oxidation events	Rationale: Has been predicted by EU fuel modelers to be important at high burnup where swelling is large. Usually this is accommodated by appropriate changes in the buffer thickness to ensure that the kernel does not come in contact with the TRISO coated and cause large mechanical stresses. Has not been shown to be a problem in current irradiation database at relatively low burnup.	Closure Criterion:

Additional Discussion

Life Cycle Phase	Factor, Characteristic or Phenomenon	Definition
Accident With Subsequent Air Intrusion	Buffer Layer Maximum fuel gaseous fission product uptake	Maximum loading of fission products that can deposit from the gas phase onto surfaces of materials surrounding the fuel kernel

Importance Rank and Rationale	Knowledge Level and Rationale	Remedy for Inadequate Knowledge/Issue Closure Criteria
Rank: L	2	Remedy:
Rationale: Not important in oxidation events; probably more important in reactivity related events.	Rationale:	Closure Criterion:

Additional Discussion

Life Cycle Phase	Factor, Characteristic or Phenomenon	Definition
Accident With Subsequent Air Intrusion	Buffer Layer Layer oxidation	Reaction of buffer layer with oxide materials in the kernel

Importance Rank and Rationale	Knowledge Level and Rationale	Remedy for Inadequate Knowledge/Issue Closure Criteria
Rank: H	5	Remedy:
Rationale: Some oxide materials in the kernel become less stable resulting in additional oxygen that can react with the buffer causing additional CO formation.	Rationale: In UO_2 excess oxygen from fission reacts with fission products and then carbon from the buffer. This is well known and can be calculated and has been measured at low burnups. In UCO fuel no oxidation is expected.	Closure Criterion:

Additional Discussion

Life Cycle Phase	Factor, Characteristic or Phenomenon	Definition
Accident With Subsequent Air Intrusion	Buffer Layer Thermal gradient	Change in temperature with distance

Importance Rank and Rationale	Knowledge Level and Rationale	Remedy for Inadequate Knowledge/Issue Closure Criteria
Rank: L	6	Remedy:
Rationale: In pebble cores, the temperature gradients are generally low because of the lower power per particle in the core. Thus, Soret effects are much less important. Thus, this effect is important as an initial condition for the accident. Under oxidation events the gradients are much smaller and thus much less important during the accident.	Rationale: Temperature gradients can drive thermal diffusion (Soret effect). Temperature gradients under normal operation are very high in prismatic cores (up to 10000 K/cm) which can cause Soret effects in fission product transport. Values of the heat of solution needed to model the fission product transport are sorely lacking.	Closure Criterion:

Additional Discussion

Life Cycle Phase	Factor, Characteristic or Phenomenon	Definition
Accident With Subsequent Air Intrusion	Buffer Layer Irradiation and thermal shrinkage	Dimension changes in the buffer layer or changes in its porosity produced by irradiation or by exposure to elevated temperatures

Importance Rank and Rationale	Knowledge Level and Rationale	Remedy for Inadequate Knowledge/Issue Closure Criteria
Rank: M	7	Remedy:
Rationale: Rapid densification can occur in the buffer under exposure to neutrons. The state of the buffer is an important initial condition in fission product modeling. Thermal densification is not expected to be important at these temperatures.	Rationale: This is fairly well known and can be calculated.	Closure Criterion:

Additional Discussion

Life Cycle Phase	Factor, Characteristic or Phenomenon	Definition
Accident With Subsequent Air Intrusion	Buffer Layer: Chemical attack by air	Rate of reaction per unit surface area as a function of temperature and partial pressure of air
	Kinetics	

Importance Rank and Rationale	Knowledge Level and Rationale	Remedy for Inadequate Knowledge/Issue Closure Criteria
Rank: M	7	Remedy:
Rationale: Overall considered to be of lower importance than the other layers in the particle.	Rationale: Oxidation rates for PyC can be adjusted to estimate rates for the buffer.	Closure Criterion:

Additional Discussion

Life Cycle Phase	Factor, Characteristic or Phenomenon	Definition
Accident With Subsequent Air Intrusion	Buffer Layer: Chemical attack by air	Modification of the reaction rate by fission products or impurities
	Catalysis	

Importance Rank and Rationale	Knowledge Level and Rationale	Remedy for Inadequate Knowledge/Issue Closure Criteria
Rank: L	3	Remedy:
Rationale: In general, the effect is felt to be less important for this layer than other layers since rapid fission product transport through the layer is already assumed.	Rationale: Reaction rate testing of low-density carbon would implicitly include the effects of any impurities on the overall oxidation. No chemical reaction rate measurements have been performed using irradiated buffer material where fission products may be in the layer. In principle sensitivity calculations can be performed with variations in the oxidation rate to bound this effect.	Closure Criterion:

Additional Discussion

Life Cycle Phase	Factor, Characteristic or Phenomenon	Definition
Accident With Subsequent Air Intrusion	Buffer Layer: Chemical attack by air	Changes in chemical form resulting from oxidizing or reducing fission products
	Changes in chemical form of fission products	

Importance Rank and Rationale	Knowledge Level and Rationale	Remedy for Inadequate Knowledge/Issue Closure Criteria
Rank: H	7	Remedy:
Rationale: This can be important because the transport behavior is dependent on the chemical form.	Rationale: This can also be calculated for a range of oxygen potentials to determine if any of the key fission products change in chemical form during the air or water ingress accident.	Closure Criterion:

Additional Discussion

Life Cycle Phase	Factor, Characteristic or Phenomenon	Definition
Accident With Subsequent Air Intrusion	Buffer Layer: Chemical attack by air Changes in graphite properties	Changes in diffusivity, porosity, adsorptivity, etc.

Importance Rank and Rationale	Knowledge Level and Rationale	Remedy for Inadequate Knowledge/Issue Closure Criteria
Rank: L	3	Remedy:
Rationale: The oxidation can change the microstructure of the buffer by creating tunnels or pathways in the matrix. Thus, because the microstructure changes, the porosity, adsorptivity, etc. can also change. Given the high porosity in the buffer and the rapid fission product transport in this layer, these effects are not considered important.	Rationale: No measurements have been made on this effect.	Closure Criterion:

Additional Discussion

Life Cycle Phase	Factor, Characteristic or Phenomenon	Definition
Accident With Subsequent Air Intrusion	Buffer Layer: Chemical attack by air	Release of graphite FP inventory
	Holdup reversal	

Importance Rank and Rationale	Knowledge Level and Rationale	Remedy for Inadequate Knowledge/Issue Closure Criteria
Rank: L	3	Remedy:
Rationale: Given the rapid transport expected in the buffer, this effect is not expected to change the transport properties significantly.	Rationale: As the oxidation process continues any fission products trapped at sites in the buffer may be released because of the thermal energy associated with the oxidation. This can be accounted for in a very simplistic yet conservative manner if details are not well known or more sophisticated models with detrapping can be used if the fundamental data needed for such models exist.	Closure Criterion:

Additional Discussion

Life Cycle Phase	Factor, Characteristic or Phenomenon	Definition
Accident With Subsequent Air Intrusion	Buffer Layer: Chemical attack by air Temperature distribution	Impact of graphite oxidation on temperature distribution through material

Importance Rank and Rationale	Knowledge Level and Rationale	Remedy for Inadequate Knowledge/Issue Closure Criteria
Rank: H	8	Remedy:
Rationale: Very important in doing an oxidation calculation is to make sure the temperature response of the material as a result of the chemical reaction is properly calculated.	Rationale: This is well known and can be done in most of the safety codes used by NRC (e.g. MELCOR). The degree of fine detail in the model may be an open question but can be handled with sensitivity studies.	Closure Criterion:

Additional Discussion

Life Cycle Phase	Factor, Characteristic or Phenomenon	Definition
Accident With Subsequent Air Intrusion	Kernel Maximum fuel temperature	Maximum fuel temperature attained by the fuel kernel during the accident

Importance Rank and Rationale	Knowledge Level and Rationale	Remedy for Inadequate Knowledge/Issue Closure Criteria
Rank: H	7	Remedy:
Rationale: Temperature is the key parameter that drives fission product migration in the coated particle fuel.	Rationale: This can be calculated and sensitivity studies can determine its overall importance in any accident scenario.	Closure Criterion:

<u>Additional Discussion</u>

Life Cycle Phase	Factor, Characteristic or Phenomenon	Definition
Accident With Subsequent Air Intrusion	Kernel	The time-dependent variation of fuel temperature with time
	Temperature vs. time transient conditions	

Importance Rank and Rationale	Knowledge Level and Rationale	Remedy for Inadequate Knowledge/Issue Closure Criteria
Rank: H	7	Remedy:
Rationale: Similar to temperature and time at temperature, the thermal response of the particle is important to calculating fission product behavior in the particle.	Rationale: Sensitivity studies can be easily performed to determine the impact of this factor on the overall progression of the accident.	Closure Criterion:

Additional Discussion

Life Cycle Phase	Factor, Characteristic or Phenomenon	Definition
Accident With Subsequent Air Intrusion	Kernel Energy Transport: Conduction within kernel	Flow of heat within a medium from a region of high temperature to a region of low temperature

Importance Rank and Rationale	Knowledge Level and Rationale	Remedy for Inadequate Knowledge/Issue Closure Criteria
Rank: M	6	Remedy:
Rationale: Needed to calculate thermal response of kernel	Rationale: Thermal conductivity of UO_2 is fairly high and reasonably well known. Conductivity of UCO is assumed to be that of UO_2. Can be varied easily in sensitivity studies to determine impact.	Closure Criterion:

Additional Discussion

Life Cycle Phase	Factor, Characteristic or Phenomenon	Definition
Accident With Subsequent Air Intrusion	Kernel Thermodynamic state of fission products	Chemical and physical state of fission products

Importance Rank and Rationale	Knowledge Level and Rationale	Remedy for Inadequate Knowledge/Issue Closure Criteria
Rank: H	7	Remedy:
Rationale: Thermodynamic state of fission products can determine volatility and mobility of the species.	Rationale: Thermodynamic studies have been performed for UO_2, UCO and UC_2 systems and chemical states of major fission products have been identified as a function of burnup and temperature. The impact of air and/or water can be evaluated.	Closure Criterion:

Additional Discussion

Life Cycle Phase	Factor, Characteristic or Phenomenon	Definition
Accident With Subsequent Air Intrusion	Kernel Oxygen flux	Mass transport of oxygen per unit surface area per unit time

Importance Rank and Rationale	Knowledge Level and Rationale	Remedy for Inadequate Knowledge/Issue Closure Criteria
Rank: L	6	Remedy:
Rationale: Less important in air and water ingress events than in traditional heatup events.	Rationale:	Closure Criterion:

Additional Discussion

Life Cycle Phase	Factor, Characteristic or Phenomenon	Definition
Accident With Subsequent Air Intrusion	Kernel Grain growth	Enlargement of grains as a result of diffusion

Importance Rank and Rationale	Knowledge Level and Rationale	Remedy for Inadequate Knowledge/Issue Closure Criteria
Rank: L	4	Remedy:
Rationale: Not important for air or water ingress events.	Rationale:	Closure Criterion:

Additional Discussion

Life Cycle Phase	Factor, Characteristic or Phenomenon	Definition
Accident With Subsequent Air Intrusion	Kernel Buffer carbon-kernel interaction	Chemical reaction between carbon and the fuel (UO_2) to form UC_2 and CO (gas)

Importance Rank and Rationale	Knowledge Level and Rationale	Remedy for Inadequate Knowledge/Issue Closure Criteria
Rank: H	6	Remedy:
Rationale: The reaction of the kernel and the buffer is known to form a "rind" of UC_2 at the interface between the two layers. Photomicrographs show a different phase that is easily distinguished optically. Such interaction can result in release of fission products.	Rationale:	Closure Criterion:

Additional Discussion

Life Cycle Phase	Factor, Characteristic or Phenomenon	Definition
Accident With Subsequent Air Intrusion	Kernel: Chemical attack by air Kinetics	Rate of reaction per unit surface area as a function of temperature and partial pressure of air

Importance Rank and Rationale	Knowledge Level and Rationale	Remedy for Inadequate Knowledge/Issue Closure Criteria
Rank: H	7 for UO_2/ 6 for UCO	Remedy:
Rationale: Oxidation kinetics are needed to understand physio-chemical changes in the kernel and effect on fission product release.	Rationale: Air oxidation of UO_2 has been studied and data are available in the literature. Less information is available on UCO.	Closure Criterion:

Additional Discussion

Life Cycle Phase	Factor, Characteristic or Phenomenon	Definition
Accident With Subsequent Air Intrusion	Kernel: Chemical attack by air Catalysis	Modification of the reaction rate by fission products or impurities

Importance Rank and Rationale	Knowledge Level and Rationale	Remedy for Inadequate Knowledge/Issue Closure Criteria
Rank: M	3	Remedy:
Rationale: Impurities can influence reaction rates.	Rationale: Reaction rate testing of UO_2/ UCO would implicitly include the effects of any impurities on the overall oxidation. Reaction rate testing of irradiated kernel material would include the effect of fission products. In principle, sensitivity calculations can be performed with variations in the oxidation rate to bound this effect.	Closure Criterion:

Additional Discussion

Life Cycle Phase	Factor, Characteristic or Phenomenon	Definition
Accident With Subsequent Air Intrusion	Kernel: Chemical attack by air Changes in chemical form of fission products	Changes in chemical form resulting from oxidizing or reducing fission products

Importance Rank and Rationale	Knowledge Level and Rationale	Remedy for Inadequate Knowledge/Issue Closure Criteria
Rank: H	7	Remedy:
Rationale: This can be important because the transport behavior is dependent on the chemical form.	Rationale: This can also be calculated for a range of oxygen potentials to determine if any of the key fission products change in chemical form during the air or water ingress accident.	Closure Criterion:

Additional Discussion

Life Cycle Phase	Factor, Characteristic or Phenomenon	Definition
Accident With Subsequent Air Intrusion	Kernel: Chemical attack by air Changes in kernel properties	Change in diffusivity, porosity, adsorptivity, etc.

Importance Rank and Rationale	Knowledge Level and Rationale	Remedy for Inadequate Knowledge/Issue Closure Criteria
Rank: M	5	Remedy:
Rationale: The oxidation can change the microstructure of the kernel and the resultant transport properties. Hyperstoichiometric uranium dioxide will behave differently than UO_2. In UCO, the oxygen will react with the carbide phase to produce more UO_2. These are important effects to determine fission product mobility in the kernel. This is rated Medium because it is difficult to see how a lot of air can get all the way to the kernel.	Rationale: Little data exist on changes in transport properties. Some data exist on integral effect of fission production.	Closure Criterion:

Additional Discussion

Appendix F.2

Detailed PIRT Submittal by the ORNL Panel Member

R. Morris

TRISO Fuel PIRT: Accident With Subsequent Air Intrusion

Life Cycle Phase	Factor, Characteristic or Phenomenon	Definition
Accident With Subsequent Air Intrusion	Fuel Element Irradiation history	The temperature, burnup and fast fluence history of the layer

Importance Rank and Rationale	Knowledge Level and Rationale	Remedy for Inadequate Knowledge/Issue Closure Criteria
Rank: H	≤ 1600 °C: 7	Remedy: None if the operating envelope remains the same, otherwise additional testing is necessary
	> 1600 °C: N/A	Remedy: N/A
Rationale: The fuel behavior is strongly related to its irradiation history. Increasing burnup and fluence beyond established limits generally degrades performance. The fraction of particles failed during normal operation is important as well as the fact that they will release first.	Rationale: (≤ 1600 °C) The Germans have collected a large database for their fuel under their specific operating conditions. Deviations from these conditions warrant additional testing. Note that the proven fuel envelope may be less demanding than that required for the turbine concepts.	Closure Criterion: Verification that the fuel can meet any new operating condition.
	Rationale (> 1600 °C) N/A	Closure Criterion: N/A

Additional Discussion

For a discussion of the best performing fuel see:

Performance Evaluation of Modern HTR TRISO Fuel, R. Gontard, H. Nabielek, HTA-1B-05/90, July 1990

Fuel Performance and Fission Product Behavior in Gas Cooled Reactors, IAEA-TECDOC-978 (1997)

Life Cycle Phase	Factor, Characteristic or Phenomenon	Definition
Accident With Subsequent Air Intrusion	Fuel Element Condensed-phase diffusion	Inter-granular diffusion and/or intra-granular solid-state diffusion

Importance Rank and Rationale	Knowledge Level and Rationale	Remedy for Inadequate Knowledge/Issue Closure Criteria
Rank: H	≤ 1600 °C: 4	Remedy: Defer to fission product transport area.
	> 1600 °C: N/A	Remedy: N/A
Rationale: The major barriers to fission product release are the particle coating layers. The diffusion through the fuel element matrix is considered to be relatively high, although it does sorb and trap some fission products. When this material is oxidized, these fission products can be released, so the inventory is important.	Rationale: (≤ 1600 °C) The fuel element matrix sorbs some of the released fission products (metals); data exist to estimate the inventory, however, chemical attack may alter things.	Closure Criterion: Diffusion and trapping coefficients for the material of interest as a function of temperature
	Rationale (> 1600 °C) N/A	Closure Criterion: N/A

Additional Discussion

Diffusion through the fuel element matrix is fairly rapid compared to the particle coating layers. Gases are not held up, but there is significant sorption of the released metals. Overall, the reactor core components can provide an attenuation factor of 10-1000 for the metallics; oxidation could release this inventory. The GT-MHR may change its matrix composition from the historical resins; if so, additional investigations may be necessary.
For examples of diffusion and sorption behavior in different HTGR materials see:

Fuel Performance and Fission Product Behavior in Gas Cooled Reactors, IAEA-TECDOC-978 (1997)

For general interest in the transport of volatile fission products through the reactor system see:

.
An analytical Study of Volatile Metallic Fission Product Release From Very High Temperature Gas-Cooled Reactor Fuel and Core, S. Mitake, et. al., Nuclear Technology, 81 (1988), pages 7-12.
Fission Product Plateout and Liftoff in the MHTGR Primary System: A Review, NUREG/CR-5647

This sorbed or plated out material could be released in the event of an accident.

Life Cycle Phase	Factor, Characteristic or Phenomenon	Definition
Accident With Subsequent Air Intrusion	Fuel Element Gas phase diffusion	Diffusion of gaseous fission products through layer (Knudsen and bulk diffusion through pore structure, and pressure driven permeation through structure). Other factors include holdup, cracking, adsorption, site poisoning, permeability, sintering, and annealing.

Importance Rank and Rationale	Knowledge Level and Rationale	Remedy for Inadequate Knowledge/Issue Closure Criteria
Rank: H	≤ 1600 °C: 7	Remedy: None
	> 1600 °C: N/A	Remedy: N/A
Rationale: The fission gases migrate rapidly through the fuel element matrix after they escape from the particle. This fact is used to monitor fuel behavior via R/B. Any damaged particles will release fission gases. Air will react in these regions.	Rationale: (≤ 1600 °C) Data shows that the gases move rapidly through the matrix material and quickly enter the coolant and/or fuel element.	Closure Criterion: None
	Rationale (> 1600 °C) N/A	Closure Criterion: N/A

Additional Discussion

Fuel Performance and Fission Product Behavior in Gas Cooled Reactors, IAEA-TECDOC-978 (1997)
Source Term Estimation for Small-Sized HTRs: Status and Further Needs, Extracted From German Safety Analysis, R. Moormann, et. al., Nuclear Technology, 135, (2001), pages 183-193
Methods and Data for HTGR Fuel Performance and Radionuclide Release Modeling during Normal Operational and Accidents for Safety Analysis, K.

Fission gases move rapidly to the coolant once they exit the particle. In a reactor they are removed by the coolant purification system so the circulating inventory is low. Transport of volatile metallics is determined by the sorption isotherms and dust. Gases released by damaged particles will rapidly move through the reactor core system.
The actual reaction of air with the core materials is more complex. For a discussion of air ingress accidents and its effect on fuel see:
Verfondern, et. al., Jul-2721

For examples of the type of modeling that has been done for transport see:

.

Fission Product Plateout and Liftoff in the MHTGR Primary System: A Review, NUREG/CR-5647

For fuel accident models see: *Compilation of Fuel Performance and Fission Product Transport Models and Database for MHTGR Design*, Martin, R.C., ORNL/NPR-91/6

Life Cycle Phase	Factor, Characteristic or Phenomenon	Definition
Accident With Subsequent Air Intrusion	Fuel Element: Transport of metallic FPs through fuel element	Chemical stoichiometry of the chemical species that includes the radioisotope of interest
	Chemical form	

Importance Rank and Rationale	Knowledge Level and Rationale	Remedy for Inadequate Knowledge/Issue Closure Criteria
Rank: H	≤ 1600 °C: 5	Remedy: Determine the need for this detailed knowledge.
	> 1600 °C: N/A	Remedy: N/A
Rationale: The chemical form of the fission product will determine how it interacts with the reactor system materials. The chemical environment of the kernel and the reactor system can be quite different and depend on the kernel composition and the coolant impurities. The kernel is expected to be somewhat oxidizing and the normal reactor system quite reducing, thus the chemical form of the fission product may change as it leaves the fuel. Once the accident starts, the environment may become oxidizing again.	Rationale: (≤ 1600 °C) Thermochemical calculations can give plausible chemical forms, but this author is not aware of any measurements confirming the chemical states.	Closure Criterion: If necessary, collect or calculate the compounds.
	Rationale (> 1600 °C) N/A	Closure Criterion: N/A

Additional Discussion

This issue of chemical forms probably should be covered under fission product transport since the reactor system has a difference chemical potential than the fuel. It will change again with the accident. Carbides may oxidize. See:

Fission Product Plateout and Liftoff in the MHTGR Primary System: A Review, NUREG/CR-5647
Chemical Behavior of Fission Products in Core Heatup Accidents in High-Temperature Gas-Cooled Reactors, R. Moormann, Nuclear Technology, 94 (1991), pages 56-67.
Source Term Estimation for Small-Sized HTRs: Status and Further Needs, Extracted From German Safety Analysis, R. Moormann, et. al., Nuclear Technology, 135, (2001), pages 183-193
Methods and Data for HTGR Fuel Performance and Radionuclide Release Modeling during Normal Operational and Accidents for Safety Analysis, K. Verfondern, et. al., Jul-2721

Life Cycle Phase	Factor, Characteristic or Phenomenon	Definition
Accident With Subsequent Air Intrusion	Fuel Element: Chemical attack by air Kinetics	Rate of reaction per unit surface area as a function of temperature and partial pressure of air

Importance Rank and Rationale	Knowledge Level and Rationale	Remedy for Inadequate Knowledge/Issue Closure Criteria
Rank: H	≤ 1600 °C: 5	Remedy: Collect the relevant data.
	> 1600 °C: N/A	Remedy: N/A
Rationale: Kinetics data is necessary to determine the reaction rate for both the matrix material and the fuel materials.	Rationale: (≤ 1600 °C) Some reaction data is available, but more specific information may be required.	Closure Criterion: Adequate data for the calculations.
	Rationale (> 1600 °C) N/A	Closure Criterion: N/A

Additional Discussion

For different reactor types a considerable amount graphite oxidation work has been done. The kinetics depend a lot on the type of material. Some results are discussed in:

Fuel Performance and Fission Product Behavior in Gas Cooled Reactors, IAEA-TECDOC-978 (1997)

Also, for graphite materials**:**

Corrosion of Nuclear-Grade Graphites: Air Oxidation of H-451, E.L. Fuller, et. al., ORNL/NPR-91/27, October 1992

Life Cycle Phase	Factor, Characteristic or Phenomenon	Definition
Accident With Subsequent Air Intrusion	Fuel Element: Chemical attack by air Catalysis	Modification of the reaction rate by fission products or impurities

Importance Rank and Rationale	Knowledge Level and Rationale	Remedy for Inadequate Knowledge/Issue Closure Criteria
Rank: H	≤ 1600 °C: 4	Remedy: Determine the sensitivity of the situation to rates. Collect the relevant data if necessary.
	> 1600 °C: N/A	Remedy: N/A
Rationale: The reactions rate can have great local variations due to catalysis from impurities or fission products.	Rationale: (≤ 1600 °C) Local rates can be quite different than global rates.	Closure Criterion: Resolution of the modeling needs or the collection of the relevant data.
	Rationale (> 1600 °C) N/A	Closure Criterion: N/A

Additional Discussion

For the effects of trace elements on graphite H-451 see:

The Effect of Trace Elements on the Surface Oxidation of H-451 Graphite, O.C. Kopp, et. al., ORNL/NPR-92/56, December 1992

Life Cycle Phase	Factor, Characteristic or Phenomenon	Definition
Accident With Subsequent Air Intrusion	Fuel Element: Chemical attack by air	Changes in chemical form resulting from oxidizing or reducing fission products
	Changes in chemical form of fission products	

Importance Rank and Rationale	Knowledge Level and Rationale	Remedy for Inadequate Knowledge/Issue Closure Criteria
Rank: H	≤ 1600 °C: 4	Remedy: Determine the need for this knowledge, collect as necessary.
	> 1600 °C: N/A	Remedy: N/A
Rationale: Changes in the chemical form of the fission products can greatly change their transport properties.	Rationale: (≤ 1600 °C) Thermochemical codes can calculate the possible chemical compounds. Little confirmation work is available.	Closure Criterion: Data to resolve uncertainties.
	Rationale (> 1600 °C) N/A	Closure Criterion: N/A

<u>Additional Discussion</u>

The forms and migration of the fission products can be complex. For some information on the chemical forms see:

Fission Product Plateout and Liftoff in the MHTGR Primary System: A Review, NUREG/CR-5647

Chemical Behavior of Fission Products in Core Heatup Accidents in High-Temperature Gas-Cooled Reactors, R. Moormann, Nuclear Technology, 94 (1991), pages 56-67.

Life Cycle Phase	Factor, Characteristic or Phenomenon	Definition
Accident With Subsequent Air Intrusion	Fuel Element: Chemical attack by air	Changes in diffusivity, porosity, adsorptivity, etc.
	Changes in graphite properties	

Importance Rank and Rationale	Knowledge Level and Rationale	Remedy for Inadequate Knowledge/Issue Closure Criteria
Rank: H	≤ 1600 °C: 4	Remedy: Determine the need for this data and collect the necessary information.
	> 1600 °C: N/A	Remedy: N/A
Rationale: Changes in graphite properties may change reaction rates and transport properties.	Rationale: (≤ 1600 °C) Some data is available for this from other reactor types.	Closure Criterion: Data and models to support the needs.
	Rationale (> 1600 °C) N/A	Closure Criterion: N/A

Additional Discussion

This issue depends on the particular graphite and matrix materials involved.

Life Cycle Phase	Factor, Characteristic or Phenomenon	Definition
Accident With Subsequent Air Intrusion	Fuel Element: Chemical attack by air	Release of graphite FP inventory
	Holdup reversal	

Importance Rank and Rationale	Knowledge Level and Rationale	Remedy for Inadequate Knowledge/Issue Closure Criteria
Rank: H	≤ 1600 °C: 4	Remedy: Determine what is in the graphite and how it moves as the graphite oxidizes.
	> 1600 °C: N/A	Remedy: N/A
Rationale: As the matrix material and graphite are consumed during the reaction, the inventory of fission products may be released or converted to a form that migrates at a higher rate.	Rationale: (≤ 1600 °C) Air ingress experiments have been conducted and the releases examined. Also, modeling has been done for this and other reactor types.	Closure Criterion: Sufficient information to model or bound the situation.
	Rationale (> 1600 °C) N/A	Closure Criterion: N/A

Additional Discussion

If the fuel is high quality and the operational temperatures below about 1300°C, only the in-service failed fuel will contribute to the release inventory. Thus, the actual material to be released may be quite small. See:

Source Term Estimation for Small-Sized HTRs: Status and Further Needs, Extracted From German Safety Analysis, R. Moormann, et. al., Nuclear Technology, 135, (2001), pages 183-193

Fuel Performance and Fission Product Behavior in Gas Cooled Reactors, IAEA-TECDOC-978 (1997)

Compilation of Fuel Performance and Fission Product Transport Models and Database for MHTGR Design, R. Martin, ORNL/NPR-91/6

Methods and Data for HTGR Fuel Performance and Radionuclide Release Modeling during Normal Operational and Accidents for Safety Analysis, K. Verfondern, et. al., Jul-2721

Life Cycle Phase	Factor, Characteristic or Phenomenon	Definition
Accident With Subsequent Air Intrusion	Fuel Element: Chemical attack by air Temperature distribution	Impact of graphite oxidation on temperature distribution through material

Importance Rank and Rationale	Knowledge Level and Rationale	Remedy for Inadequate Knowledge/Issue Closure Criteria
Rank: H	≤ 1600 °C: 4	Remedy: Determine the data needed to be collected.
	> 1600 °C: N/A	Remedy: N/A
Rationale: The temperature distribution needs to be known to predict fuel performance and the course of the accident. Both afterheat and heat of combustion need to be known.	Rationale: (≤ 1600 °C) Graphite oxidation codes have been developed and similar cases run.	Closure Criterion: Sufficient information to resolve the issue.
	Rationale (> 1600 °C) N/A	Closure Criterion: N/A

Additional Discussion

Life Cycle Phase	Factor, Characteristic or Phenomenon	Definition
Accident With Subsequent Air Intrusion	Outer PyC Layer Gas-phase diffusion	Diffusion of gaseous fission products through layer (Knudsen and bulk diffusion through pore structure, and pressure driven permeation through structure)

Importance Rank and Rationale	Knowledge Level and Rationale	Remedy for Inadequate Knowledge/Issue Closure Criteria
Rank: H	≤ 1600 °C: 5	Remedy: Insure that proper PyC is manufactured. Material properties are difficult to characterize.
	> 1600 °C: N/A	Remedy: N/A
Rationale: The PyC layers hold fission gases well. The diffusion coefficients are generally quite low. The biggest concern is the rupture of the layer and the release of gases (if other layers are bad). This layer may be attacked by air.	Rationale: (≤ 1600 °C) A great deal of testing has been conduced on PyC at the temperatures of interest. The primary concern is fabricating the proper material and its loss during the accident.	Closure Criterion: Test fuel performs as expected
	Rationale (> 1600 °C) N/A	Closure Criterion: N/A

Additional Discussion

Extensive testing has been done of the PyC for BISO and TRISO fuels under helium conditions, less so under air/steam see:

Performance Evaluation of Modern HTR TRISO Fuel, R. Gontard, H. Nabielek, HTA-1B-05/90, July 1990

Fuel Performance and Fission Product Behavior in Gas Cooled Reactors, IAEA-TECDOC-978 (1997)

Nuclear Technology, 35, Number 2 (entire issue devoted to coated particle fuels)

If the OpyC is unbreached, the helium heatup issues generally apply. If the layer is damaged or burned away, then the loss of OPyC issues would apply.

Life Cycle Phase	Factor, Characteristic or Phenomenon	Definition
Accident With Subsequent Air Intrusion	Outer PyC Layer Condensed-phase diffusion	Inter-granular diffusion and/or intra-granular solid-state diffusion

Importance Rank and Rationale	Knowledge Level and Rationale	Remedy for Inadequate Knowledge/Issue Closure Criteria
Rank: H	≤ 1600 °C: 7	Remedy: None
	> 1600 °C: N/A	Remedy: N/A
Rationale: Metallic fission products generally diffuse through the layer rapidly at high temperatures. Its loss would make some difference, but the primary issue would be exposing the SiC to the air.	Rationale: (≤ 1600 °C) The OPyC offers little holdup to metallics at accident temperatures.	Closure Criterion: None
	Rationale (> 1600 °C) N/A.	Closure Criterion: N/A

Additional Discussion

Extensive testing has been done of the PyC for in helium BISO and TRISO fuels; less has been done for air/steam. See:

Performance Evaluation of Modern HTR TRISO Fuel, R. Gontard, H. Nabielek, HTA-1B-05/90, July 1990

Fuel Performance and Fission Product Behavior in Gas Cooled Reactors, IAEA-TECDOC-978 (1997)

Nuclear Technology, 35, Number 2 (entire issue devoted to coated particle fuels)

Life Cycle Phase	Factor, Characteristic or Phenomenon	Definition
Accident With Subsequent Air Intrusion	Outer PyC Layer Layer oxidation	Uptake of oxygen by the layer through a chemical reaction

Importance Rank and Rationale	Knowledge Level and Rationale	Remedy for Inadequate Knowledge/Issue Closure Criteria
Rank: H	≤ 1600 °C: 4	Remedy: Determine the conditions of interest and collect the necessary data.
	> 1600 °C: N/A	Remedy: N/A
Rationale: The oxidation rate determines the life of this layer under air ingress. Generally, a bulk rate is assumed rather than detailed behavior.	Rationale: (≤ 1600 °C) Testing has been done, but it is of a more integral nature.	Closure Criterion: Resolution of the data gaps.
	Rationale (> 1600 °C) N/A	Closure Criterion: N/A

Additional Discussion

For information on fuel exposure in steam/air see:

Source Term Estimation for Small-Sized HTRs: Status and Further Needs, Extracted From German Safety Analysis, R. Moormann, et. al., Nuclear Technology, 135, (2001), pages 183-193

Fuel Performance and Fission Product Behavior in Gas Cooled Reactors, IAEA-TECDOC-978 (1997)

Compilation of Fuel Performance and Fission Product Transport Models and Database for MHTGR Design, R. Martin, ORNL/NPR-91/6

Methods and Data for HTGR Fuel Performance and Radionuclide Release Modeling during Normal Operational and Accidents for Safety Analysis, K. Verfondern, et. al., Jul-2721

Life Cycle Phase	Factor, Characteristic or Phenomenon	Definition
Accident With Subsequent Air Intrusion	Outer PyC Layer Stress state (compression/tension)	The state of the forces induced by external forces that are acting across the layer to resist movement

Importance Rank and Rationale	Knowledge Level and Rationale	Remedy for Inadequate Knowledge/Issue Closure Criteria
Rank: M	≤ 1600 °C: 6	Remedy: Review and collect new data for the codes if necessary. Material properties are the major issue.
	> 1600 °C: N/A	Remedy: N/A
Rationale: The stress state of the OPyC helps keep a compression force on the SiC. Failure of the OPyC by oxidation increases the likelihood of SiC failure.	Rationale: (≤ 1600 °C) The fuel design codes include these calculations. (Assumes the PyC is irradiation stable)	Closure Criterion: Adequate test fuel performance.
	Rationale (> 1600 °C) N/A	Closure Criterion: N/A

Additional Discussion

Revised MHTGR High-Temperature Fuel Performance Models, R.C. Martin, ORNL/NPR-92/16

Methods and Data for HTGR Fuel Performance and Radionuclide Release Modeling during Normal Operational and Accidents for Safety Analysis, K.

See the PIRT Design Table for references on fuel design. Also see the accident models. The most common accident model is pressure vessel failure. See: Verfondern, et. al., Jul-2721

Compilation of Fuel Performance and Fission Product Transport Models and Database for MHTGR Design, Martin, R.C., ORNL/NPR-91/6

Revised MHTGR High-Temperature Fuel Performance Models, R.C. Martin, ORNL/NPR-92/16

Fuel Performance and Fission Product Behavior in Gas Cooled Reactors, IAEA-TECDOC-978 (1997)

Life Cycle Phase	Factor, Characteristic or Phenomenon	Definition
Accident With Subsequent Air Intrusion	Outer PyC Layer Intercalation	Trapping of species between sheets of the graphite structure

Importance Rank and Rationale	Knowledge Level and Rationale	Remedy for Inadequate Knowledge/Issue Closure Criteria
Rank: L	≤ 1600 °C: 2	Remedy: Review data to determine if it is important.
	> 1600 °C: N/A	Remedy: N/A
Rationale: Small amounts of material may be trapped in the layer, but the material sorbed in the matrix is expected to be much larger.	Rationale: (≤ 1600 °C) Some work has been done in this area, but it has not been an important driver.	Closure Criterion: None
	Rationale (> 1600 °C) N/A	Closure Criterion: N/A

Additional Discussion

With good SiC, the fission product transport to the OPyC is very low. Some new modeling efforts are determining if this is an important factor.

Life Cycle Phase	Factor, Characteristic or Phenomenon	Definition
Accident With Subsequent Air Intrusion	Outer PyC Layer Trapping	Adsorption of fission products on defects

Importance Rank and Rationale	Knowledge Level and Rationale	Remedy for Inadequate Knowledge/Issue Closure Criteria
Rank: L	≤ 1600 °C: 3	Remedy: Review data to determine if it is important.
	> 1600 °C: N/A	Remedy: N/A
Rationale: Some trapping is used in the modeling and it may play a role in the transport, but the FPs in the matrix appears to be the major concern.	Rationale: (≤ 1600 °C) Some modeling has looked at this	Closure Criterion: None
	Rationale (> 1600 °C) N/A	Closure Criterion: N/A

Additional Discussion

With good SiC, the fission product transport to the OPyC is very low. Current modeling efforts are investigating this effect. Even if it is a real effect, it may be consumed by general data uncertainties.

Life Cycle Phase	Factor, Characteristic or Phenomenon	Definition
Accident With Subsequent Air Intrusion	Outer PyC Layer Cracking	Lengths, widths and numbers of cracks produced in layer during operation or an accident

Importance Rank and Rationale	Knowledge Level and Rationale	Remedy for Inadequate Knowledge/Issue Closure Criteria
Rank: H	≤ 1600 °C: 5 (models determine failure rather than cracks)	Remedy: Better data and model for fuel performance, especially PyC behavior.
	> 1600 °C: N/A	Remedy: N/A
Rationale: Failure of the OPyC affects the likelihood of SiC failure and exposes it to air/steam. Cracking of particle layers can result in particle failure. One intact PyC can retain gases, but metallic release will be high. Modeling often assumes that particles fail by overpressure rather than a small crack. A crack is assumed to equal failure.	Rationale: (≤ 1600 °C) Fuel models have been developed to model normal and accident behavior. Particles are assumed to fail when they meet some weakness criteria based on a layer stress. Details of cracks are not modeled (yet). Agreement has been good for high quality fuel	Closure Criterion: Models that predict fuel behavior under normal and accident conditions. Does one need cracks or just failure? This adds a lot of complexity.
	Rationale (> 1600 °C) N/A	Closure Criterion: N/A

Additional Discussion

For some work on examining the effects of cracks on fuel performance and general models see:

Consideration of the Effects on Fuel Particle Behavior from Shrinkage Cracks in the Inner Pyrocarbon Layer, G.Miller, et. al., Journal of Nuclear Materials, 295 (2001), pages 205-212.

Key Differences in the Fabrication, Irradiation and Safety Testing of U.S. and German TRISO-coated Particle Fuel and Their Implications on Fuel Performance, D.A. Petti, et. al Nuclear Engineering and Design, 222 (2003) 281-297.
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MHTGR TRISO-P Fuel Failure Evaluation Report, DOE-HTGR-90390*Compilation of Fuel Performance and Fission Product Transport Models and Database for MHTGR Design*, Martin, R.C., ORNL/NPR-91/6

Methods and Data for HTGR Fuel Performance and Radionuclide Release Modeling during Normal Operational and Accidents for Safety Analysis, K. Verfondern, et. al., Jul-2721

Compilation of Fuel Performance and Fission Product Transport Models and Database for MHTGR Design, Martin, R.C., ORNL/NPR-91/6

Revised MHTGR High-Temperature Fuel Performance Models, R.C. Martin, ORNL/NPR-92/16

Fuel Performance and Fission Product Behavior in Gas Cooled Reactors, IAEA-TECDOC-978 (1997)

Life Cycle Phase	Factor, Characteristic or Phenomenon	Definition
Accident With Subsequent Air Intrusion	Outer PyC Layer: Chemical attack by air	Rate of reaction per unit surface area as a function of temperature and partial pressure of air
	Kinetics	

Importance Rank and Rationale	Knowledge Level and Rationale	Remedy for Inadequate Knowledge/Issue Closure Criteria
Rank: H	≤ 1600 °C: 4	Remedy: Determine conditions and perform testing.
	> 1600 °C: N/A	Remedy: N/A
Rationale: The reaction rate determines how long the layer will last and support or protect the SiC.	Rationale: (≤ 1600 °C) Much work has been done, but the results are sensitive to materials.	Closure Criterion: Collect the required data.
	Rationale (> 1600 °C) N/A	Closure Criterion: N/A

Additional Discussion

Some work has been done in this area, but specific rates and mechanisms have not been isolated: *Methods and Data for HTGR Fuel Performance and Radionuclide Release Modeling during Normal Operational and Accidents for Safety Analysis*, K. Verfondern, et. al., Jul-2721

Compilation of Fuel Performance and Fission Product Transport Models and Database for MHTGR Design, Martin, R.C., ORNL/NPR-91/6

Fuel Performance and Fission Product Behavior in Gas Cooled Reactors, IAEA-TECDOC-978 (1997)

Reactivity of Graphite and Fueled Graphite Spheres with Oxidizing Gases, J.P. Blakely, ORNL-TM-751, February 1964

The particular material under relevant conditions needs to be examined, as there can be considerable variation in results.

Life Cycle Phase	Factor, Characteristic or Phenomenon	Definition
Accident With Subsequent Air Intrusion	Outer PyC Layer: Chemical attack by air Catalysis	Modification of the reaction rate by fission products or impurities

Importance Rank and Rationale	Knowledge Level and Rationale	Remedy for Inadequate Knowledge/Issue Closure Criteria
Rank: M	≤ 1600 °C: 3	Remedy: Determine if it is relevant or important
	> 1600 °C: N/A	Remedy: N/A
Rationale: A catalysis can increase the reaction rate in the layer and hasten its failure.	Rationale: (≤ 1600 °C) This is an unexplored area for fuel, but the graphite air reaction has seen much work.	Closure Criterion: Collect the effects of catalysis if necessary.
	Rationale (> 1600 °C) N/A	Closure Criterion: N/A

Additional Discussion

If the fission product inventory in the PyC is low and its loss does not significantly increase the SiC failure probably, then this issue may be unimportant.

For the effects of trace elements on graphite H-451 see:

The Effect of Trace Elements on the Surface Oxidation of H-451 Graphite, O.C. Kopp, et. al., ORNL/NPR-92/56, December 1992
A literature search should come up with some material on catalysis for PyC. It is likely to be sensitive to the exact nature of the materials.

Life Cycle Phase	Factor, Characteristic or Phenomenon	Definition
Accident With Subsequent Air Intrusion	Outer PyC Layer: Chemical attack by air	Changes in chemical form resulting from oxidizing or reducing fission products
	Changes in chemical form of fission products	

Importance Rank and Rationale	Knowledge Level and Rationale	Remedy for Inadequate Knowledge/Issue Closure Criteria
Rank: H	≤ 1600 °C: 4	Remedy: Determine the need for this knowledge, collect as necessary.
	> 1600 °C: N/A	Remedy: N/A
Rationale: Changes in the chemical form of the fission products can greatly change their transport properties.	Rationale: (≤ 1600 °C) Thermochemical codes can calculate the possible chemical compounds. Little confirmation work is available.	Closure Criterion: Collect data to resolve uncertainties
	Rationale (> 1600 °C) N/A	Closure Criterion: N/A

Additional Discussion

If the inventory of the layer is low, this issue may be of little practical importance. The forms and migration of the fission products can be complex. For some information on the chemical forms see:

Fission Product Plateout and Liftoff in the MHTGR Primary System: A Review, NUREG/CR-5647

Chemical Behavior of Fission Products in Core Heatup Accidents in High-Temperature Gas-Cooled Reactors, R. Moormann, Nuclear Technology, 94 (1991), pages 56-67.

Life Cycle Phase	Factor, Characteristic or Phenomenon	Definition
Accident With Subsequent Air Intrusion	Outer PyC Layer: Chemical attack by air	Changes in diffusivity, porosity, adsorptivity, etc.
	Changes in graphite properties	

Importance Rank and Rationale	Knowledge Level and Rationale	Remedy for Inadequate Knowledge/Issue Closure Criteria
Rank: M	≤ 1600 °C: 1	Remedy: Determine if this item is relevant.
	> 1600 °C: N/A	Remedy: N/A
Rationale: The modeling is not performed at this level; generally, the layer is assumed to disappear at some rate.	Rationale: (≤ 1600 °C) Not examined in this detail.	Closure Criterion: Collect relevant detail.
	Rationale (> 1600 °C) N/A.	Closure Criterion: N/A

Additional Discussion

This level of detail may not be necessary if all one needs is time to significant fuel releases as the failure of the SiC may dominate.

Life Cycle Phase	Factor, Characteristic or Phenomenon	Definition
Accident With Subsequent Air Intrusion	Outer PyC Layer: Chemical attack by air	Release of graphite FP inventory
	Holdup reversal	

Importance Rank and Rationale	Knowledge Level and Rationale	Remedy for Inadequate Knowledge/Issue Closure Criteria
Rank: L	≤ 1600 °C: 3	Remedy: Determine the conditions of interest and collect the necessary data.
	> 1600 °C: N/A	Remedy: N/A
Rationale: As the OPyC is burned away; any inventory of fission products will be released. The inventory of this layer is low for high quality fuel.	Rationale: (≤ 1600 °C) Some air ingress experiments have been done.	Closure Criterion: Determine the relevance of this need and collect data.
	Rationale (> 1600 °C) N/A	Closure Criterion: N/A

Additional Discussion

If the fuel performs as expected, the inventory of this layer will be very low. Thus, the actual details of its release may not be important. The greater problem will be that its loss exposes the SiC to air. For a summary of burning data see:

Compilation of Fuel Performance and Fission Product Transport Models and Database for MHTGR Design, Martin, R.C., ORNL/NPR-91/6

Fuel Performance and Fission Product Behavior in Gas Cooled Reactors, IAEA-TECDOC-978 (1997)

Life Cycle Phase	Factor, Characteristic or Phenomenon	Definition
Accident With Subsequent Air Intrusion	Outer PyC Layer: Chemical attack by air Temperature distribution	Impact of graphite oxidation on temperature distribution through material

Importance Rank and Rationale	Knowledge Level and Rationale	Remedy for Inadequate Knowledge/Issue Closure Criteria
Rank: H	≤ 1600 °C: 5	Remedy: Determine if the uncertainty in the temperatures is acceptable. Refine models and collect data as necessary.
	> 1600 °C: N/A	Remedy: N/A
Rationale: The temperature determines the reaction rates and thus how fast the layer is attacked.	Rationale: (≤ 1600 °C) Enough modeling has been done to reasonably estimate the temperatures.	Closure Criterion: Adequate data for calculations.
	Rationale (> 1600 °C) N/A	Closure Criterion: N/A

Additional Discussion

Life Cycle Phase	Factor, Characteristic or Phenomenon	Definition
Accident With Subsequent Air Intrusion	SiC Layer Gas-phase diffusion	Diffusion of gaseous fission products through layer (Knudsen and bulk diffusion through pore structure, and pressure driven permeation through structure)

Importance Rank and Rationale	Knowledge Level and Rationale	Remedy for Inadequate Knowledge/Issue Closure Criteria
Rank: H	≤ 1600 °C: 4	Remedy: Determine relevance of this issue and collect data if necessary.
	> 1600 °C: N/A	Remedy: N/A
Rationale: The SiC is an important barrier to fission products. Its damage will allow fission product to migrate. It is assumed that the OPyC has been destroyed so that air can reach the layer. Also, note that the IPyC must also fail for gas release.	Rationale: (≤ 1600 °C) Germans have done extensive testing in this area with a helium atmosphere. The major problem is attack of the layer. Some work has been done in this area. Extensive work to collect diffusion coefficients has not been done.	Closure Criterion: Resolution of the uncertainties.
	Rationale (> 1600 °C) N/A	Closure Criterion: N/A

Additional Discussion

Much work has been done in a helium atmosphere, but less has been done with air. See:

Compilation of Fuel Performance and Fission Product Transport Models and Database for MHTGR Design, Martin, R.C., ORNL/NPR-91/6

Fuel Performance and Fission Product Behavior in Gas Cooled Reactors, IAEA-TECDOC-978 (1997)

Methods and Data for HTGR Fuel Performance and Radionuclide Release Modeling during Normal Operational and Accidents for Safety Analysis, K. Verfondern, et. al., Jul-2721

Life Cycle Phase	Factor, Characteristic or Phenomenon	Definition
Accident With Subsequent Air Intrusion	SiC Layer Condensed-phase diffusion	Inter-granular diffusion and/or intra-granular solid-state diffusion

Importance Rank and Rationale	Knowledge Level and Rationale	Remedy for Inadequate Knowledge/Issue Closure Criteria
Rank: H	≤ 1600 °C: 4	Remedy: Outline the course of the accident and collect the relevant data.
	> 1600 °C: N/A	Remedy: N/A
Rationale: The SiC is the major barrier to the release of metallic fission products. It is assumed that the OPyC has been removed and air/steam is attacking the SiC.	Rationale: (≤ 1600 °C) Integral experiments exposing a particle to air and steam have been done.	Closure Criterion: The course of the accident and the necessary data.
	Rationale (> 1600 °C) N/A	Closure Criterion: N/A

Additional Discussion

Much work has been done in a helium atmosphere, but less has been done with air. See:

Compilation of Fuel Performance and Fission Product Transport Models and Database for MHTGR Design, Martin, R.C., ORNL/NPR-91/6

Fuel Performance and Fission Product Behavior in Gas Cooled Reactors, IAEA-TECDOC-978 (1997)

Methods and Data for HTGR Fuel Performance and Radionuclide Release Modeling during Normal Operational and Accidents for Safety Analysis, K. Verfondern, et. al., Jul-2721

Life Cycle Phase	Factor, Characteristic or Phenomenon	Definition
Accident With Subsequent Air Intrusion	SiC Layer	Decline in the quality of the layer due to thermal loading
	Thermal deterioration/decomposition	

Importance Rank and Rationale	Knowledge Level and Rationale	Remedy for Inadequate Knowledge/Issue Closure Criteria
Rank: H	≤ 1600 °C: 4	Remedy: If 1600°C and the irradiation envelope are adequate then okay; otherwise testing may be necessary, especially if air/steam contact layer.
	> 1600 °C: N/A	Remedy: N/A
Rationale: The loss of the SiC will result in the release of metallics even if the PyCs are in good shape. The loss of the OPyC will probably result in accelerated failure due to loss of strength.	Rationale: (≤ 1600 °C) Extensive testing at 1600°C has shown it to be a "safe" limit, but exposure to air/steam may accelerate the process.	Closure Criterion: Accident definition and the uncertainties with air/steam resolved.
	Rationale (> 1600 °C) N/A	Closure Criterion: N/A

Additional Discussion

1600°C has been used as the maximum temperature; it is conservative and some researchers feel that 1650-1700°C may be allowable, but the air exposure my greatly change the situation. The modeling approach to this situation needs to be resolved. This is a complex issue. Some references:

Compilation of Fuel Performance and Fission Product Transport Models and Database for MHTGR Design, Martin, R.C., ORNL/NPR-91/6

Fuel Performance and Fission Product Behavior in Gas Cooled Reactors, IAEA-TECDOC-978 (1997)

Methods and Data for HTGR Fuel Performance and Radionuclide Release Modeling during Normal Operational and Accidents for Safety Analysis, K. Verfondern, et. al., Jul-2721

Life Cycle Phase	Factor, Characteristic or Phenomenon	Definition
Accident With Subsequent Air Intrusion	SiC Layer Fission product corrosion	Attack of layer by fission products, e.g., Pd

Importance Rank and Rationale	Knowledge Level and Rationale	Remedy for Inadequate Knowledge/Issue Closure Criteria
Rank: H	≤ 1600 °C: 7	Remedy: None, if the particle operating temperature/time is below an acceptable damage limit.
	> 1600 °C: N/A	Remedy: N/A
Rationale: Some fission products may migrate to the SiC layer and damage it. This corrosion process is a function of temperature. The corrosion mostly occurs during normal operation at the higher temperatures and weakens the particle for the accident. At the higher accident temperatures, thermal decomposition effects dominate.	Rationale: (≤ 1600 °C) This effect has been studied both in-pile and out of pile. Controlling the maximum operating temperature is a major factor.	Closure Criterion: Insure that the operating conditions are acceptable
	Rationale (> 1600 °C) N/A	Closure Criterion: N/A

Additional Discussion

Palladium is one element that is of great concern for high temperature corrosion of SiC and temperature is an important driving factor. Corrosion rates are strong functions of temperature. See the other PIRT Tables and:

Fission Product Pd-SiC Interaction in Irradiated Coated-Particle Fuels, T.N. Tiegs, Nuclear Technology, 57, pages 389-398.

Silicon Carbide Corrosion in High-Temperature Gas-Cooled Reactor Fuel Particles, H. Grubmeier, et. al., Nuclear Technology, 35 (1977), pages 413-427

Out-of-Reactor Studies of Fission Product-Silicon Carbide Interactions in HTGR Fuel Particles, R. Lauf, et. al., Journal of Nuclear Materials, 120 (1984), pages 6-30

Carbon Monoxide-Silicon Carbide Interaction in HTGR Fuel Particles, K. Minato, et. al., Journal of Materials Science, 26 (1991), pages 2379-2388

Life Cycle Phase	Factor, Characteristic or Phenomenon	Definition
Accident With Subsequent Air Intrusion	SiC Layer Heavy metal diffusion	Diffusion of heavy metals through layer

Importance Rank and Rationale	Knowledge Level and Rationale	Remedy for Inadequate Knowledge/Issue Closure Criteria
Rank: L	≤ 1600 °C: 5	Remedy: None
	> 1600 °C: N/A	Remedy: N/A
Rationale: Diffusion of heavy metal through the particle could result is the redistribution of fissile material.	Rationale: (≤ 1600 °C) To this author's knowledge, heavy metal diffusion through the SiC is not a problem.	Closure Criterion: None
	Rationale (> 1600 °C) N/A	Closure Criterion: N/A

Additional Discussion

Significant migration of fissile material through SiC during an accident is not an issue at the temperatures of interest. See: *Compilation of Fuel Performance and Fission Product Transport Models and Database for MHTGR Design*, Martin, R.C., ORNL/NPR-91/6

Life Cycle Phase	Factor, Characteristic or Phenomenon	Definition
Accident With Subsequent Air Intrusion	SiC Layer Layer oxidation	Uptake of oxygen by the layer through a chemical reaction

Importance Rank and Rationale	Knowledge Level and Rationale	Remedy for Inadequate Knowledge/Issue Closure Criteria
Rank: H	≤ 1600 °C: 4	Remedy: Determine chemical conditions and release time for the relevant case.
	> 1600 °C: N/A	Remedy: N/A
Rationale: Oxidation of the SiC layer will destroy its fission product retention capability. A major issue is whether SiO or SiO_2 is produced. SiO_2 will produce a layer that impedes mass transfer while SiO is volatile. Also, if the IPyC breaks, the SiC layer may be exposed to CO that could slowly corrode it. This is less of a concern for UCO fuel.	Rationale: (≤ 1600 °C) Experiments have been done with particles and spheres.	Closure Criterion: Resolution of release rates.
	Rationale (> 1600 °C) N/A	Closure Criterion: N/A

<u>Additional Discussion</u>

This is a complex issue. Some references:

Compilation of Fuel Performance and Fission Product Transport Models and Database for MHTGR Design, Martin, R.C., ORNL/NPR-91/6

Fuel Performance and Fission Product Behavior in Gas Cooled Reactors, IAEA-TECDOC-978 (1997)

Methods and Data for HTGR Fuel Performance and Radionuclide Release Modeling during Normal Operational and Accidents for Safety Analysis, K. Verfondern, et. al., Jul-2721
CO corrosion can be a problem at the higher pressures and temperatures if a crack in the IPyC allows access to the SiC. Controlling the IPyC properties and controlling the CO by using UCO or gettering the fuel can mitigate this problem. See other PIRT tables and:

Carbon Monoxide-Silicon Carbide Interaction in HTGR Fuel Particles, K. Minato, et. al., Journal of Materials Science, 26 (1991), pages 2379-2388

Life Cycle Phase	Factor, Characteristic or Phenomenon	Definition
Accident With Subsequent Air Intrusion	SiC Layer Fission product release through undetected defects	Passage of fission products from the buffer region through defects in the SiC layer

Importance Rank and Rationale	Knowledge Level and Rationale	Remedy for Inadequate Knowledge/Issue Closure Criteria
Rank: M	≤ 1600 °C: 7	Remedy: Defer to fuel fabrication
	> 1600 °C: N/A	Remedy: N/A
Rationale: Defective SiC will allow gas transport if the PyCs both fail. This is more of a manufacturing issue that shows up when the fuel is stressed.	Rationale: (≤ 1600 °C) This is a manufacturing issue that shows up during accident conditions.	Closure Criterion: None
	Rationale (> 1600 °C) N/A	Closure Criterion: N/A

Additional Discussion

The SiC layer can be damaged during compact fabrication by iron impurities. The particles will still retain gases as long as one of the PyCs is good. See the PIRT on Manufacturing Design. It is not known if the chemical attack will worsen the situation.

Life Cycle Phase	Factor, Characteristic or Phenomenon	Definition
Accident With Subsequent Air Intrusion	SiC Layer Fission product release through failures, e.g. cracking	Passage of fission products from the buffer region through regions in the SiC layer that fail during operation or an accident

Importance Rank and Rationale	Knowledge Level and Rationale	Remedy for Inadequate Knowledge/Issue Closure Criteria
Rank: H	≤ 1600 °C: 4	Remedy: If the fuel is used outside of its tested region, more testing is needed.
	> 1600 °C: N/A	Remedy: N/A
Rationale: Failure of the SiC will allow fission gas to pass through it. If the PyC remains good, the gas will not be released, if not, the gas will be released. Metallics will be released in both cases. See previous SiC entries.	Rationale: (≤ 1600 °C) C Accident models have been compared to experiments to approximately model the situation. If material properties are consistent, useful predictions can be made, however chemical attack issues can change the results.	Closure Criterion: Resolution of identified concerns.
	Rationale (> 1600 °C) N/A	Closure Criterion: N/A

Additional Discussion

Most SiC failure models are based on pressure vessel failure. More recent models are considering cracking. See the other PIRT Tables and:

Revised MHTGR High-Temperature Fuel Performance Models, R.C. Martin, ORNL/NPR-92/16
Methods and Data for HTGR Fuel Performance and Radionuclide Release Modeling during Normal Operational and Accidents for Safety Analysis, K. Verfondern, et. al., Jul-2721
MHTGR TRISO-P Fuel Failure Evaluation Report, DOE-HTGR-90390, 1993
Fuel Performance and Fission Product Behavior in Gas Cooled Reactors, IAEA-TECDOC-978 (1997)

Life Cycle Phase	Factor, Characteristic or Phenomenon	Definition
Accident With Subsequent Air Intrusion	SiC Layer Thermodynamics of the SiC-fission product system	Chemical form of fission products including the effects of solubility, intermetallics, and chemical activity

Importance Rank and Rationale	Knowledge Level and Rationale	Remedy for Inadequate Knowledge/Issue Closure Criteria
Rank: H	≤ 1600 °C: 7	Remedy: None, if the particle operating temperature/time is below an acceptable damage limit.
	> 1600 °C: N/A	Remedy: N/A
Rationale: Some fission products may migrate to the SiC layer and damage it. This corrosion process is a function of temperature. See the entry on corrosion. If the SiC fails and air/steam enters, the oxidation state may increase, which may not be bad.	Rationale: (≤ 1600 °C) This effect has been studied both in-pile and out of pile. Controlling the maximum operating temperature is a major factor.	Closure Criterion: Acceptable performance.
	Rationale (> 1600 °C) N/A	Closure Criterion: N/A

Additional Discussion

See entries on corrosion and the other PIRT Tables. Also see entries on UCO. One of the goals of kernel design is to stabilize the corrosive elements so they do not migrate to the SiC. Also, determine if air attack kernel.
During normal or accident conditions, the SiC can crack or break due to over pressure or an interaction with cracked PyC. High temperatures increase the pressure in a particle. Above 1600 °C or so, decomposition begins to weaken the SiC and it can fail.

For some work on examining the effects of cracks on fuel performance and general models see the other PIRT tables and:

Consideration of the Effects on Fuel Particle Behavior from Shrinkage Cracks in the Inner Pyrocarbon Layer, G.Miller, et. al., Journal of Nuclear Materials, 295 (2001), pages 205-212.

Key Differences in the Fabrication, Irradiation and Safety Testing of U.S. and German TRISO-coated Particle Fuel and Their Implications on Fuel Performance, D.A. Petti, et. al., INEEL/EXT-02-00300

Revised MHTGR High-Temperature Fuel Performance Models, R.C. Martin, ORNL/NPR-92/16

Methods and Data for HTGR Fuel Performance and Radionuclide Release Modeling during Normal Operational and Accidents for Safety Analysis, K. Verfondern, et. al., Jul-2721

MHTGR TRISO-P Fuel Failure Evaluation Report, DOE-HTGR-90390, 1993

Fuel Performance and Fission Product Behavior in Gas Cooled Reactors, IAEA-TECDOC-978 (1997)

Life Cycle Phase	Factor, Characteristic or Phenomenon	Definition
Accident With Subsequent Air Intrusion	SiC Layer Sintering	Change of graphite microstructure as a function of temperature

Importance Rank and Rationale	Knowledge Level and Rationale	Remedy for Inadequate Knowledge/Issue Closure Criteria
Rank: L	≤ 1600 °C: 7	Remedy: None if temperatures are below 1600 °C, an air environment may modify this.
	> 1600 °C: N/A	Remedy: N/A
Rationale: SiC doesn't appear to suffer any significant changes at normal operating conditions and survives at 1600 °C without large changes.	Rationale: (≤ 1600 °C) Extensive testing at 1600 °C for hundreds of hours has shown the good behavior of SiC.	Closure Criterion: None
	Rationale (> 1600 °C) N/A	Closure Criterion: N/A

Additional Discussion

The major challenge is to reproduce the SiC that performed so well in past testing. The exposure to air is expected to lead to corrosion effects rather than sintering effects. The loss of the SiC integrity is the major issue.

Life Cycle Phase	Factor, Characteristic or Phenomenon	Definition
Accident With Subsequent Air Intrusion	SiC Layer: Chemical attack by air Kinetics	Rate of reaction per unit surface area as a function of temperature and partial pressure of air

Importance Rank and Rationale	Knowledge Level and Rationale	Remedy for Inadequate Knowledge/Issue Closure Criteria
Rank: H	≤ 1600 °C: 4	Remedy: Determine chemical conditions and release time for the relevant case.
	> 1600 °C: N/A	Remedy: N/A
Rationale: The rates determine how long the SiC will last. Also, oxidation of the SiC layer will destroy its fission product retention capability. A major issue is whether SiO or SiO_2 is produced. SiO_2 will produce a layer that impedes mass transfer while SiO is volatile.	Rationale: (≤ 1600 °C) Experiments have been done with particles.	Closure Criterion: Resolution of release rates.
	Rationale (> 1600 °C) N/A	Closure Criterion: N/A

<u>Additional Discussion</u>

This is a complex issue because of the SiO or SiO_2 issue and mass transfer. Some references:

Compilation of Fuel Performance and Fission Product Transport Models and Database for MHTGR Design, Martin, R.C., ORNL/NPR-91/6

Fuel Performance and Fission Product Behavior in Gas Cooled Reactors, IAEA-TECDOC-978 (1997)

Methods and Data for HTGR Fuel Performance and Radionuclide Release Modeling during Normal Operational and Accidents for Safety Analysis, K. Verfondern, et. al., Jul-2721

Life Cycle Phase	Factor, Characteristic or Phenomenon	Definition
Accident With Subsequent Air Intrusion	SiC Layer: Chemical attack by air Catalysis	Modification of the reaction rate by fission products or impurities

Importance Rank and Rationale	Knowledge Level and Rationale	Remedy for Inadequate Knowledge/Issue Closure Criteria
Rank: L	≤ 1600 °C: 1	Remedy: Estimate the potential for this to occur.
	> 1600 °C: N/A	Remedy: N/A
Rationale: A catalysis could influence the reaction rate of SiC with water or air and thus greatly increase the rate of thinning.	Rationale: (≤ 1600 °C) This is unexplored.	Closure Criterion: Resolution of the issue.
	Rationale (> 1600 °C) N/A	Closure Criterion: N/A

<u>Additional Discussion</u>

Little is known about this, but experiments have not revealed any sort of problem. A literature review may be a way to quickly determine if this area needs to be explored more.

Life Cycle Phase	Factor, Characteristic or Phenomenon	Definition
Accident With Subsequent Air Intrusion	SiC Layer: Chemical attack by air	Changes in chemical form resulting from oxidizing or reducing fission products
	Changes in chemical form of fission products	

Importance Rank and Rationale	Knowledge Level and Rationale	Remedy for Inadequate Knowledge/Issue Closure Criteria
Rank: H	≤ 1600 °C: 4	Remedy: Determine the need for this knowledge, collect as necessary.
	> 1600 °C: N/A	Remedy: N/A
Rationale: Changes in the chemical form of the fission products can greatly change their transport properties. Once the SiC fails, the potential for significant particle releases increase.	Rationale: (≤ 1600 °C) Thermochemical codes can calculate the possible chemical compounds. Little confirmation work is available.	Closure Criterion: Collect data to resolve uncertainties
	Rationale (> 1600 °C) N/A	Closure Criterion: N/A

Additional Discussion

The forms and migration of the fission products can be complex. For some information on the chemical forms see:

Fission Product Plateout and Liftoff in the MHTGR Primary System: A Review, NUREG/CR-5647

Chemical Behavior of Fission Products in Core Heatup Accidents in High-Temperature Gas-Cooled Reactors, R. Moormann, Nuclear Technology, 94 (1991), pages 56-67.

Life Cycle Phase	Factor, Characteristic or Phenomenon	Definition
Accident With Subsequent Air Intrusion	SiC Layer: Chemical attack by air	Changes in diffusivity, porosity, adsorptivity, etc.
	Changes in SiC properties	

Importance Rank and Rationale	Knowledge Level and Rationale	Remedy for Inadequate Knowledge/Issue Closure Criteria
Rank: H	≤ 1600 °C: 1	Remedy: Determine if this item is relevant.
	> 1600 °C: N/A	Remedy: N/A
Rationale: The modeling is not performed at this level; generally, the layer is assumed to disappear at some rate.	Rationale: (≤ 1600 °C) Not examined in this detail.	Closure Criterion: Collect relevant detail.
	Rationale (> 1600 °C) N/A	Closure Criterion: N/A

Additional Discussion

This level of detail may not be necessary if all one needs is time to significant fuel releases as the SiC fails.

Life Cycle Phase	Factor, Characteristic or Phenomenon	Definition
Accident With Subsequent Air Intrusion	SiC Layer: Chemical attack by air	Release of SiC FP inventory
	Holdup reversal	

Importance Rank and Rationale	Knowledge Level and Rationale	Remedy for Inadequate Knowledge/Issue Closure Criteria
Rank: L	≤ 1600 °C: 3	Remedy: Determine the conditions of interest and collect the necessary data
	> 1600 °C: N/A	Remedy: N/A
Rationale: As the SiC is removed; any inventory of fission products will be released. The inventory of this layer is low for high quality fuel.	Rationale: (≤ 1600 °C) Some air ingress work has been done.	Closure Criterion: Determine the relevance of this need and collect data.
	Rationale (> 1600 °C) N/A	Closure Criterion: N/A

<u>**Additional Discussion**</u>

If the fuel performs as expected, the inventory of this layer will be very low. Thus, the actual details of its release may not be important. The greater problem is that its loss exposed the high inventory kernel. See:

Compilation of Fuel Performance and Fission Product Transport Models and Database for MHTGR Design, Martin, R.C., ORNL/NPR-91/6

Fuel Performance and Fission Product Behavior in Gas Cooled Reactors, IAEA-TECDOC-978 (1997)

Life Cycle Phase	Factor, Characteristic or Phenomenon	Definition
Accident With Subsequent Air Intrusion	SiC Layer: Chemical attack by air Temperature distribution	Impact of SiC oxidation on temperature distribution through material

Importance Rank and Rationale	Knowledge Level and Rationale	Remedy for Inadequate Knowledge/Issue Closure Criteria
Rank: H	≤ 1600 °C: 5	Remedy: Determine if the uncertainty in the temperatures is acceptable. Refine models and collect data as necessary.
	> 1600 °C: N/A	Remedy: N/A
Rationale: The temperature determines the reaction rates and thus how fast the layer is attacked.	Rationale: (≤ 1600 °C) Enough modeling has been done to reasonably estimate the temperatures.	Closure Criterion: Adequate data for calculations.
	Rationale (> 1600 °C) N/A	Closure Criterion: N/A

Additional Discussion

Life Cycle Phase	Factor, Characteristic or Phenomenon	Definition
Accident With Subsequent Air Intrusion	Inner PyC Layer Gas-phase diffusion	Diffusion of gaseous fission products through layer (Knudsen and bulk diffusion through pore structure, and pressure driven permeation through structure)

Importance Rank and Rationale	Knowledge Level and Rationale	Remedy for Inadequate Knowledge/Issue Closure Criteria
Rank: H	≤ 1600 °C: 4	Remedy: None at present
	> 1600 °C: N/A	Remedy: N/A
Rationale: Gas diffusion through the PyCs is generally quite low at the temperatures of interest. The SiC layer must be breeched for the gases to get out. If the SiC layer has been damaged, the failure likelihood of the IPyC is increased. If attack of the IPyC occurs, significant release will soon follow.	Rationale: (≤ 1600 °C) Gas diffusion through the PyCs has been shown to be quite low. The issue is the layer behavior after is has been attacked. Some integral testing has been done.	Closure Criterion: Acceptable test fuel behavior
	Rationale (> 1600 °C) N/A	Closure Criterion: Acceptable test fuel behavior

Additional Discussion

Extensive testing has been done on various fuels over a range of temperatures. The challenge is to reproduce this good material. See:

Performance Evaluation of Modern HTR TRISO Fuel, R. Gontard, H. Nabielek, HTA-1B-05/90, July 1990
Fuel Performance and Fission Product Behavior in Gas Cooled Reactors, IAEA-TECDOC-978 (1997)
Fission-Product Release During Postirradiation Annealing of Several Types of Coated Fuel Particles, R.E. Bullock, Journal of Nuclear Materials, 125 (1984), pages 304-319

The concern is how the chemical attack affects the layer. For accident models see:

Compilation of Fuel Performance and Fission Product Transport Models and Database for MHTGR Design, Martin, R.C., ORNL/NPR-91/6
Revised MHTGR High-Temperature Fuel Performance Models, R.C. Martin, ORNL/NPR-92/16
Methods and Data for HTGR Fuel Performance and Radionuclide Release Modeling during Normal Operational and Accidents for Safety Analysis, K. Verfondern, et. al., Jul-2721

Life Cycle Phase	Factor, Characteristic or Phenomenon	Definition
Accident With Subsequent Air Intrusion	Inner PyC Layer Condensed-phase diffusion	Inter-granular diffusion and/or intra-granular solid-state diffusion

Importance Rank and Rationale	Knowledge Level and Rationale	Remedy for Inadequate Knowledge/Issue Closure Criteria
Rank: M	≤ 1600 °C: 4	Remedy: None, nothing can be done
	> 1600 °C: N/A	Remedy: N/A
Rationale: The diffusion of metallic fission products through the PyCs is known to be fairly high. Only modest credit can be taken for PyC as a barrier or release delay for metallics. Any chemical attack will only enhance the diffusion.	Rationale: (≤ 1600 °C) The PyCs are generally assumed to provide limited retention to metallic fission products at accident temperatures. Chemical attack may make the situation worse.	Closure Criterion: None
	Rationale (> 1600 °C) N/A	Closure Criterion: N/A

Additional Discussion

For a discussion of PyC and metallics see:

Nuclear Technology, 35, Number 2, Fission Product Release Section, pages 457-526

For the higher accident temperatures, the PyCs are assumed to have essentially no resistance to metallic transport. The PyC offers some impedance to metallic transport, but is not a major barrier. Chemical attack will worsen the situation, but the SiC layer is the important one.

Life Cycle Phase	Factor, Characteristic or Phenomenon	Definition
Accident With Subsequent Air Intrusion	Inner PyC Layer Pressure loading (Fission products)	Stress loading of the layer by increased pressure from fission products

Importance Rank and Rationale	Knowledge Level and Rationale	Remedy for Inadequate Knowledge/Issue Closure Criteria
Rank: H	≤ 1600 °C: 7	Remedy: Proper design and fabrication
	> 1600 °C: N/A	Remedy: N/A
Rationale: Depending on the particular configuration, the PyC layers can help keep the SiC in compression. Loss of a PyC layer can increase the probability of SiC failure.	Rationale: (≤ 1600 °C) Pressure can be controlled by particle design, burnup, and kernel composition. Analysis and designs are available	Closure Criterion: Acceptable fuel performance
	Rationale (> 1600 °C) N/A	Closure Criterion: N/A

Additional Discussion

According to the fuel models, the PyC functions as an important load-bearing component of the fuel particle. See the PIRT Design Table for more information concerning the stresses. Loss of other layers due to chemical attack influences the structural stability of the entire particle.

A major concern is the proper material properties – see the Manufacturing Design PIRT

Life Cycle Phase	Factor, Characteristic or Phenomenon	Definition
Accident With Subsequent Air Intrusion	Inner PyC Layer Pressure loading (Carbon monoxide)	Stress loading of the layer by carbon monoxide by increased pressure

Importance Rank and Rationale	Knowledge Level and Rationale	Remedy for Inadequate Knowledge/Issue Closure Criteria
Rank: H	≤ 1600 °C: 7	Remedy: Control pressure by design
	> 1600 °C: N/A	Remedy: N/A
Rationale: High CO product will result in high particle pressures, especially at the higher accident temperatures. Changing the kernel composition can control CO production.	Rationale: (≤ 1600 °C) Pressure can be controlled by particle design, burnup, and kernel composition. Analysis and designs are available.	Closure Criterion: Proof testing of final fuel design
	Rationale (> 1600 °C) N/A	Closure Criterion: N/A

Additional Discussion

For a discussion on kernel design to minimize CO and immobilize key fission products see:

Stoichiometric Effects on Performance of High-Temperature Gas-Cooled Reactor Fuels from the U-C-O System, F.J. Homan, et. al., Nuclear Technology, 35, pages 428-441.
See the other PIRT Tables for fuel design issues.

Life Cycle Phase	Factor, Characteristic or Phenomenon	Definition
Accident With Subsequent Air Intrusion	Inner PyC Layer Layer oxidation	Reaction of pyrolytic graphic with oxygen released from the kernel.

Importance Rank and Rationale	Knowledge Level and Rationale	Remedy for Inadequate Knowledge/Issue Closure Criteria
Rank: H	≤ 1600 °C: 3	Remedy: Collect relevant data
	> 1600 °C: N/A	Remedy: N/A
Rationale: Defects or cracks in the OPyC and SiC can allow air/stem to enter the particle and oxidize the IPyC. This will release fission gases and provide a direct path to the kernel.	Rationale: (≤ 1600 °C) This behavior is similar to the burn leach tests used to determine fuel quality. The rates are assumed to be the same as for OPyC	Closure Criterion: Reasonable calculational basis.
	Rationale (> 1600 °C) N/A	Closure Criterion: N/A

Additional Discussion

If both the OPyC and the SiC are breeched, then the particle is releasing.

Performance Evaluation of Modern HTR TRISO Fuel, R. Gontard, H. Nabielek, HTA-1B-05/90, July 1990
Fuel Performance and Fission Product Behavior in Gas Cooled Reactors, IAEA-TECDOC-978 (1997)
Fission-Product Release During Postirradiation Annealing of Several Types of Coated Fuel Particles, R.E. Bullock, Journal of Nuclear Materials, 125 (1984), pages 304-319

For accident models see:

Compilation of Fuel Performance and Fission Product Transport Models and Database for MHTGR Design, Martin, R.C., ORNL/NPR-91/6
Revised MHTGR High-Temperature Fuel Performance Models, R.C. Martin, ORNL/NPR-92/16
Methods and Data for HTGR Fuel Performance and Radionuclide Release Modeling during Normal Operational and Accidents for Safety Analysis, K. Verfondern, et. al., Jul-2721

Life Cycle Phase	Factor, Characteristic or Phenomenon	Definition
Accident With Subsequent Air Intrusion	Inner PyC Layer Stress state (compression/tension)	The state of the forces induced by external forces that are acting across the layer to resist movement

Importance Rank and Rationale	Knowledge Level and Rationale	Remedy for Inadequate Knowledge/Issue Closure Criteria
Rank: H	≤ 1600 °C: 7	Remedy: Control pressure by design
	> 1600 °C: N/A	Remedy: N/A
Rationale: Failure of the PyC can increase the likelihood of SiC failure. See the previous pressure loading entries.	Rationale: (≤ 1600 °C) Pressure can be controlled by particle design, burnup, and kernel composition. Analysis and designs are available	Closure Criterion: Proof testing of final fuel design
	Rationale (> 1600 °C) N/A	Closure Criterion: N/A

Additional Discussion

See the table entries about pressure loading and also the PIRT Design Tables.

Life Cycle Phase	Factor, Characteristic or Phenomenon	Definition
Accident With Subsequent Air Intrusion	Inner PyC Layer Cracking	Lengths, widths and numbers of cracks produced in layer during accident

Importance Rank and Rationale	Knowledge Level and Rationale	Remedy for Inadequate Knowledge/Issue Closure Criteria
Rank: H	≤ 1600 °C: 4 (failure only, cracking is not calculated)	Remedy: Review and collect new data for the codes if necessary.
	> 1600 °C: N/A	Remedy: N/A
Rationale: Failure of the IPyC affects the likelihood of SiC failure. See the entry on stress state. The lengths, widths, and number of cracks don't really matter – the failure does. Many models assume the SiC layer will dominate the particle failure. Effects of chemical attack may not be included.	Rationale: (≤ 1600 °C) Fuel models have been developed to model normal and accident behavior. Particles are assumed to fail when they meet some weakness criteria rather based a layer stress.	Closure Criterion: Models that predict fuel behavior under normal and accident conditions. Does one need cracks or just failure? This adds a lot of complexity.
	Rationale (> 1600 °C) N/A	Closure Criterion: N/A

Additional Discussion

For some work on examining the effects of cracks on fuel performance and general models see:

Under accident conditions, a pressure vessel type failure model has been used with the particle failing when the pressure exceeds a critical value. The accident models may not include all the chemical attack effects.

Consideration of the Effects on Fuel Particle Behavior from Shrinkage Cracks in the Inner Pyrocarbon Layer, G.Miller, et. al., Journal of Nuclear Materials, 295 (2001), pages 205-212.
Key Differences in the Fabrication, Irradiation and Safety Testing of U.S. and German TRISO-coated Particle Fuel and Their Implications on Fuel Performance, D.A. Petti, et. al., INEEL/EXT-02-00300

MHTGR TRISO-P Fuel Failure Evaluation Report, DOE-HTGR-90390

Compilation of Fuel Performance and Fission Product Transport Models and Database for MHTGR Design, Martin, R.C., ORNL/NPR-91/6
Revised MHTGR High-Temperature Fuel Performance Models, R.C. Martin, ORNL/NPR-92/16
Methods and Data for HTGR Fuel Performance and Radionuclide Release Modeling during Normal Operational and Accidents for Safety Analysis, K. Verfondern, et. al., Jul-2721
Fuel Performance and Fission Product Behavior in Gas Cooled Reactors, IAEA-TECDOC-978 (1997)

Massive pyrocarbon failure In HRB-21 due to a design flaw (seal coats) resulted in cracks that appear to have compromised the SiC and resulted in releases. (ORNL)

Life Cycle Phase	Factor, Characteristic or Phenomenon	Definition
Accident With Subsequent Air Intrusion	Inner PyC Layer Intercalation	Trapping of species between sheets of the graphite structure

Importance Rank and Rationale	Knowledge Level and Rationale	Remedy for Inadequate Knowledge/Issue Closure Criteria
Rank: L	≤ 1600 °C: 2	Remedy: None
	> 1600 °C: N/A	Remedy: N/A
Rationale: This layer is likely to be saturated with fission products and this effect may only make a minor difference.	Rationale: (≤ 1600 °C) This situation has not caused problems	Closure Criterion: None
	Rationale (> 1600 °C) N/A	Closure Criterion: N/A

Additional Discussion

Some modeling is looking at this situation.

Life Cycle Phase	Factor, Characteristic or Phenomenon	Definition
Accident With Subsequent Air Intrusion	Inner PyC Layer: Chemical attack by air Kinetics	Rate of reaction per unit surface area as a function of temperature and partial pressure of air

Importance Rank and Rationale	Knowledge Level and Rationale	Remedy for Inadequate Knowledge/Issue Closure Criteria
Rank: H	≤ 1600 °C: 4	Remedy: Review data and perform tests to fill in gaps.
	> 1600 °C: N/A	Remedy: N/A
Rationale: This is the last barrier before exposing the kernel. Metals are being released, but gases are still retained.	Rationale: (≤ 1600 °C) Some testing has been done on the reaction of steam with matrix material and graphite.	Closure Criterion: Sufficient data to resolve gaps.
	Rationale (> 1600 °C) N/A	Closure Criterion: N/A

Additional Discussion

Air attack of the IPyC means that the OPyC and SiC layers have all been breeched. In this case, the particle is probably just about gone. It may not be worthwhile to model this in detail as failure is near. See:

Source Term Estimation for Small-Sized HTRs: Status and Further Needs, Extracted From German Safety Analysis, R. Moormann, et. al., Nuclear Technology, 135, (2001), pages 183-193

Fuel Performance and Fission Product Behavior in Gas Cooled Reactors, IAEA-TECDOC-978 (1997)

Compilation of Fuel Performance and Fission Product Transport Models and Database for MHTGR Design, R. Martin, ORNL/NPR-91/6

Methods and Data for HTGR Fuel Performance and Radionuclide Release Modeling during Normal Operational and Accidents for Safety Analysis, K. Verfondern, et. al., Jul-2721

Life Cycle Phase	Factor, Characteristic or Phenomenon	Definition
Accident With Subsequent Air Intrusion	Inner PyC Layer: Chemical attack by air	Modification of the reaction rate by fission products or impurities
	Catalysis	

Importance Rank and Rationale	Knowledge Level and Rationale	Remedy for Inadequate Knowledge/Issue Closure Criteria
Rank: M	≤ 1600 °C: 1	Remedy: Determine if it is relevant or important
	> 1600 °C: N/A	Remedy: N/A
Rationale: A catalysis can increase the reaction rate in the layer and hasten its failure.	Rationale: (≤ 1600 °C) This is an unexplored area.	Closure Criterion: Collect the effects of catalysis if necessary.
	Rationale (> 1600 °C) N/A.	Closure Criterion: N/A

Additional Discussion

For the effects of trace elements on graphite H-451 see:

The Effect of Trace Elements on the Surface Oxidation of H-451 Graphite, O.C. Kopp, et. al., ORNL/NPR-92/56, December 1992
A literature search should come up with some material on catalysis for PyC. It is likely to be sensitive to the exact nature of the materials.

Life Cycle Phase	Factor, Characteristic or Phenomenon	Definition
Accident With Subsequent Air Instrusion	Inner PyC Layer: Chemical attack by air Changes in chemical form of fission products	Changes in chemical form resulting from oxidizing or reducing fission products

Importance Rank and Rationale	Knowledge Level and Rationale	Remedy for Inadequate Knowledge/Issue Closure Criteria
Rank: H	≤ 1600 °C: 4	Remedy: Determine the need for this knowledge, collect as necessary.
	> 1600 °C: N/A	Remedy: N/A
Rationale: Changes in the chemical form of the fission products can greatly change their transport properties. Once the SiC fails, the potential for significant particle releases increase. The greatest change may come from the reaction of UC and the change in kernel structure.	Rationale: (≤ 1600 °C) Thermochemical codes can calculate the possible chemical compounds. Little confirmation work is available.	Closure Criterion: Collect data to resolve uncertainties
	Rationale (> 1600 °C) N/A	Closure Criterion: N/A

Additional Discussion

The forms and migration of the fission products can be complex. For some information on the chemical forms see:

Fission Product Plateout and Liftoff in the MHTGR Primary System: A Review, NUREG/CR-5647

Chemical Behavior of Fission Products in Core Heatup Accidents in High-Temperature Gas-Cooled Reactors, R. Moormann, Nuclear Technology, 94 (1991), pages 56-67.

Life Cycle Phase	Factor, Characteristic or Phenomenon	Definition
Accident With Subsequent Air Intrusion	Inner PyC Layer: Chemical attack by air	Changes in diffusivity, porosity, adsorptivity, etc.
	Changes in graphite properties	

Importance Rank and Rationale	Knowledge Level and Rationale	Remedy for Inadequate Knowledge/Issue Closure Criteria
Rank: M	≤ 1600 °C: 2	Remedy: Determine if this level of detail is really needed for the safety case.
	> 1600 °C: N/A	Remedy: N/A
Rationale: It may not be necessary to examine the PyC to this level of detail. An integral weakening or failure rate may be sufficient.	Rationale: (≤ 1600 °C) This area has not been examined in detail. Many of the tests have been integral tests on fuel elements and particles.	Closure Criterion: Resolution of the problem and the needed data.
	Rationale (> 1600 °C) N/A	Closure Criterion: N/A

Additional Discussion

The level of detail needed by the models needs to be examined. This will be expensive and difficult information to get. It is also like to be sensitive to the exact material nature.

Life Cycle Phase	Factor, Characteristic or Phenomenon	Definition
Accident With Subsequent Air Intrusion	Inner PyC Layer: Chemical attack by air	Release of graphite FP inventory
	Holdup reversal	

Importance Rank and Rationale	Knowledge Level and Rationale	Remedy for Inadequate Knowledge/Issue Closure Criteria
Rank: L	≤ 1600 °C: 2	Remedy: Determine if this is really important.
	> 1600 °C: N/A	Remedy: N/A
Rationale: The destruction of this layer will expose the kernel/buffer and a large fission product inventory.	Rationale: (≤ 1600 °C) This individual parameter has not been studied in much detail.	Closure Criterion: Resolution of its importance.
	Rationale (> 1600 °C) N/A	Closure Criterion: N/A

Additional Discussion

Once the particle layers have been breached, the kernel is exposed. The inventory now available for release will dwarf the minor inventories in the layers.

Life Cycle Phase	Factor, Characteristic or Phenomenon	Definition
Accident With Subsequent Air Intrusion	Inner PyC Layer: Chemical attack by air Temperature distribution	Impact of graphite oxidation on temperature distribution through material

Importance Rank and Rationale	Knowledge Level and Rationale	Remedy for Inadequate Knowledge/Issue Closure Criteria
Rank: H	≤ 1600 °C: 4	Remedy: Determine if the uncertainty in the temperatures is acceptable. Refine models and collect data as necessary.
	> 1600 °C: N/A	Remedy: N/A
Rationale: The temperature determines the rate at which the layer is attacked.	Rationale: (≤ 1600 °C) Enough modeling has been done to reasonably estimate the temperatures	Closure Criterion: Adequate data for calculations.
	Rationale (> 1600 °C) N/A	Closure Criterion: N/A

Additional Discussion

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Life Cycle Phase	Factor, Characteristic or Phenomenon	Definition
Accident With Subsequent Air Intrusion	Buffer Layer Gas-phase diffusion	Diffusion of gaseous fission products through layer (Knudsen and bulk diffusion through pore structure, and pressure driven permeation through structure)

Importance Rank and Rationale	Knowledge Level and Rationale	Remedy for Inadequate Knowledge/Issue Closure Criteria
Rank: H	≤ 1600 °C: 7	Remedy: None
	> 1600 °C: N/A	Remedy: N/A
Rationale: The buffer layer is designed to be a void to collect the gases released from the kernel. The problem would be if it weren't porous.	Rationale: (≤ 1600 °C) The buffer layer appears to work as planned. Gases are expected to diffusive through this layer.	Closure Criterion: None
	Rationale (> 1600 °C) N/A	Closure Criterion: N/A

Additional Discussion

Once this layer is exposed, the kernel is essentially exposed.

Life Cycle Phase	Factor, Characteristic or Phenomenon	Definition
Accident With Subsequent Air Intrusion	Buffer Layer Condensed-phase diffusion	Inter-granular diffusion and/or intra-granular solid-state diffusion

Importance Rank and Rationale	Knowledge Level and Rationale	Remedy for Inadequate Knowledge/Issue Closure Criteria
Rank: H	≤ 1600 °C: 7	Remedy: None
	> 1600 °C: N/A	Remedy: N/A
Rationale: The buffer layer is essentially void volume and is not expected to offer resistance to transport. Some material may be sorbed on this layer.	Rationale: (≤ 1600 °C) The buffer layer appears to work as planned. Fission products are expected to diffusive through this layer.	Closure Criterion: None
	Rationale (> 1600 °C) N/A	Closure Criterion: N/A

Additional Discussion

Once this layer is exposed, the kernel is essentially exposed.

Life Cycle Phase	Factor, Characteristic or Phenomenon	Definition
Accident With Subsequent Air Intrusion	Buffer Layer Response to kernel swelling	Mechanical reaction of the layer to the growth of the kernel via swelling

Importance Rank and Rationale	Knowledge Level and Rationale	Remedy for Inadequate Knowledge/Issue Closure Criteria
Rank: H	≤ 1600 °C: 5	Remedy: None
	> 1600 °C: N/A	Remedy: N/A
Rationale: The buffer layer must be weak enough that it will deform or crush without transmitting high forces to the IPyC as the kernel distorts.	Rationale: (≤ 1600 °C) All evidence to date indicates that the buffer layer performs as expected.	Closure Criterion: None
	Rationale (> 1600 °C) N/A	Closure Criterion: N/A

Additional Discussion

In the accident fuel testing done to date, no evidence of adverse buffer reaction to kernel swelling was apparent.

Life Cycle Phase	Factor, Characteristic or Phenomenon	Definition
Accident With Subsequent Air Intrusion	Buffer Layer	Maximum loading of fission products that can deposit from the gas phase onto surfaces of materials surrounding the fuel kernel
	Maximum fuel gaseous fission product uptake	

Importance Rank and Rationale	Knowledge Level and Rationale	Remedy for Inadequate Knowledge/Issue Closure Criteria
Rank: H	≤ 1600 °C: 7	Remedy: None
	> 1600 °C: N/A	Remedy: N/A
Rationale: The buffer layer must have sufficient void volume to control the pressure from released fission gases and CO.	Rationale: (≤ 1600 °C) All evidence to date indicates that the buffer layer performs as expected.	Closure Criterion: None
	Rationale (> 1600 °C) N/A	Closure Criterion: N/A

<u>Additional Discussion</u>

This is really a design issue. See the PIRT Design Table.

Life Cycle Phase	Factor, Characteristic or Phenomenon	Definition
Accident With Subsequent Air Intrusion	Buffer Layer Layer oxidation	Reaction of buffer layer with oxide materials in the kernel.

Importance Rank and Rationale	Knowledge Level and Rationale	Remedy for Inadequate Knowledge/Issue Closure Criteria
Rank: L	≤ 1600 °C: 7	Remedy: None
	> 1600 °C: N/A	Remedy: N/A
Rationale: A small portion of the layer is oxidized by the excess oxygen released form the kernel. This is of no consequence, as the layer has no structural function. It is of no consequence if the buffer is oxidized by air/steam as the particle is already failed.	Rationale: (≤ 1600 °C) No problem ahs been observed. The basic problem is CO production that has been outlined elsewhere.	Closure Criterion: None
	Rationale (> 1600 °C) N/A	Closure Criterion: N/A

Additional Discussion

See the discussions on the use of UCO to control CO pressure.

Life Cycle Phase	Factor, Characteristic or Phenomenon	Definition
Accident With Subsequent Air Intrusion	Buffer Layer Thermal gradient	Change in temperature with distance

Importance Rank and Rationale	Knowledge Level and Rationale	Remedy for Inadequate Knowledge/Issue Closure Criteria
Rank: L	≤ 1600 °C: 7	Remedy: None
	> 1600 °C: N/A	Remedy: N/A
Rationale: During accident conditions, the particle gradient is low because the power production is low relative to operating conditions and heat transfer is no longer driven by strong convection	Rationale: (≤ 1600 °C) The codes can compute these temperatures.	Closure Criterion: None
	Rationale (> 1600 °C) N/A	Closure Criterion: N/A

Additional Discussion

It is not likely that the chemical reactions will generate thermal gradients that are comparable with normal operation.

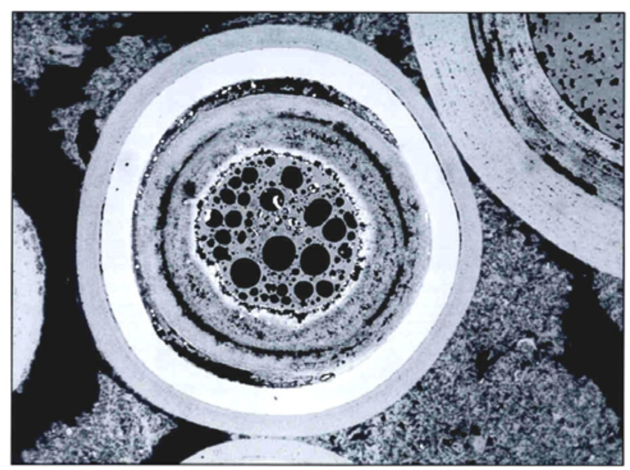
Life Cycle Phase	Factor, Characteristic or Phenomenon	Definition
Accident With Subsequent Air Intrusion	Buffer Layer	Dimension changes in the buffer layer or changes in its porosity produced by irradiation or by exposure to elevated temperatures
	Irradiation and thermal shrinkage	

Importance Rank and Rationale	Knowledge Level and Rationale	Remedy for Inadequate Knowledge/Issue Closure Criteria
Rank: M	≤ 1600 °C: 6	Remedy: None
	> 1600 °C: N/A	Remedy: N/A
Rationale: Ideally, the buffer layer should isolate the kernel from the IPyC, but small cracks or limited shrinkage do not seem to cause trouble. Most of these changes would have taken place during normal operation.	Rationale: (≤ 1600 °C) Modest buffer shrinkage and small cracks don't seem to result in problems	Closure Criterion: None
	Rationale (> 1600 °C) N/A	Closure Criterion: N/A

Additional Discussion

One concern is that cracks could offer a direct path for corrosive fission products to the SiC if the IPyC also breaks. Some current modeling is looking at this.

In this high burnup Pu kernel (ORNL), considerable shrinkage took place in the buffer layer and the IPyC separated from the SiC. While one would like to see less behavior of this sort, the particle performed well under irradiation.



R71558 (C9900515-03) 200x — 20 μm

Life Cycle Phase	Factor, Characteristic or Phenomenon	Definition
Accident With Subsequent Air Intrusion	Buffer Layer: Chemical attack by air Kinetics	Rate of reaction per unit surface area as a function of temperature and partial pressure of air

Importance Rank and Rationale	Knowledge Level and Rationale	Remedy for Inadequate Knowledge/Issue Closure Criteria
Rank: M	≤ 1600 °C: 3	Remedy: Determine if this affect is of any real importance.
	> 1600 °C: N/A	Remedy: N/A
Rationale: The particle has failed by the time this layer is attacked. The additional loss of the buffer may not make much difference.	Rationale: (≤ 1600 °C) Some data and modeling is available. Integral tests on particles and fuel elements have been performed.	Closure Criterion: Resolution of the importance.
	Rationale (> 1600 °C) N/A	Closure Criterion: N/A

Additional Discussion

Once the other layers have been attacked, the buffer offers very little impedance to fission product migration.

Life Cycle Phase	Factor, Characteristic or Phenomenon	Definition
Accident With Subsequent Air Intrusion	Buffer Layer: Chemical attack by air	Modification of the reaction rate by fission products or impurities
	Catalysis	

Importance Rank and Rationale	Knowledge Level and Rationale	Remedy for Inadequate Knowledge/Issue Closure Criteria
Rank: M	≤ 1600 °C: 1	Remedy: Determine if it is relevant or important
	> 1600 °C: N/A	Remedy: N/A
Rationale: Catalysis can increase the reaction rate in the layer and hasten its failure.	Rationale: (≤ 1600 °C) This is an unexplored area.	Closure Criterion: Collect the effects of catalysis if necessary.
	Rationale (> 1600 °C) N/A.	Closure Criterion: N/A

Additional Discussion

For the effects of trace elements on graphite H-451 see:

The Effect of Trace Elements on the Surface Oxidation of H-451 Graphite, O.C. Kopp, et. al., ORNL/NPR-92/56, December 1992
A literature search should come up with some material on catalysis for PyC. It is likely to be sensitive to the exact nature of the materials.

Life Cycle Phase	Factor, Characteristic or Phenomenon	Definition
Accident With Subsequent Air Intrusion	Buffer Layer: Chemical attack by air	Changes in chemical form resulting from oxidizing or reducing fission products
	Changes in chemical form of fission products	

Importance Rank and Rationale	Knowledge Level and Rationale	Remedy for Inadequate Knowledge/Issue Closure Criteria
Rank: H	≤ 1600 °C: 4	Remedy: Determine the need for this knowledge, collect as necessary.
	> 1600 °C: N/A	Remedy: N/A
Rationale: Changes in the chemical form of the fission products can greatly change their transport properties. The greatest change may come from the reaction of UC and the change in kernel structure	Rationale: (≤ 1600 °C) Thermochemical codes can calculate the possible chemical compounds. Little confirmation work is available.	Closure Criterion: Collect data to resolve uncertainties
	Rationale (> 1600 °C) N/A	Closure Criterion: N/A

Additional Discussion

The forms and migration of the fission products can be complex. For some information on the chemical forms see:

Fission Product Plateout and Liftoff in the MHTGR Primary System: A Review, NUREG/CR-5647

Chemical Behavior of Fission Products in Core Heatup Accidents in High-Temperature Gas-Cooled Reactors, R. Moormann, Nuclear Technology, 94 (1991), pages 56-67.

Life Cycle Phase	Factor, Characteristic or Phenomenon	Definition
Accident With Subsequent Air Intrusion	Buffer Layer: Chemical attack by air	Changes in diffusivity, porosity, adsorptivity, etc.
	Changes in graphite properties	

Importance Rank and Rationale	Knowledge Level and Rationale	Remedy for Inadequate Knowledge/Issue Closure Criteria
Rank: L	≤ 1600 °C: 2	Remedy: Determine if this level of detail is really needed for the safety case.
	> 1600 °C: N/A	Remedy: N/A
Rationale: It may not be necessary to examine the PyC to this level of detail. An integral weakening or failure rate may be sufficient.	Rationale: (≤ 1600 °C) This area has not been examined in detail. Many of the tests have been integral tests on fuel elements and particles.	Closure Criterion: Resolution of the problem and the needed data.
	Rationale (> 1600 °C) N/A	Closure Criterion: N/A

<u>Additional Discussion</u>

The level of detail needed by the models needs to be examined. This will be expensive and difficult information to get. It is also like to be sensitive to the exact material nature

Life Cycle Phase	Factor, Characteristic or Phenomenon	Definition
Accident With Subsequent Air Intrusion	Buffer Layer: Chemical attack by air	Release of graphite FP inventory
	Holdup reversal	

Importance Rank and Rationale	Knowledge Level and Rationale	Remedy for Inadequate Knowledge/Issue Closure Criteria
Rank: L	≤ 1600 °C: 2	Remedy: Determine if this is really important.
	> 1600 °C: N/A	Remedy: N/A
Rationale: The destruction of this layer will expose the kernel and a large fission product inventory.	Rationale: (≤ 1600 °C) This individual parameter has not been studied in much detail.	Closure Criterion: Resolution of its importance.
	Rationale (> 1600 °C) N/A	Closure Criterion: N/A.

Additional Discussion

Once the particle layers have been breached, the kernel is exposed. The inventory now available for release will dwarf the minor inventories in the layers.

Life Cycle Phase	Factor, Characteristic or Phenomenon	Definition
Accident With Subsequent Air Intrusion	Buffer Layer: Chemical attack by air	Impact of graphite oxidation on temperature distribution through material
	Temperature distribution	

Importance Rank and Rationale	Knowledge Level and Rationale	Remedy for Inadequate Knowledge/Issue Closure Criteria
Rank: H	≤ 1600 °C: 4	Remedy: Determine if the uncertainty in the temperatures is acceptable. Refine models and collect data as necessary.
	> 1600 °C: N/A	Remedy: N/A
Rationale: The temperature determines the rate at which the layer is attacked.	Rationale: (≤ 1600 °C) Enough modeling has been done to reasonably estimate the temperatures	Closure Criterion: Adequate data for calculations.
	Rationale (> 1600 °C) N/A	Closure Criterion: N/A

Additional Discussion

Life Cycle Phase	Factor, Characteristic or Phenomenon	Definition
Accident With Subsequent Air Intrusion	Kernel Maximum fuel temperature	Maximum fuel temperature attained by the fuel kernel during the accident

Importance Rank and Rationale	Knowledge Level and Rationale	Remedy for Inadequate Knowledge/Issue Closure Criteria
Rank: H	≤ 1600 °C: 7	Remedy: Insure that core models are up to date.
	> 1600 °C: N/A	Remedy: N/A
Rationale: The SiC layer is the primary barrier, but diffusion through the kernel does delay the release somewhat. The kernel retains a considerable amount of material and release is a function of temperature.	Rationale: (≤ 1600 °C) The core codes should be good enough to calculate the temperatures.	Closure Criterion: Acceptable uncertainties.
	Rationale (> 1600 °C) N/A	Closure Criterion: N/A

Additional Discussion

For a study comparing the relative contributions of core and fuel materials and fission product retention see: *An Analytical Study of Volatile Metallic Fission Product Release From Very High Temperature Gas-Cooled Reactor Fuel and Core*, S. Mitake, et. al., Nuclear Technology, 81, 7-12.

Life Cycle Phase	Factor, Characteristic or Phenomenon	Definition
Accident With Subsequent Air Intrusion	Kernel Temperature vs. time transient conditions	The time-dependent variation of fuel temperature with time

Importance Rank and Rationale	Knowledge Level and Rationale	Remedy for Inadequate Knowledge/Issue Closure Criteria
Rank: H	≤ 1600 °C: 7	Remedy: None, expect to watch for hot spots
	> 1600 °C: N/A	Remedy: N/A
Rationale: The temperature history of the fuel is important. Higher temperature operation even if it is followed by lower temperature operation can result in greater corrosion problems. High temperatures also increase fission product diffusion.	Rationale: (≤ 1600 °C) Modern codes can computer the time history of the fuel. The greatest problem is material property uncertainties.	Closure Criterion: Calculations within the needed uncertainties.
	Rationale (> 1600 °C) N/A	Closure Criterion: N/A

Additional Discussion

This is really a core design issue.

Life Cycle Phase	Factor, Characteristic or Phenomenon	Definition
Accident With Subsequent Air Intrusion	Kernel Energy Transport: Conduction within kernel	Flow of heat within a medium from a region of high temperature to a region of low temperature

Importance Rank and Rationale	Knowledge Level and Rationale	Remedy for Inadequate Knowledge/Issue Closure Criteria
Rank: M	≤ 1600 °C: 7	Remedy: None
	> 1600 °C: N/A	Remedy: N/A
Rationale: The kernel conductivity determines the kernel peak temperature. The kernel is fairly small, so modest changes in conductivity won't matter much. Higher temperatures could result in greater diffusion of fission products out of the kernel.	Rationale: (≤ 1600 °C) These numbers have been measured for the fuels of interest. No major issues are associated with them.	Closure Criterion: None
	Rationale (> 1600 °C) N/A	Closure Criterion: N/A

Additional Discussion

Kernel conductivity depends on the kernel composition and changes as the kernel burns up. The small size of the kernel limits these effects in coated particle fuel.

Life Cycle Phase	Factor, Characteristic or Phenomenon	Definition
Accident With Subsequent Air Intrusion	Kernel Thermodynamic state of fission products	Chemical and physical state of fission products

Importance Rank and Rationale	Knowledge Level and Rationale	Remedy for Inadequate Knowledge/Issue Closure Criteria
Rank: H	≤ 1600 °C: 4	Remedy: If fuel kernels other than UO_2 are to be used, testing is required to assure that they work as expected.
	> 1600 °C: N/A	Remedy: N/A
Rationale: The chemical state of the fission products determines how they will migrate and the temperature dependence. It is desirable to oxidize some fission products without producing CO. Air and steam could cause additional changes by reacting with the UCO.	Rationale: (≤ 1600 °C) A considerable amount of work has been done kernel composition to limit the migration of fission products and control CO pressure. However, only UO_2 has been extensively tested in a high quality fuel. Also, the kernel will oxide with air and water.	Closure Criterion: Demonstrated performance under the conditions of interest
	Rationale (> 1600 °C) N/A	Closure Criterion: N/A

<u>Additional Discussion</u>

For a discussion on kernel design to minimize CO and immobilize key fission products see:

Stoichiometric Effects on Performance of High-Temperature Gas-Cooled Reactor Fuels from the U-C-O System, F.J. Homan, et. al., Nuclear Technology, 35, pages 428-441.

The effect of Water Vapor on the Release of Gaseous Fission Products from High-Temperature Gas-Cooled Reactor Fuel Compacts Containing Exposed Uranium Oxycarbide Fuel, B. Myers, DOE-HTGR-88486

Life Cycle Phase	Factor, Characteristic or Phenomenon	Definition
Accident With Subsequent Air Intrusion	Kernel Oxygen flux	Mass transport of oxygen per unit surface area per unit time

Importance Rank and Rationale	Knowledge Level and Rationale	Remedy for Inadequate Knowledge/Issue Closure Criteria
Rank: L	≤ 1600 °C: 3	Remedy: Determine if this area is of any significance
	> 1600 °C: N/A	Remedy: N/A
Rationale: The mass of oxygen from the kernel will determine the rate at which CO is formed and particle pressure. Since the particles are designed assuming maximum pressure, the rate does not seem that important, but his area is somewhat unexplored. Oxygen coming in due to air/water will oxidize the kernel. See previous entry.	Rationale: (≤ 1600 °C) Some work has been done in this area. The full implications are not clear.	Closure Criterion: Resolution of the issue.
	Rationale (> 1600 °C) N/A	Closure Criterion: N/A

Additional Discussion

Tests have shown that the oxygen does not immediately leave the kernel, leading to a somewhat lower CO pressure than normally would occur. This effect is probably more important for low burnup fuel than high burnup fuel. Upcoming tests on German fuel at higher burnups should shed more light on the oxygen issue. See:

Production of Carbon Monoxide During Burn-up of UO_2 Kerneled HTR Fuel Particles, E. Proksch, et. al., Journal of Nuclear Materials, 107 (1982) pages 280-285.

Influence of Irradiation Temperature, Burnup, and Fuel Composition on Gas Pressure (Xe, Kr, CO, CO2) in Coated Particle Fuels, G.W. Horsley, et. al., Journal of the American Ceramic Society, 59, Number 1-2, pages 1-4.

Life Cycle Phase	Factor, Characteristic or Phenomenon	Definition
Accident With Subsequent Air Intrusion	Kernel Grain growth	Enlargement of grains as a result of diffusion

Importance Rank and Rationale	Knowledge Level and Rationale	Remedy for Inadequate Knowledge/Issue Closure Criteria
Rank: L	≤ 1600 °C: 3	Remedy: None at present
	> 1600 °C: N/A	Remedy: N/A
Rationale: Kernel grain growth has not been an issue. The higher burnups of coated particles fuels often results in the destruction of any structure. Gas release could be higher, but this issue hasn't come up.	Rationale: (≤ 1600 °C) The grain growth issue appears to be less important with coated particle fuel because the layers form the fission product boundary.	Closure Criterion: None at present
	Rationale (> 1600 °C) N/A	Closure Criterion: N/A

Additional Discussion

Unlike LWR fuel, the grain structure appears to be less important.

Life Cycle Phase	Factor, Characteristic or Phenomenon	Definition
Accident With Subsequent Air Intrusion	Kernel	Chemical reaction between carbon and the fuel (UO2 or UOC) to form UC2 and CO (gas)
	Buffer carbon-kernel interaction	

Importance Rank and Rationale	Knowledge Level and Rationale	Remedy for Inadequate Knowledge/Issue Closure Criteria
Rank: L	≤ 1600 °C: 5	Remedy: None
	> 1600 °C: N/A	Remedy: N/A
Rationale: A significant problem in this area has not been observed.	Rationale: (≤ 1600 °C) Reactions of this nature can be investigated using thermochemical codes. Nothing has come up to date.	Closure Criterion: None
	Rationale (> 1600 °C) N/A	Closure Criterion: N/A

<u>Additional Discussion</u>

This issue is discussed to some extent in: *Stoichiometric Effects on Performance of High-Temperature Gas-Cooled Reactor Fuels from the U-C-O System*, F.J. Homan, et. al., Nuclear Technology, 35, pages 428-441.

Life Cycle Phase	Factor, Characteristic or Phenomenon	Definition
Accident With Subsequent Air Intrusion	Kernel: Chemical attack by air Kinetics	Rate of reaction per unit surface area as a function of temperature and partial pressure of air

Importance Rank and Rationale	Knowledge Level and Rationale	Remedy for Inadequate Knowledge/Issue Closure Criteria
Rank: H	≤ 1600 °C: 3	Remedy: Determine the need for this information.
	> 1600 °C: N/A	Remedy:N/A
Rationale: As the kernel is oxidized, it can change its structure and release fission products in a small burst. The rate at which this happens may be important if a significant number of kernels are exposed or particles fail.	Rationale: (≤ 1600 °C) The details effects on kernels have not been studied. Some integral testing has been done with particles and fuel elements.	Closure Criterion: Resolve this issue for accident cases.
	Rationale (> 1600 °C) N/A	Closure Criterion: N/A

Additional Discussion

For some information on fuel under oxidizing conditions see:

Compilation of Fuel Performance and Fission Product Transport Models and Database for MHTGR Design, Martin, R.C., ORNL/NPR-91/6

Fuel Performance and Fission Product Behavior in Gas Cooled Reactors, IAEA-TECDOC-978 (1997)

Life Cycle Phase	Factor, Characteristic or Phenomenon	Definition
Accident With Subsequent Air Intrusion	Kernel: Chemical attack by air Catalysis	Modification of the reaction rate by fission products or impurities

Importance Rank and Rationale	Knowledge Level and Rationale	Remedy for Inadequate Knowledge/Issue Closure Criteria
Rank: L	≤ 1600 °C: 1	Remedy: Determine if relevant.
	> 1600 °C: N/A	Remedy: N/A
Rationale: A catalysis could increase the reaction rate and accelerate releases, but it doesn't appear that there are any good candidates.	Rationale: (≤ 1600 °C) Unknown	Closure Criterion: Collection of relevant data.
	Rationale (> 1600 °C) N/A	Closure Criterion: N/A

Additional Discussion

Accelerated releases from the kernel under accident conditions due to catalysis have not been explored.

Life Cycle Phase	Factor, Characteristic or Phenomenon	Definition
Accident With Subsequent Air Intrusion	Kernel: Chemical attack by air Changes in chemical form of fission products	Changes in chemical form resulting from oxidizing or reducing fission products

Importance Rank and Rationale	Knowledge Level and Rationale	Remedy for Inadequate Knowledge/Issue Closure Criteria
Rank: H	≤ 1600 °C: 4	Remedy: Determine the need for this knowledge, collect as necessary.
	> 1600 °C: N/A	Remedy: N/A
Rationale: Changes in the chemical form of the fission products can greatly change their transport properties. The greatest change may come from the reaction of UC and the change in kernel structure	Rationale: (≤ 1600 °C) Thermochemical codes can calculate the possible chemical compounds. Little confirmation work is available	Closure Criterion: Collect data to resolve uncertainties
	Rationale (> 1600 °C) N/A	Closure Criterion: N/A

Additional Discussion

The forms and migration of the fission products can be complex. For some information on the chemical forms see:

Fission Product Plateout and Liftoff in the MHTGR Primary System: A Review, NUREG/CR-5647

Chemical Behavior of Fission Products in Core Heatup Accidents in High-Temperature Gas-Cooled Reactors, R. Moormann, Nuclear Technology, 94 (1991), pages 56-67.

Fuel Performance and Fission Product Behavior in Gas Cooled Reactors, IAEA-TECDOC-978 (1997)

Life Cycle Phase	Factor, Characteristic or Phenomenon	Definition
Accident With Subsequent Air Intrusion	Kernel: Chemical attack by air Changes in kernel properties	Changes in diffusivity, porosity, adsorptivity, etc.

Importance Rank and Rationale	Knowledge Level and Rationale	Remedy for Inadequate Knowledge/Issue Closure Criteria
Rank: M	≤ 1600 °C: 4	Remedy: Determine the relevance of this situation
	> 1600 °C: N/A	Remedy: N/A
Rationale: If the kernel restructures because of oxidation, it can release some its stored inventory of fission products, mostly gases.	Rationale: (≤ 1600 °C) Testing has been done for LWR fuel. Some of this information may be useful for HTGR fuel.	Closure Criterion: Relevance of this situation and any data.
	Rationale (> 1600 °C) N/A.	Closure Criterion: N/A

Additional Discussion

The amount of damaged fuel determines how significant this issue is. If the fuel performs as advertised, then it may not matter. See *Fuel Performance and Fission Product Behavior in Gas Cooled Reactors*, IAEA-TECDOC-978 (1997)

Appendix F.3

Detailed PIRT Submittal by the SNL Panel Member

F. A. Powers

TRISO Fuel PIRT: Accident With Subsequent Air Intrusion

This PIRT is based more on geometry than it is on phenomenology, despite the name. The PIRT seems to be attempting to identify the critical component of the coated particle fuel structure that deserves the most attention. This is done at the expense of identifying the critical phenomena that need to be understood to anticipate the behavior of the fuel in normal and off normal circumstances. As a result questions are asked repetitively about each of the major elements of the fuel perhaps to see if one or more of the elements are more vulnerable than others. The questions do not illuminate in any detail the type of information that must be derived for coated particle fuel or the types of testing that must be done to gather the information. For instance, lumped within the simple question of gas phase diffusion are bulk and Knudsen diffusion. Though the question is repeated for each layer even when the layers are very similar, such as inner and outer PyC, there is no request for details of the materials that would be essential to estimate Knudsen versus bulk diffusion such as porosity and tortuosity. There is no indication of whether tests of permeability need to be done for layers in situ or such data can be obtained from macroscopic samples of analog material. We do not know from the PIRT whether phenomena such as thermal diffusion require testing to be done in prototypic gradients or just known gradients. We do not know from the PIRT whether diffusion must be considered as approximately binary diffusion or has to be viewed as a multicomponent process. This focus on the structure at the expense of phenomena limits the utility of the PIRT for the design of fuel models and experimental studies. Perhaps, the PIRT is more useful in other respects because of its focus on structure.

Life Cycle Phase	Factor, Characteristic or Phenomenon	Definition
Accident With Subsequent Air Intrusion	Fuel Element Irradiation history	The temperature, burnup and fast fluence history of the layer

Importance Rank and Rationale	Knowledge Level and Rationale	Remedy for Inadequate Knowledge/Issue Closure Criteria
Rank: H	Level: 3	Remedy:There is a need for studies of the energetics of radiation damage to the materials making up the coated particle fuel layers. (Damage to the kernel is of lesser interest). The needed information can probably be obtained by thermal analysis of specimens irradiated under prototypic conditions for varying lengths of time. There is further need for information on the kinetics of oxidant reactions and reactions of nitrogen with the materials as functions of temperature.
Rationale: The fast fluence history of the layers will dictate how much radiation damage is built into the materials. This will affect the kinetics of reaction. Also as reaction proceeds, the radiation damage energy will be released augmenting the energy of chemical reactions with the layers	Rationale: We have some knowledge of the radiation damage that can develop in carbon materials at the operating temperatures of interest for this work. We don't have such information about the specific materials involved in the coated particle fuel. Furthermore, we don't have data or models on the effects of radiation damage on the kinetics of oxidant interactions with the materials	Closure Criterion:

Additional Discussion

Life Cycle Phase	Factor, Characteristic or Phenomenon	Definition
Accident With Subsequent Air Intrusion	Fuel Element Condensed phase diffusion	Inter grannular diffusion and/or intra-grannular solid-state diffusion

Importance Rank and Rationale	Knowledge Level and Rationale	Remedy for Inadequate Knowledge/Issue Closure Criteria
Rank: M	Level: 1	Remedy: The essential remedy is to wait until a specific and reproducible material is specified. Then the material has to be characterized in terms of grain size and orientation as well as in terms of the surface and grain boundary diffusion coefficients of irradiated material. Diffusion studies will have to take into account the fact that the material will not be isothermal. Rather there will be necessarily a temperature gradient across the material from the fuel particles (which are the source of the decay heat) and the coolant. A major issue to confront here is whether the release modeling should be so complete that it considers release limitations by the matrix material surrounding the fuel particles. It would not be an unreasonable conservatism to neglect this barrier to release since it appear unlikely that there will soon be useful experimental data to validate models of the barrier
Rationale: Grain boundary and surface diffusion of fission products will be faster mechanisms of mass transport of fission products from the perimeter of the fuel particles to the surfaces of the matrix material and into the reactor coolant system from where they can escape into the plant environment. Surface diffusion and grain boundary diffusion are notoriously sensitive to impurity concentrations of the material. They are also sensitive to the grain sizes and the preferential orientation of grains. Presumably they are also sensitive to the irradiation of the material though I am not familiar with definitive studies of this issue. Diffusion in the systems will be complicated by the presence of a thermal gradient across the material.	Rationale: The bulk matrix material has not been specified and certainly has not been characterized sufficiently to estimate diffusion coefficients for the fission products. There are of course no measured data because the specification of the material has not yet been made. Studies of generic material may provide some guidance.	Closure Criterion:

Additional Discussion

Life Cycle Phase	Factor, Characteristic or Phenomenon	Definition
Accident With Subsequent Air Intrusion	Fuel Element Gas diffusion	Diffusion of gaseous fission products through layer (Knudsen and bulk diffusion through pore structure, and pressure driven permeation through structure) Other factors include holdup craking adsorption, site poisoning, permeability, sintering and annealing

Importance Rank and Rationale	Knowledge Level and Rationale	Remedy for Inadequate Knowledge/Issue Closure Criteria
Rank: H	Level: 4	Remedy: The gas phase mass transport across elements from multi-point sources is a sufficiently complicated process that it is probably useful to set up models now and test them against models used for catalysts and the like. Detailed analyses of the issue will have to wait until there are real data on the fuel matrix materials that will be used in the reactor. A major issue to confront here is whether the release modeling should be so complete that it considers release limitations by the matrix material surrounding the fuel particles. It would not be an unreasonable conservatism to neglect this barrier to release since it appear unlikely that there will soon be useful experimental data to validate models of the barrier
Rationale: Vapor transport through pores and voids in the matrix material will be the fastest mechanism of mass transport of fission products from the fuel particle surfaces to the boundary of the fuel elements, The transport may driven by pressure differences or it may be by diffusion (either chemical or Knudsen). The presence of a thermal gradient will affect the diffusion process. It may be necessary to develop the diffusion equations to include thermal diffusion. Certainly the mass transport will have to address multicomponent effects using something like the Stefan Maxwell equations rather than Fickian diffusion equations	Rationale: The physics of the process is relative well understood and, indeed, fairly sophisticated models of this kind of mass transport have been developed by the catalyst community. What we don't know with any detail is the speciation of the fission product vapors or the pore and void structure of the matrix material. Diffusion coefficients for the vapors can be estimated with surprisingly good reliability from simple first order Chapman Enskog theory. Second order theory must be used to estimate thermal diffusion coefficients which (continued next column)	Closure Criterion: (continued from previous column) may not be negligible if the thermal gradients are large and if there are gases that have low molecular weights relative to the fission product vapors. Application of models of this type to the issue is not possible now because we do not have data on the material such as its void and porosity structure and its permeability

Additional Discussion

Life Cycle Phase	Factor, Characteristic or Phenomenon	Definition
Accident With Subsequent Air Intrusion	Fuel Element: Transport of metallic FPs through fuel element Chemical form	Chemical stoichiometry of the chemical species that includes the radioisotope of interest

Importance Rank and Rationale	Knowledge Level and Rationale	Remedy for Inadequate Knowledge/Issue Closure Criteria
Rank: H A major issue to confront here is whether the release modeling should be so complete that it considers release limitations by the matrix material surrounding the fuel particles. It would not be an unreasonable conservatism to neglect this barrier to release since it appear unlikely that there will soon be useful experimental data to validate models of the barrier	Level: 4	Remedy: There needs to be an agreed upon thermodynamic data base for the important species arising in the analysis of fission product release at these gas-cooled reactors. Much of the data in this base could be borrowed from existing databases. There needs also to be a search for possible species many of which have been identified in the literature but not characterized sufficiently to include in data bases now available.
Rationale: metallic fission products are going to be transported through the matrix material primarily as vapors. The effective vapor pressures of the metallic fission products depend on their gas phase speciation. There have been fairly limited investigations of the speciation of the fission products in the strongly reducing environment of the fuel element. Certainly the elemental forms will be important. What is of interest is whether there are more exotic species such as carbonyls and carbides and even cyanides that can augment the vapor pressures significantly. A reliable database on the thermodynamics of fission product species appropriate for this kind of a reducing environment (At least prior to oxidant intrusion) has not been assembled. Existing databases treat primarily elements, oxides and in some cases hydroxides. Once the oxidant (air) intrudes, these other possible vapor species as well as vapor phase hydrides need to be considered to know the vapor pressures of the fission products	Rationale: Elemental vapor pressures are rather well established for most of the fission products. Databases exist for most oxides and some hydroxides. Hydride, carbonyl, carbide data are scattered in the literature and have not been systematized nor has there been a systematic survey to identify more exotic vapor species. Polyatomic vapor species become less important as temperatures increase and pressures decrease.	Closure Criterion:

Life Cycle Phase	Factor, Characteristic or Phenomenon	Definition
Accident With Subsequent Air Intrusion	Fuel Element: Chemical attack by air Kinetics	Rate of reaction per unit surface area as a function of temperature and partial pressure of air

Importance Rank and Rationale	Knowledge Level and Rationale	Remedy for Inadequate Knowledge/Issue Closure Criteria
Rank: H	Level: 4	Remedy: Any model of fission product release will have to be capable of addressing the multiple effects of oxidation.
Rationale: The intrusion of oxidant, in this case air, will have several effects : Alter the ambient oxygen potential and consequently the speciation and volatility of fission products Convert carbon into carbon monoxide, etc. and in doing so open pathways for vapor transport through the fuel element to the reactor coolant system thereby facilitating release of radionuclides Impart heat to the element and alter the temperature distribution within the element The kinetics of attack on the matrix material is important since the depletion of oxidant by the reactions reduces the attack that is possible on fuel particles themselves. An interesting issue in the case of air intrusion is reactions of nitrogen. Presumably some production of cyanogens occurs. Cyanides of metals such as fission product metals are often considered analogous to the rather volatile halides of the same metals. Does the production of cyanogens alter the vapor phase speciation of fission products and enhance the volatility of fission products normally considered refractory? Unfortunately, there does not seem to have been a systematic study of the volatile cyanides of pertinent metals in the literature.	Rationale: There is a lot of information about air interactions with generic graphitic materials though obviously nothing specifically for the material that will be used in gas-cooled reactor fuel. What we know is that at lower temperatures the attack by oxidant is not uniform. Attack is along preferential locations. Catalysis can be responsible for this localized attack and catalysis is discussed further below. In the absence of catalysis oxidation of graphite seems to be at energetic sites such as those found on cracks and pore networks of the material. This means that solid material gets converted to gas to open channels for gas phase mass transport from the fuel particles through the matrix material. It also means that kinetics of oxidant attack on graphite should differ between normal material and irradiated material though it is not entirely clear how much the kinetics differ. One possibility is that irradiation will make the attack more homogeneous since the defects introduced by irradiation will be much like energetic sites on the walls of cracks and pore networks. Investigation of the kinetics of oxidation as a function of temperature is made complicated by the additional release of energy as material displace by irradiation from normal crystal sites reacts. At very high temperatures, the attack on graphite by oxidant becomes more uniform and the effects of catalysis less dominant. Still the overall issues of oxidation remain.	Closure Criterion:

Additional Discussion

Life Cycle Phase	Factor, Characteristic or Phenomenon	Definition
Accident With Subsequent Air Intrusion	Fuel Element: Chemical attack by air Catalysis	Modification of the reaction rate by fission products or impurities

Importance Rank and Rationale	Knowledge Level and Rationale	Remedy for Inadequate Knowledge/Issue Closure Criteria
Rank: H	Level: 5	Remedy:Catalysis will have to recognized in modeling of the oxidation of graphite.
Rationale: the oxidation of graphite is catalyzed especially at lower temperatures. The catalysis arises because of the adsorption step $O_2(gas) = 2\ O\ (surface)$ That preceeds reaction with carbon and the desorption step $CO(surface) = CO(gas)$ Catalysis is by materials deposited on the surface of the graphite. Because of this, catalytic attack is localized and leads to pits being bored into the material. The depth of attack in these pits vastly exceeds the expected uniform erosion. In the case of fuel elements, pit attack can result in oxidant boring into the regions of fuel particles. Many materials catalyze the oxidation. Common contaminants such as iron catalyze attack. Such fission products such as cesium and palladium are known to catalyze attack.	RationaleThere is information in the literature on catalytic oxidation of generic graphites. Nothing can be said to be particularly applicable to the graphite to be used in the reactors. There has not been a systematic survey of catalysts by the fission products of interest for graphite reactors. Catalysis becomes of decreasing interest at very elevated temperatures – It is difficult to investigate because the catalysts vaporize from the surface. This may not be an excuse to ignore the issue here. The transport of radionuclides will involve transient adsorption and desorption along the transport pathway. During residence on the surface the material can catalyze reaction of the surface and the opening of the flow pathway	Closure Criterion:

Additional Discussion

Life Cycle Phase	Factor, Characteristic or Phenomenon	Definition
Accident With Subsequent Air Intrusion	Fuel Element: Chemical attack by air	Changes in chemical form resulting from oxidizing or reducing fission products
	Changes in chemical form of fission products	

Importance Rank and Rationale	Knowledge Level and Rationale	Remedy for Inadequate Knowledge/Issue Closure Criteria
Rank: H	Level: 4	Remedy Any modeling of the fission product release from gas reactor fuels will have to include a careful thermodynamic assessment of both the condensed and vapor phase speciation. It may require that this speciation assessment is spatially dependent:
Rationale: Vapor pressures of many of the fission products are strong functions of the ambient oxygen potential. In the regions of oxidant attack the oxygen potential may be much higher than the bulk average oxygen potential of the reactor core. The higher oxygen potential can enhance the vaporization of fission products like Pd, Ru, Mo. It can inhibit the vaporization of fission products like Ba, Sr, La, Ce. An intriguing concept is the possibility that nitrogen will react with carbon to form cyanogens that will subsequently react to form pseudo halides of the metals. N_2 (gas) + 2C = $(CN)_2$ $(CN)_2$ + Ru = $Ru(CN)_2$ (gas) Since pseudohalides like halides are typically quite volatile, this could enhance the vaporization of some radionuclides. At high temperatures, vapor phase nitrides (as well as carbides) could contribute to the volatility of the fission products.	Rationale: The speciation of fission products in the environment of air attack on graphite have not been explored very thoroughly though the basis for such an exploration can be done. The data base is not well established and there has not been a careful survey to identify unusual species like carbides and cyanides that might contribute to the vaporization of fission products	Closure Criterion:

Life Cycle Phase	Factor, Characteristic or Phenomenon	Definition
Accident With Subsequent Air Intrusion	Fuel Element: Chemical attack by air Changes in graphite properties	Changes in diffusivity, porosity, adsorptivity, etc.

Importance Rank and Rationale	Knowledge Level and Rationale	Remedy for Inadequate Knowledge/Issue Closure Criteria
Rank: H	Level: 2	Remedy:This modeling of the oxidation along pathways for mass transport could be a very challenging feature of a fission product release model. Whether the development of such a model needs to be done or not depends on whether credit is taken for the barrier to fission product release provided by the matrix material.
Rationale: As noted above, especially at lower temperatures, oxidant attack on graphite is localized, not uniform and the localized attack is on the regions that will facilitate gas phase mass transport of fission product vapors through the fuel matrix like cracks and pore networks, the attack opens these pathways and makes transport easier	Rationale: The prediction of the effects of oxidant attack on the pathways is challenging. There has been some work in the chemical engineering field on analogous issues that could serve as a basis for modeling this phenomenon.	Closure Criterion:
	The effects of oxidant attack on cracks and pore networks become less important as temperature become very high and the attack becomes more uniform.	

<u>Additional Discussion</u>

Life Cycle Phase	Factor, Characteristic or Phenomenon	Definition
Accident With Subsequent Air Intrusion	Fuel Element: Chemical attack by air Holdup reversal	Release of graphite FP inventory

Importance Rank and Rationale	Knowledge Level and Rationale	Remedy for Inadequate Knowledge/Issue Closure Criteria
Rank: L	Level: 5	Remedy: It is not clear that this phenomenon needs to be included in a model. Certainly it does not need to be included if the barrier to release presented by the matrix is neglected as a conservative measure that considerably relieves the challenges in estimating releases for risk assessments.
Rationale: It is known that energetic sites will adsorb fission product vapors and create some holdup of the release of radionuclides. It is not evident that there are enough of these sites to cause the holdup of a significant fraction of the radionuclide inventory. It is known that chemical reactions that destroy energetic sites or even the intrusion of polarizable gases that will compete for site occupancy can result in the release of the adsorbed fission products. But, if the desorption does not involve a large fraction of the inventory of particular class of fission products the phenomenon is not significant	Rationale We probably do not have sufficient data on the holdup to make quantitatively defensible estimates of the holdup. We do know enough to make simple qualitative arguments about its significance Holdup on the matrix surfaces is less important at high temperatures because of the high vapor pressures of the fission product species of interest. Though we certainly know less about holdup on the surfaces at high temperature than we know at low temperatures, we probably know enough to say that if the importance of the phenomenon is questionable at low temperatures, it certainly is unimportant at very high temperatures.	Closure Criterion:

Additional Discussion

Life Cycle Phase	Factor, Characteristic or Phenomenon	Definition
Accident With Subsequent Air Intrusion	Fuel Element: Chemical attack by air Temperature distribution	Impact of graphite oxidation on temperature distribution through material

Importance Rank and Rationale	Knowledge Level and Rationale	Remedy for Inadequate Knowledge/Issue Closure Criteria
Rank: H	Level: 6	Remedy: If the barrier to fission product release posed by the matrix material is to be considered a fairly sophisticated model of gas phase mass transport will be needed. (A completely similar model will be needed also for mass transport in the fuel particles themselves. Once developed the same model can be used in both places) Modeling of fission product transport by gas phase processes will be important both because these are the fastest transport processes and because it is unlikely that we will ever have good, reproducible data on the release of fission products from fuel elements for the range of accidents that will be of interest for risk assessments.
Rationale: Temperature distributions along the transport paths for fission products will affect the vapor pressures of these fission products. The temperature gradients will also affect the gas phase mass transport of fission products (It will also affect condensed phase mass transport though here this process is taken to be much less important than gas phase mass transport) the effect is both to the chemical diffusion of vapors and to the thermal diffusion	Rationale: Given the details of the gas phase mass transport paths (which are not currently available) it should be possible to estimate the effects of temperature distribution on the transport of fission product vapors from the fuel particles to the surfaces of the fuel element exposed to the atmosphere of the reactor coolant system. Many things will have to be estimated. Fickian diffusion may not be the appropriate basis for the calculation of transport of multicomponent gas which may include light molecular weight species such as CO along with heavy molecular weight species like the fission product (continued next column)	Closure Criterion: (Continued from previous column) vapors. Though we can estimate chemical diffusion coefficients using perturbations of Chapman Enskog theory, it is more challenging to estimate the thermal diffusion coefficients of polyatomic species (Third order expansion of determinants versus first order expansion). A further complication will be the need to allow for Knudsen diffusion and pressure driven flow in the case of very limited flow pathways for release. Though the problem is doable, it is not trivially doable.
	The reliability of predictions of gas phase mass transport decreases with increasing temperature because of the increasing influence of inelastic collisions Otherwise things are the same as above though Knudsen diffusion becomes more important at higher temperatures	

Life Cycle Phase	Factor, Characteristic or Phenomenon	Definition
Accident With Subsequent Air Intrusion	Outer PyC Layer Gas Phase Diffusion	Diffusion of gaseous fission products through layer (Knudsen and bulk diffusion through pore structure, and pressure driven permeation through structure)

Importance Rank and Rationale	Knowledge Level and Rationale	Remedy for Inadequate Knowledge/Issue Closure Criteria
Rank: H	Level: 6	Remedy: Any model of fission product transport within the fuel particle will have to include a gas phase mass transport model recognizing bulk diffusion, pressure driven flow and Knudsen diffusion
Rationale: These gas phase mass transport processes are the fastest ways for fission products released from the kernel to cross the Outer PyC layer.	Rationale: Given the geometry and nature of the pore and crack network in the layer it is possible to calculate the gas phase mass transport across the layer. We can estimate most of the gas phase diffusion coefficients. The mass transport is probably not modeled well by Fickian diffusion and one will have to develop a multicomponent diffusion model much like the membrane models that have been developed in the chemical engineering literature. It may be necessary to include in these models the effects of thermal diffusion especially if the gas includes both low molecular weight species such as CO (MW=28) and fission product vapor species (MW>100) and temperature gradients are significant as they surely must be to get decay heat out of the particle. The most complicated part of the modeling will be to treat the geometries of the layer as a (continued next column)	Closure Criterion: (continued from previous column) whole and the pore, crack and void network in the layer. We know the layers will not by spherically symmetric. Does the deviation from symmetry have a significant effect on the rate of transport? Similarly the layers will not be uniformly thick and this may create short circuits or preferred pathways for mass transport. We do not have good data on the pore and void network. We are not likely to get adequate data from microscopic analysis. The cracks pores and voids that are of interest are too small to readily identify and detect and microscopic examinations will never yield anything but a biased estimate of the concentration and sizes of the networks. Transport data are needed, but it is not readily apparent how such data are obtained for the microscopic layers of the particles.
	The situation is much the same at elevated temperatures though gas phase mass transport becomes an even more dominant mechanism simply because the gas phase concentrations are higher. The ability to estimate diffusion coefficients and thermal diffusion coefficients for polyatomic vapor species begins to degrade because inelastic collision become more important	

Life Cycle Phase	Factor, Characteristic or Phenomenon	Definition
Accident With Subsequent Air Intrusion	Outer PyC Layer Condensed phase diffusion	Intergrannular diffusion and'or intra-grannular solid-state diffusion

Importance Rank and Rationale	Knowledge Level and Rationale	Remedy for Inadequate Knowledge/Issue Closure Criteria
Rank: M	Level: 2	Remedy: Any model of fission product transport across the Outer PyC layer will have to include these process though it is likely that even with only modest vapor pressures the gas phase mass transport processes will be more important mechanisms. The diffusion process has the same problems discussed above. Spherical symmetry may be an overly crude approximation as may be the assumption that the layer is uniformly thick.
Rationale: Fission products that are not volatile will be transported across the barrier posed by the outer PyC layer by the condensed phase diffusion processes. Bulk diffusion is the slowest of these a low temperatures, but it has the highest activation energy so it does eventually become the dominant process. Even if the metals have only small vapor pressures, gas phase mass transport of fission products may still be the dominant mechanism for most fission products. There do appear to be some exceptions such as the transport of Ag.	Rationale: We donot have surface and grain boundary diffusion coefficients for the fission products and materials of interest here and surface and grain boundary diffusion are likely to be the dominant condensed phase transport processes. These coefficients cannot be estimated. They have to be measured and they are notoriously sensitive to impurities accumulated on the grain surfaces and at the grain boundaries	Closure Criterion:
	At sufficiently high temperatures (and it by no means established that 1600 is sufficiently high) bulk diffusion of fission products will be dominant transport processes for nonvolatile species. We do not have useful bulk diffusion coefficients for irradiated material. The need for irradiated material is to be emphasized since it is known that radiation defects can act as traps for diffusing species	

Additional Discussion

Life Cycle Phase	Factor, Characteristic or Phenomenon	Definition
Accident With Subsequent Air Intrusion	Outer PyC Layer Layer oxidation	Reaction of pyrolytic graphite with oxygen released from the kernel

Importance Rank and Rationale	Knowledge Level and Rationale	Remedy for Inadequate Knowledge/Issue Closure Criteria
Rank: H	Level: 2	Remedy: Analysis of fission product release during air intrusion or water intrusion accidents will have to account for the effects of oxidant on the integrity of the outer PyC layer. It will have to be a kinetic analysis so that the analyst will know how much oxidant survives the interaction with the layer to attack other regions of the fuel particle.
Rationale: Oxidant can reach the Outer PyC layer either coming from oxygen evolved from the fuel kernel or oxidant intruding into the core (air or water). It is likely that the source of oxidant coming form the fuel will be sufficiently weak that most of this oxidant will be consumed by reactions with graphite etc. before it can reach the Outer PyC layer in any form other than CO. Oxidant from intrusive sources will have to survive reactions with graphitic materials along its transport path to the fuel particle. When it does survive this transport the results can be catastrophic with respect to fission product transport across the PyC layer. The oxidant will thin the layer, but more importantly localized attack on energetically preferred sites will result in widening and smoothing the cracks and pores through the layer thereby facilitating gas phase mass transport across the layer. The oxidation reactions can also heat the layer	Rationale: The oxidation reactions kinetics are enormously sensitive to impurities that can catalyze reactions. Fission products themselves may act as catalysts. Though we have some data on the oxidation reactions, we do not have data on the specific material. Without these data accurate quantitative analysis of the oxidation process at the Outer PyC layer is really not possible The situation becomes a little simpler at very high temperatures where the kinetics are less affected by the catalytic processes and proceed in a more uniform process. Still we donot have validated kinetic models.	Closure Criterion:

Additional Discussion

Life Cycle Phase	Factor, Characteristic or Phenomenon	Definition
Accident With Subsequent Air Intrusion	Outer PyC Layer Stress state (compression/tension)	The state of the forces induced by external forces that are acting across the layer to resist movement

Importance Rank and Rationale	Knowledge Level and Rationale	Remedy for Inadequate Knowledge/Issue Closure Criteria
Rank: L	Level: 2	Remedy: it isn't clear that any remedy is needed
Rationale:This is a more important issue during normal operations since it can result in rupture of the layer prior to the accident . Thermal expansion may cause some stresses on the layer and it would be of interest to know if rupture can occur	RationaleWe really don' t know much about these forces	Closure Criterion:

Additional Discussion

Life Cycle Phase	Factor, Characteristic or Phenomenon	Definition
Accident With Subsequent Air Intrusion	Outer PyC Layer Intercalation	Trapping of species between sheets of the graphite structure

Importance Rank and Rationale	Knowledge Level and Rationale	Remedy for Inadequate Knowledge/Issue Closure Criteria
Rank: L	Level: 2	Remedy: no remedy needed
Rationale: It is known that energetic sites in the PyC layer will provide sites for fission product deposition and holdup. There can be a preference for fission products to migrate toward the basal planes of the graphite structure and be intercalated. It is not apparent that sufficient concentrations of sites will be formed to holdup a significant fraction of the radionuclide inventory of the fuel particle. Eventually oxidation or thermal annealing will eliminate these energetic sites and lead to the desorption of fission products that have been attracted to the sites. The elevated temperatures will eventually move fission products from the intercalation sites as well.	Rationale: We don't really know how much holdup can occur At sufficiently high temperatures there really will not be any holdup since the vapor pressures of the fission products will be so high	Closure Criterion:

Additional Discussion

Life Cycle Phase	Factor, Characteristic or Phenomenon	Definition
Accident With Subsequent Air Intrusion	Outer PyC Layer Trapping	Adsorption of fission products on defects

Importance Rank and Rationale	Knowledge Level and Rationale	Remedy for Inadequate Knowledge/Issue Closure Criteria
Rank: L	Level: 2	Remedy: no remedy needed
Rationale: It is known that energetic sites in the PyC layer will provide sites for fission product deposition and holdup. There can be a preference for fission products to migrate toward the basal planes of the graphite structure and be intercalated. It is not apparent that sufficient concentrations of sites will be formed to holdup a significant fraction of the radionuclide inventory of the fuel particle. Eventually oxidation or thermal annealing will eliminate these energetic sites and lead to the desorption of fission products that have been attracted to the sites. The elevated temperatures will eventually move fission products from the intercalation sites as well.	Rationale: We don't really know how much holdup can occur At sufficiently high temperatures there really will not be any holdup since the vapor pressures of the fission products will be so high	Closure Criterion:

Additional Discussion

Life Cycle Phase	Factor, Characteristic or Phenomenon	Definition
Accident With Subsequent Air Intrusion	Outer PyC Layer Cracking	Lengths, widths and numbers of cracks produced in layer during accident

Importance Rank and Rationale	Knowledge Level and Rationale	Remedy for Inadequate Knowledge/Issue Closure Criteria
Rank: H	Level: 1	Remedy:It is clear that any model of fission product transport through the fuel particles has to recognize the possibility of cracks in the material providing a short pathway for transport. Whether the cracking has to be modeled or cracking is input to the transport model is a decision that must be made. This decision may well rest on whether cracking occurs during the accident transient or is primarily a process that occurs during normal operations.
Rationale: Cracks through the layer facilitate gas phase mass transport of fission products across the layer	Rationale: It is not apparent that we are in any position to predict the cracking of the layers under any circumstances let alone under accident circumstances. It may not be practical to predict cracking and we will have to rely on empirical evidence for cracks. This is a challenge since cracks that can affect fission product release rates may be very difficult to detect microscopically	Closure Criterion:

Additional Discussion

Life Cycle Phase	Factor, Characteristic or Phenomenon	Definition
Accident With Subsequent Air Intrusion	Outer PyC Layer:Chemical attack by air Kinetics	Rate of reaction per unit surface area as a function of temperature and partial pressure of air

Importance Rank and Rationale	Knowledge Level and Rationale	Remedy for Inadequate Knowledge/Issue Closure Criteria
Rank: H	Level: 2	Remedy: Analysis of fission product release during air intrusion or water intrusion accidents will have to account for the effects of oxidant on the integrity of the outer PyC layer. It will have to be a kinetic analysis so that the analyst will know how much oxidant survives the interaction with the layer to attack other regions of the fuel particle.:
Rationale: Oxidant can reach the Outer PyC layer either coming from oxygen evolved from the fuel kernel or oxidant intruding into the core (air or water). It is likely that the source of oxidant coming form the fuel will be sufficiently weak that most of this oxidant will be consumed by reactions with graphite etc. before it can reach the Outer PyC layer in any form other than CO. Oxidant from intrusive sources will have to survive reactions with graphitic materials along its transport path to the fuel particle. When it does survive this transport the results can be catastrophic with respect to fission product transport across the PyC layer. The oxidant will thin the layer, but more importantly localized attack on energetically preferred sites will result in widening and smoothing the cracks and pores through the layer thereby facilitating gas phase mass transport across the layer. The oxidation reactions can also heat the layer	Rationale: The oxidation reactions kinetics are enormously sensitive to impurities that can catalyze reactions. Fission products themselves may act as catalysts. Though we have some data on the oxidation reactions, we do not have data on the specific material. Without these data accurate quantitative analysis of the oxidation process at the Outer PyC layer is really not possible The situation becomes a little simpler at very high temperatures where the kinetics are less affected by the catalytic processes and proceed in a more uniform process. Still we do not have validated kinetic models.	Closure Criterion:

Additional Discussion

Life Cycle Phase	Factor, Characteristic or Phenomenon	Definition
Accident With Subsequent Air Intrusion	Outer PyC Layer: Chemical attack by air Catalysis	Modification of the reaction rate by fission products or impurities

Importance Rank and Rationale	Knowledge Level and Rationale	Remedy for Inadequate Knowledge/Issue Closure Criteria
Rank: H	Level: 4	Remedy: Models of fission product transport that include the effects of oxidation will have to take into account catalysis. That is oxidation of pure material cannot be the kinetic data base the model uses.
Rationale: catalysis by impurities will affect the oxidation rates of the PyC layer. Catalysis can be caused by fission products. Defects introduced by the irradiation of the layer may also accelerate the reaction kinetics in such a way that the catalytic effects are not detectable. However, the biggest effect of catalysis is to open up pore networks and facilitate the transport of radionuclides across the layer. Defects and reactive sites are very likely to be most concentrated in these networks.	Rationale: We don't have good models of the catalysis of oxidation of the materials of specific interest by the fission products or the radiation defects.	Closure Criterion:
	Catalysis is much less important at high temperatures where the reaction rates are inherently high and the fission products are quite volatile. Though we don't know more about high temperature catalysis, we don't need to know as much so our relative knowledge level is higher	

Additional Discussion

Life Cycle Phase	Factor, Characteristic or Phenomenon	Definition
Accident With Subsequent Air Intrusion	Outer PyC Layer: Chemical attack by air	Changes in chemical form resulting from oxidizing or reducing fission products
	Changes in chemical form of fission products	

Importance Rank and Rationale	Knowledge Level and Rationale	Remedy for Inadequate Knowledge/Issue Closure Criteria
Rank: H	Level: 5	Remedy: Fission product transport models will have to have the capability to evolve the chemical forms of the fission products as the ambient conditions change with respect to both chemical potentials and temperatures.
Rationale: The high local oxygen potential will change the fission product chemical form making some more volatile and some less volatile	Rationale: We have databases that will allow us to do some exploration of the change in chemical form of the fission products in the vicinity of regions of higher oxidation potential. We do not have information on more exotic species like pseudo halides such as cyanides that may affect the volatility of some of the more refractor fission products.	Closure Criterion:

Additional Discussion

Life Cycle Phase	Factor, Characteristic or Phenomenon	Definition
Accident With Subsequent Air Intrusion	Outer PyC Layer: Chemical attack by air Changes in graphite properties	Changes in diffusivity, porosity, adsorptivity, etc.

Importance Rank and Rationale	Knowledge Level and Rationale	Remedy for Inadequate Knowledge/Issue Closure Criteria
Rank: H	Level: 3	Remedy: Oxidation effects on fission product transport will have to be considered. Data on the change in the permeability of material as reactions progress would be useful.
Rationale: The important effect of oxidation aside from changing the volatilities of the fission products is to open pathways for the transport of the fission products from the fuel kernels to the outside of the fuel particles.	Rationale It is difficult to predict quantitatively how the oxidation will change the transport pathways	Closure Criterion:
	same as above, however at higher temperature when oxidation kinetics are rapid, the reactions take place more uniformly and act more to ablate material (shorten the transport distance) than to open the flow pathways	

Additional Discussion

Life Cycle Phase	Factor, Characteristic or Phenomenon	Definition
Accident With Subsequent Air Intrusion	Outer PyC Layer: Chemical attack by air	Release of graphite FP inventory
	Holdup reversal	

Importance Rank and Rationale	Knowledge Level and Rationale	Remedy for Inadequate Knowledge/Issue Closure Criteria
Rank: L	Level: 4	Remedy:It is not evident a remedy is needed until there is some demonstration that the holdup is significant from a risk perspective
Rationale: oxidation reaction will destroy energetic sites that have absorbed fission products and thus release the fission products. It is not apparent that absorption of fission products on energetic sites holdups enough of the releasable inventory of fission products for this reactive desorption process to be risk important	Rationale: We don't have data on the adsorption. We do know that reactions will reverse it	Closure Criterion:
	At such high temperatures the adsorption of fission product vapors has probably been thermally reversed prior to reaction	

Additional Discussion

Life Cycle Phase	Factor, Characteristic or Phenomenon	Definition
Accident With Subsequent Air Intrusion	Outer PyC Layer: Chemical attack by air Temperature distribution	Impact of graphite oxidation on temperature distribution through material

Importance Rank and Rationale	Knowledge Level and Rationale	Remedy for Inadequate Knowledge/Issue Closure Criteria
Rank: H	Level: 3	Remedy:Any fission product transport model will require good, local temperature descriptions including the effects of chemical reactions on these temperatures
Rationale: Chemical reactions can heat the layer and change the thermal gradients across the layer – both of which will affect fission product transport	Rationale: We generally know enough about the heat of reaction. Combining this with the less well known kinetics of reaction and the heat that comes from destroying irradiation produced defects should allow a calculation of the effects of reaction on temperatures. The thermal conduction calculation is a challenge as delineated above	Closure Criterion:

Additional Discussion

Life Cycle Phase	Factor, Characteristic or Phenomenon	Definition
Accident With Subsequent Air Intrusion	SiC Layer Gas phase diffusion	Diffusion of gaseous fission products through layer (Knudsen and bulk diffusion through pore structure, and pressure driven permeation through structure)

Importance Rank and Rationale	Knowledge Level and Rationale	Remedy for Inadequate Knowledge/Issue Closure Criteria
Rank: H	Level: 6	Remedy: Any model of fission product transport within the fuel particles will have to include an gas phase mass transport model recognizing bul diffusion, pressure driven flow and Knudsen diffusion The mechanistic detail with which a model could be constructed is probably not supported by adequate characterization of the irradiated layer. It may be necessary to adopt a more empirical modeling retaining perhaps the functional forms suggested by the theory of mass transport through porous materials.
Rationale: Gas phase mass transport across the SiC layer through cracks or through the pore and void network in the material will be by far the fastest mechanism for mass transport of fission products across this layer	Rationale: Given the geometry and nature of the pore and crack network in the layer it is possible to calculate the gas phase mass transport across the layer. We can estimate most of the gas phase diffusion coefficients about as accurately as they can be measured. The mass transport probably cannot be calculated using Fickian diffusion and neglecting temperature gradients in the material. A multicomponent model similar in nature to the models of mass transport across membranes used widely in the chemical engineering field will have to be used. It may be necessary to recognize the effects of thermal diffusion if the temperature gradients are large and there are significant differences in the molecular weights of gases. This may well be the case especially inside the SiC layer which will be	Closure Criterion: (continued from previous column)
	The situation is largely the same at high temperatures as at low temperatures though the speciation of the gas phase fission products becomes more complicated.	

Life Cycle Phase	Factor, Characteristic or Phenomenon	Definition
Accident With Subsequent Air Intrusion	SiC Layer Condensed phase diffusion	Inter-grannular diffusion and/or intra-grannular solid-state diffusion

Importance Rank and Rationale	Knowledge Level and Rationale	Remedy for Inadequate Knowledge/Issue Closure Criteria
Rank: M	Level: 2	Remedy: Modeling of fission product transport will have to include the modeling of condensed phase mass transport.
Rationale: Fission products that are not volatile will transport across the layer by diffusion. At low temperatures, grain boundary diffusion and surface diffusion will be the more rapid processes. Because the activation energy for bulk diffusion is highest, it will become, eventually the dominant mechanism of mass transport as the temperature is increased. Still, even if the fission product has only a very small vapor pressure, gas phase mass transport may outstrip condensed phase diffusion processes. There are some exceptions to this. Ag seems to be capable of fast transport across the layer and this fast transport has been ascribed to condensed phase diffusion although there are not the data necessary to conclusively demonstrate this.	Rationale: We really don't have good condensed phase diffusion coefficients for fission products during bulk, surface or grain boundary diffusion for the specific material that is of interest. Bulk diffusion coefficients from analogous materials may be adequate IF the defects in the crystal lattices produced by irradiation don't act as traps for diffusing species. Grain boundary and surface diffusion coefficients depend so much on the impurity levels at surfaces and grain boundaries where these impurities accumulate, that it would be difficult to ascribe significance to data sets for anything except the actual material of the layer including the correct crystallite orientation etc. pressurized with CO from the reaction of carbon (continued next column)	Closure Criterion: (continued from previous column) materials with the urania fuel kernel. Complication in the analysis come about if the deviations from spherical symmetry of the layer are significant and if the variations in the layer thickness is significant. Characterization of the pore, void or crack network in the layer is most important and quite challenging since the voids or cracks that can be effective for mass transport are not easily detected by microscopic examination. It is furthermore quite difficult to average sets of visual observations of cracks and voids to come up with a suitable 'average' description for the analysis of mass transport. What would really be desirable would be permeability measurements of the layer. It is of course not practical to make such measurements.

Additional Discussion

Life Cycle Phase	Factor, Characteristic or Phenomenon	Definition
Accident With Subsequent Air Intrusion	SiC Layer Thermal deterioration/decomposition	Decline in the quality of the layer due to thermal loading

Importance Rank and Rationale	Knowledge Level and Rationale	Remedy for Inadequate Knowledge/Issue Closure Criteria
Rank: M	Level: 3	Remedy: no remedy may be needed.
Rationale: SiC is a most peculiar material. There have been reports of phase changes in the material from cubic to hexagonal at elevated temperatures. Modern phase diagrams do not reflect this phase change. It may be more important that the material is subject to polytypism based on the hexagonal structure. If the formation of the layer does not yield the thermodynamically stable product, thermal annealing during the temperature transient of an accident could cause some restructuring that will create pathways for gas phase mass transport. It might also be possible during a thermal transient for the heavily radiation damaged material to restructure to relieve the accumulation of strain energy of the irradiation defects (A sort of analogy to the formation of the rim in heavily irradiated fuel!). This restructuring could well lead to gas phase mass transport paths that will facilitate the transport of fission products released from the fuel kernel across the layer.	Rationale: To quantitatively examine this issue we would have to have considerable data on the product of the particle formation process to see if polytypism occurs and also to see if radiation restructuring can occur during an accident temperature transient. Then we would need data to see how annealing affected the permeability of the layer The situation is the same as above for lower temperatures	Closure Criterion:

Additional Discussion

Life Cycle Phase	Factor, Characteristic or Phenomenon	Definition
Accident With Subsequent Air Intrusion	SiC Layer Fission product corrosion	Attack of layer by fission products, e.g., Pd

Importance Rank and Rationale	Knowledge Level and Rationale	Remedy for Inadequate Knowledge/Issue Closure Criteria
Rank: L	Level: 3	Remedy: At this juncture it appears to me that holdup by chemical reaction with the SiC layer can be neglected until there is evidence that this important for more important radionuclides than Pd.
Rationale: Chemcial attack on the layer by fission products will affect transport across the layer and certainly may affect the transport of the fission product doing the transporting since it will be converted to a more stable form which may be less volatile. It is however to become excessively concerned over this since the fission product inventory of the kernel is not large enough to produce massive damage to the layer that will affect the transport of all fission products. There is only one example of significant attack and that is with Pd which is not an especially important fission product from an accident consequences view point. The attack by Pd may suggest other noble metals such as Ru and Mo will produce similar attack. There would have to be substantial evidence of this to rate the process of higher signficance.	RationaleWe don't have a comprehensive survey of the attack on SiC by fission products in part because SiC under reducing conditions is not an especially reactive material.	Closure Criterion:

Additional Discussion

Life Cycle Phase	Factor, Characteristic or Phenomenon	Definition
Accident With Subsequent Air Intrusion	SiC Layer Heavy metal diffusion	Diffusion of heavy metals through layer

Importance Rank and Rationale	Knowledge Level and Rationale	Remedy for Inadequate Knowledge/Issue Closure Criteria
Rank: M	Level: 2	Remedy: Modeling of fission product transport will have to include the modeling of condensed phase mass transport
Rationale: Fission products that are not volatile will transport across the layer by diffusion. At low temperatures, grain boundary diffusion and surface diffusion will be the more rapid processes. Because the activation energy for bulk diffusion is highest, it will become, eventually the dominant mechanism of mass transport as the temperature is increased. Still, even if the fission product has only a very small vapor pressure, gas phase mass transport may outstrip condensed phase diffusion processes. There are some exceptions to this. Ag seems to be capable of fast transport across the layer and this fast transport has been ascribed to condensed phase diffusion although there are not the data necessary to conclusively demonstrate this.	Rationale: We really don't have good condensed phase diffusion coefficients for fission products during bulk, surface or grain boundary diffusion for the specific material that is of interest. Bulk diffusion coefficients from analogous materials may be adequate IF the defects in the crystal lattices produced by irradiation don't act as traps for diffusing species. Grain boundary and surface diffusion coefficients depend so much on the impurity levels at surfaces and grain boundaries where these impurities accumulate, that it would be difficult to ascribe significance to data sets for anything except the actual material of the layer including the correct crystallite orientation etc.	Closure Criterion:

Additional Discussion

Life Cycle Phase	Factor, Characteristic or Phenomenon	Definition
Accident With Subsequent Air Intrusion	SiC Layer Layer oxidation	Uptake of oxygen by the layer through a chemical reaction

Importance Rank and Rationale	Knowledge Level and Rationale	Remedy for Inadequate Knowledge/Issue Closure Criteria
Rank: L	Level: 5	Remedy: No remedy needed.
Rationale: I distinguish here between the reaction of SiC with oxidant to form CO and SiO and the uptake to form nominally SiOC. This later uptake can only progress to the point of saturation. It will only be important if it causes swelling or decrepitation of the SiC layer and I can find no evidence that it does. All my experience is with higher oxygen potentials where SiO is not stable and SiO2 is the condensed product of reaction and this SiO2 does act to occlude surfaces which would interfere in gas phase mass transport at the highest temperatures. SiO, a vapor in the temperature ranges of interest could condense elsewhere in the particle and have some ramifications on the transport of fission products.	Rationale: There is a lot of information about the response of SiC to oxidizing conditions of various oxygen potentials. I don't' find information that indicates processes during uptake that would affect fission product transport (but see below when reaction is discussed)	Closure Criterion:

Additional Discussion

Life Cycle Phase	Factor, Characteristic or Phenomenon	Definition
Accident With Subsequent Air Intrusion	SiC Layer Fission product release through defects	Passage of fission gas from the buffer region through defects in the SiC layer

Importance Rank and Rationale	Knowledge Level and Rationale	Remedy for Inadequate Knowledge/Issue Closure Criteria
Rank: H	Level: 1	Remedy: This mechanism probably cannot be modeled mechanistically. It will have to be treated by providing empirical evidence of the change in layer permeability as irradiation progresses.
Rationale: Defects introduced into the SiC lattice by manufacture or by irradiation will become mobile at elevated temperatures and accumulate to form dislocations that themselves will lead to the formation of porosity networks. These networks will provide a pathway for gas phase mass transport that will be the dominant mechanism for fission product transport across the layer.	Rationale: We don't have the information to assess this process now	Closure Criterion:

Additional Discussion

Life Cycle Phase	Factor, Characteristic or Phenomenon	Definition
Accident With Subsequent Air Intrusion	SiC Layer Fission product release through failures, e.g. craking	Passage of fission gas from the buffer region through regions in the SiC layer that fail during operations or an accident

Importance Rank and Rationale	Knowledge Level and Rationale	Remedy for Inadequate Knowledge/Issue Closure Criteria
Rank: H	Level: 4	Remedy: Mechanistic modeling of gas phase mass transport across a failed layer of SiC may not be undertaken though it can be done. A true failure of the layer may be taken somewhat but not greatly conservatively as meaning the layer no longer poses a barrier to fission product transport.
Rationale: SiC layer failure will permit the venting of accumulated fission product vapors and the ongoing releases of fission product vapors as they escape the fuel kernel and reach the SiC layer	Rationale: We don't have information that allows us to know when SiC layers fail or how massive the failures are. If we had this information it should not be difficult to model the gas phase mass transport across the layer through the failure locations.	Closure Criterion:

Additional Discussion

Life Cycle Phase	Factor, Characteristic or Phenomenon	Definition
Accident With Subsequent Air Intrusion	SiC Layer Thermodynamics of the SiC-fission product system	Include solubility, intermetallics, and chemical activity

Importance Rank and Rationale	Knowledge Level and Rationale	Remedy for Inadequate Knowledge/Issue Closure Criteria
Rank: M	Level: 2	Remedy: The remedy is some compatibility studies of fission products with SiC
Rationale: Fission products that dissolve in the SiC lattice will be stabilized and will be held from release at least temporarily. It does not appear, however, that this is major factor in the release of the more important, volatile fission products like I, Cs, Xe, Kr, Te etc. It may be more important for some of the transition metal fission products. Certainly Pd actually can react with SiC. Similarly Zr might react. It would also be of interest to know if other materials interacted badly with SiC, but even if we knew of some bad interactions involving materials other than fission products, we would have to have some idea of how these materials came into contact with the SiC within a fuel particle.	Rationale: There is amazingly little information about the phase relationships in the Si-C-FP systems of interest.	Closure Criterion:

Additional Discussion

Life Cycle Phase	Factor, Characteristic or Phenomenon	Definition
Accident With Subsequent Air Intrusion	SiC Layer Sintering	Change of graphite microstructure as a function of temperature

Importance Rank and Rationale	Knowledge Level and Rationale	Remedy for Inadequate Knowledge/Issue Closure Criteria
Rank: L	Level: 6	Remedy no remedy necessary:
Rationale: I do not find anything to suggest that changes in the microstructure of graphite will affect the SiC layer there may be some information suggesting that bonding of the graphite to the SiC affects the integrity of this layer, but it has nothing to do with microstructure issues	Rationale : there is really quite a lot of information about the sintering of SiC in the literature. It does not necessarily cover the entire region of interest nor does it address the effects of the fission product species on the sintering process. It should, however, be sufficient to estimate the magnitudes of any effects attributable to sintering on fission product transport. Far more important than simple, classic sintering will the thermal annealing of the radiation-induced defects in the SiC structure	Closure Criterion:

Additional Discussion

Life Cycle Phase	Factor, Characteristic or Phenomenon	Definition
Accident With Subsequent Air Intrusion	SiC Layer: Chemical attack by air Kinetics	Rate of reaction per unit surface area as a function of temperature and partial pressure of air

Importance Rank and Rationale	Knowledge Level and Rationale	Remedy for Inadequate Knowledge/Issue Closure Criteria
Rank: H	Level: 4	Remedy:The key issues are whether sufficient oxidant survives transport through the core and the matrix material to reach the SiC and whether oxidant in the viscinity of the SiC layer will react to open pathways for gas phase mass transport across the layer or only leads to homogeneous ablation of layer material as the gases SiO and CO. Clearly actual data are needed and these should be collected for irradiated material since the dislocations produced by the irradiation should be more reactive than normal materials
Rationale: The rate of oxidation will be important to know. The rate will be complicated in regions of oxygen potential where there is a change from both products of oxidation being gases (SiO and CO) and higher oxygen potentials where the silicon-bearing product is condensed SiO2. More important than the homogeneous reaction kinetics will be how the reaction rates are affected by radiation-produced defects and the presence of pores and voids in the SiC. We will want to know if there is preferential attack in the voids that leads to the opening of pathways for gas phase mass transport of fission products through the layer or simple material ablation thinning the transport path across the layer. It will also be of interest to know if the SiC will react with the nitrogen component of air once the oxygen has been depleted to form silicon nitride and cyanogens, etc.	Rationale: there is some data in the literature on the air oxidation of SiC. Most of these data are for higher oxygen potentials than are likely to exist at the layer within the fuel particle. The database does not include information on highly irradiated material. A further complication is that SiC produced in a dynamic fashion such as is done in the manufacture of the coated particle fuels may still exhibit polytyism and not be in the stable crystallographic state for which measurements of reaction kinetics done in other technical disciplines have been directed. Especially at temperatures in excess of about 1800 K, and at higher oxygen potentials, product SiO2 will be liquid and will occlude the surface so that oxidation rates are controlled by transport across the viscous layer.	Closure Criterion:

Additional Discussion

Life Cycle Phase	Factor, Characteristic or Phenomenon	Definition
Accident With Subsequent Air Intrusion	SiC Layer: Chemical attack by air Catalysis	Modification of the reaction rate by fission products or impurities

Importance Rank and Rationale	Knowledge Level and Rationale	Remedy for Inadequate Knowledge/Issue Closure Criteria
Rank: L	Level: 2	Remedy No remedy needed:
Rationale: I am not aware of data indicating that the oxidation of SiC is catalyzed. There are some indications that impurities, notably iron, can accentuate the rates of attack and lead to attack along the grain boundaries, but this is really not catalysis.	Rationale: I am not aware of a data base that would suggest catalysis	Closure Criterion:
	The situation at higher temperatures is much the same as above and catalysis becomes less important at higher temperatures where reaction rates can be sufficiently fast that mass transport of oxidant will control the rate of reaction	

Additional Discussion

Life Cycle Phase	Factor, Characteristic or Phenomenon	Definition
Accident With Subsequent Air Intrusion	SiC Layer: Chemical attack by air	Changes in chemical form resulting from oxidizing or reducing fission products
	Changes in chemical form of fission products	

Importance Rank and Rationale	Knowledge Level and Rationale	Remedy for Inadequate Knowledge/Issue Closure Criteria
Rank: H	Level: 6	Remedy:It will be essential in the analysis of fission product transport to track the speciation of the fission products as changes in ambient temperature, pressure and chemical potentials occur including the ambient potentials of oxygen
Rationale:An elevated oxygen potential can lead to changes in the chemical forms of the fission products making some more volatile and some less volatile. There is a reasonable understanding of this. Less certain is whether nitrogen from air can react with the fission products or carbon to produce species such as cyanides that have higher vapor pressures than would otherwise be expected. Vapor phase nitrides are now getting substantial attention in the molecular vapor literature. Solid thermochemical databases have not been developed for these species though it is known that some fission products can form stable vapor phase nitrides.	Rationale: There is a reasonable data base to calculate the speciation of fission products as a function of the oxygen potential. The issue may focus on the local oxygen potential and not the core wide average oxygen potential which will be dictated by the equilibrium: $2\ CO = CO_2 + C$ There has not been a systematic survey of the effects of species like cyanogens and the formation of pseudohalides of the fission product elements to produce elevated vapor pressures	Closure Criterion:

Additional Discussion

Life Cycle Phase	Factor, Characteristic or Phenomenon	Definition
Accident With Subsequent Air Intrusion	SiC Layer: Chemical attack by air Changes in SiC properties	Changes in diffusivity, porosity, adsorptivity, etc.

Importance Rank and Rationale	Knowledge Level and Rationale	Remedy for Inadequate Knowledge/Issue Closure Criteria
Rank: M	Level: 2	Remedy A more far ranging data base on the oxidation of SiC and its effects on bulk material permeability would help resolve whether this is an issue of concern or not.:
Rationale:The clear concern is that oxidation of SiC opens pathways for gas phase mass transport because the attack is preferentially at pores, and void networks. I am not aware of data that shows this to be the case, but it is certainly possible for this to happen since the material at the boundaries of porosity in the SiC will be more energetic and reactive than material in the bulk. Also, because reactions with SiC are essentially slow there may be some preferential attack. Its significance depends both on the nature of SiC oxidation and the availability of oxidant to reach the SiC	Rationale: No data base for oxidation of the particular material in the coated particle fuels which will certainly be badly defected by irradiation and may exhibit some polytypism that makes it different than bulk annealed materials	Closure Criterion:

Additional Discussion

Life Cycle Phase	Factor, Characteristic or Phenomenon	Definition
Accident With Subsequent Air Intrusion	SiC Layer: Chemical attack by air	Release of SiC FP inventory
	Holdup reversal	

Importance Rank and Rationale	Knowledge Level and Rationale	Remedy for Inadequate Knowledge/Issue Closure Criteria
Rank: L	Level: 1	Remedy no remedy needed:
Rationale: Chemical reaction of oxidant with energetic sites that have adsorbed fission products will destroy the site and release any retained, volatile fission product. It is not clear that adsorption will retain a sufficient fraction of the radionuclide inventory to make this oxidative release of risk significance.	Rationale There appear to be only anecdotal accounts of fission product retention on the dislocations introduced by irradiation and no quantitative data on the adsorption isotherms	Closure Criterion:
	The issue becomes of less interest at elevated temperatures both because energetic sites anneal thermally and because the vapor pressures of important fission products become so high that there is no significant retention even on energetic sites	

Additional Discussion

Life Cycle Phase	Factor, Characteristic or Phenomenon	Definition
Accident With Subsequent Air Intrusion	SiC Layer: Chemical attack by air Temperature distribution	Impact of SiC oxidation on temperature distribution through material

Importance Rank and Rationale	Knowledge Level and Rationale	Remedy for Inadequate Knowledge/Issue Closure Criteria
Rank: H	Level: 6	Remedy: Fission product transport analyses will require a detailed prediction of the temperature distributions throughout the coated particle fuel.
Rationale: The oxidation of SiC is not iso-enthalpic so we know that the temperature distribution will be changed by chemical reaction. As noted elsewhere temperature distributions can affect both the volatility and the transport of fission products across a layer	Rationale: It should be possible to calculate the effect of oxidation on the temperature distributions across the layer since the heats of reaction are known for the bulk material and may be estimated when the involve the destruction of a radiation induced defect in the SiC lattice. It is necessary to have detailed knowledge of the reaction kinetics to do this calculation	Closure Criterion:

<u>Additional Discussion</u>

Life Cycle Phase	Factor, Characteristic or Phenomenon	Definition
Accident With Subsequent Air Intrusion	Inner PyC Layer Gas Phase Diffusion	Diffusion of gaseous fission products through layer (Knudsen and bulk diffusion through pore structure, and pressure driven permeation through structure)

Importance Rank and Rationale	Knowledge Level and Rationale	Remedy for Inadequate Knowledge/Issue Closure Criteria
Rank: H	Level: 6	Remedy: Any model of fission product transport within the fuel particle will have to include a gas phase mass transport model recognizing bulk gaseous diffusion, pressure driven flow and Knudsen diffusion
Rationale: Gas phase mass transport is the fastest mechanism to move fission products release from the fuel kernel across the barrier posed by the inner PyC layer	Rationale: Given the geometry and nature of the pore and crack network through the layer it should be possible to calculate the gas phase mass transport across the layer. We can estimate the gas phase diffusion coefficients for most of the dominant gaseous species. The diffusion process itself probably cannot be modeled as strictly Fickian diffusion. One will have develop a multicomponent diffusionmodel much like the membrane modesl that have been developed in the chemical engineering literature. It may be necessary to include in these models the effects of thermal diffusion especially since we will have low molecular weight species (CO MW=28) migrating along the same paths as the high molecular weight (>100) fission product vapor species. The importance of this will depend on the magnitude of the thermal gradients across the layer which surely must be significant given the relatively high conductivity and the need to move the decay heat away from the fuel kernel.	Closure Criterion:

Additional Discussion

Life Cycle Phase	Factor, Characteristic or Phenomenon	Definition
Accident With Subsequent Air Intrusion	Inner PyC Layer Condensed phase diffusion)	Inter-grannular and/or intra-grannular solid-state diffusion

Importance Rank and Rationale	Knowledge Level and Rationale	Remedy for Inadequate Knowledge/Issue Closure Criteria
Rank: M	Level: 2	Remedy: Any model of fission product transport across the inner PyC layer will have to include the condensed phase mass transport process to account for mass transport of fission products when the layer does not have pore and crack networks to facilitate gas phase mass transport across the layer
Rationale: Fission products that are not volatile will be transported across the inner PyC layer by the condensed phase diffusion processes. Bulk diffusion is the slowest of these at low temperatures but it has the highest activation energy so it does eventually become the dominant process. Even if the metals have only small vapor pressures, gas phase mass transport of fission products may still be the dominant mechanism for mass transport	Rationale We do not have surface and grain boundary diffusion coefficients to model the mass transport of fission products across the layer at lower temperatures. These cannot be estimated or transferred from studies of analogous materials since they are notoriously sensitive to the precise grain structure and the nature of impurities at the grain boundaries. We don't even have a data set of bulk diffusion coefficients for the PyC layer of demonstrated reliability. The most complicated part of the modeling will be a realistic portrayal of the layer geometry and the pore and crack networks. It is tempting to model the layer as a spherical shell, but this Continued next column	Closure Criterion: (continued from previous column) is only justified if the deviations from spherical are not sufficient to provide a short circuit pathway in some regions. Similarly, it will be tempting to treat the layer as uniform in thickness though it never will really be. We do not have meaningful data on the pore and crack network. These networks may change if there is reaction with the intruding gases. We may not be able to derive useful descriptions of the pore and crack networks through the layer from microscopic examinations of these networks. Cracks and channels to small to be readily identified in microscopic analyses can be effective in the transport of material across the layer.
	At sufficiently high temperatures bulk diffusion will be the dominant condensed phase mass transport process This process is very sensitive to the presence of defects produced by irradiation acting as traps for diffusing species and we don't seem to have data on this.	

Additional Discussion

Life Cycle Phase	Factor, Characteristic or Phenomenon	Definition
Accident With Subsequent Air Intrusion	Inner PyC Layer Pressure loading (Fission products)	Stress loading of the layer by fission products by increased pressure

Importance Rank and Rationale	Knowledge Level and Rationale	Remedy for Inadequate Knowledge/Issue Closure Criteria
Rank: L	Level: 2	Remedy to evaluate the pressure drop one would have to have some estimate of the permeability of the layer:
Rationale: Pressure loading will more likely be by CO pressure produced by the reaction of carbon with the fuel kernel. The loading will probably be on the SiC layer rather than the inner PyC layer though it is possible that there will be some pressure drop across the layer	Rationale: We need permeability data that seem not to exist to estimate the pressure drop across the layer. If this is significant then the layer can act at least temporarily as a barrier to fission product transport. But, if the pressure drop is significant then the layer is likely to rupture and completely lose its effectiveness as a barrier as the accident progresses and additional pressurization from both CO build up and fission product release occurs	Closure Criterion:

Additional Discussion

Life Cycle Phase	Factor, Characteristic or Phenomenon	Definition
Accident With Subsequent Air Intrusion	Inner PyC Layer Pressure loading (Carbon monoxide)	Stress loading of the layer by carbon monoxide by increased pressure

Importance Rank and Rationale	Knowledge Level and Rationale	Remedy for Inadequate Knowledge/Issue Closure Criteria
Rank: L	Level: 2	Remedy:no remedy needed
Rationale:The loading by CO should dominate that by fission products. Still it is not evident that the layer will have a substantial pressure retaining capability and the SiC layer is a more important layer for this.	Rationale: We need permeability data that seem not to exist to estimate the pressure drop across the layer. If this is significant then the layer can act at least temporarily as a barrier to fission product transport. But, if the pressure drop is significant then the layer is likely to rupture and completely lose its effectiveness as a barrier as the accident progresses and additional pressurization from both CO build up and fission product release occurs)	Closure Criterion:

Additional Discussion

Life Cycle Phase	Factor, Characteristic or Phenomenon	Definition
Accident With Subsequent Air Intrusion	Inner PyC Layer Layer oxidation	Reaction of pyrolytic graphite with oxygen released from the kernel

Importance Rank and Rationale	Knowledge Level and Rationale	Remedy for Inadequate Knowledge/Issue Closure Criteria
Rank: H	Level: 2	Remedy:Analysis of fission product transport will have to treat the effects of oxidants and ascertain if oxidants can reach the inner PyC layer. If so, the possibility of preferential and even catalyzed oxidation of the layer will have to be considered. Decent data sets on the reactions of the specific materials with oxidants are really needed.
Rationale: This high importance is assigned under the presumption that oxidant can reach the layer. The oxidant that comes is more likely to be from the fuel kernel than from the gases intruding in the accident scenario. Intruding gases will have to pass over an awful lot of reactive material before they can reach the inner PyC layer. On the other hand oxidant from the fuel will have to pass through a buffer layer of carbon to reach the inner PyC layer. If the oxidant reaches the material it can cause thinning of the layer (probably not especially important) or opening of the pathways for gas phase mass transport of fission products making the transport by gas phase processes even more rapid.	Rationale: The layer really does not take up oxidant. It reacts to form CO (and other equivalent species such as C2O and C2O3) that vaporize. The reactions are enormously sensitive to catalysis and fission products can act as catalysts. We don't have a lot of data on which fission products will produce catalysis, We do know that Cs can catalyze the oxidation of C. We also know that irradiation makes the material more reactive. More than just rate of reaction data for the specific material, we need to know if the reaction takes place uniformly over the surface or if there is preferential reaction especially to open pathways for the gas phase transport of fission products across the layer	Closure Criterion:
	same as above though catalysis is not an issue at very high temperatures where the oxidation reaction are rapid	

Additional Discussion

Life Cycle Phase	Factor, Characteristic or Phenomenon	Definition
Accident With Subsequent Air Intrusion	Inner PyC Layer Stress state (compression/tension)	The state of the forces induced by external forces that are acting across the layer to resist movement

Importance Rank and Rationale	Knowledge Level and Rationale	Remedy for Inadequate Knowledge/Issue Closure Criteria
Rank: L	Level: 2	Remedy: Models or data to predict rupture of the layer are needed. These models may be nothing more than criteria identifying conditions for which layer integrity can no longer be assured.
Rationale: It is known that stress state can affect both condensed phase and gas phase diffusion across a layer, but this is a pretty subtle effect. More important is whether the layer stays in tact or is ruptured and allows essentially unimpeded gas phase mass transport across the layer, but this is treated in other questions	Rationale:We don't really know much about the forces and especially forces induced by the radiation caused growth of materials	Closure Criterion:

Additional Discussion

Life Cycle Phase	Factor, Characteristic or Phenomenon	Definition
Accident With Subsequent Air Intrusion	Inner PyC Layer Cracking	Lengths, widths and numbers of cracks produced in layer during accident

Importance Rank and Rationale	Knowledge Level and Rationale	Remedy for Inadequate Knowledge/Issue Closure Criteria
Rank: H	Level: 1	Remedy: Any model of the fission product transport across the inner PyC layer will have to admit to the possibility of cracks – perhaps quite narrow cracks – developing in the layer from radiation-induced growth or thermal expansion or mechanical forces on the layer including pressurization examined above.
Rationale:Any cracking of the layer will create effective pathways for gas phase mass transport across the layer	Rationale: We are not really in the position to predict cracking of the layer. Though there are data in abundance for PyC they are not for the specific material in the fuel particle and not for the material subjected to thermal transients and irradiation of the type that will be seen by the PyC layer	Closure Criterion:

Additional Discussion

Life Cycle Phase	Factor, Characteristic or Phenomenon	Definition
Accident With Subsequent Air Intrusion	Inner PyC Layer Intercalation	Trapping of species between sheets of the graphite structure

Importance Rank and Rationale	Knowledge Level and Rationale	Remedy for Inadequate Knowledge/Issue Closure Criteria
Rank: M	Level: 2	Remedy:WE need some sort of data or analyses to show whether intercalation will be an effective holdup mechanism for fission product release.
Rationale: Intercalation could act as a holdup mechanism for fission products. Intercalation usually occurs during the simultaneous condensation of vapors and graphitic material. Intercalation could occur because of the radiation displacements of materials. Intercalation is known to be an effective way to trap potassium in graphite and so it might be effective in trapping Cs in the graphite. Still, it is not evident that so much of the radionulcide inventory can be trapped in the layer that this is risk-significant issue	Rationale: I have no data on intercalation as a dynamic process either during an accident or during fuel operations	Closure Criterion:
	Intercalation will reverse at very high temperatures and not be an issue	

Additional Discussion

Life Cycle Phase	Factor, Characteristic or Phenomenon	Definition
Accident With Subsequent Air Intrusion	Inner PyC Layer: Chemical attack by air Kinetics	Rate of reaction per unit surface area as a function of temperature and partial pressure of air

Importance Rank and Rationale	Knowledge Level and Rationale	Remedy for Inadequate Knowledge/Issue Closure Criteria
Rank: H	Level: 5	Remedy: kinetic data on both the reactions of oxygen and the reactions of nitrogen with the specific material of the inner PyC layer will be needed. As important as the spedific reaction kinetics – which may be just mass transport limitations for this particular case – will be information on the nature of the attack and in particular whether the attack is uniform or is localized so that it enhances the pathways available for gas phase mass transport through the layer.
Rationale: A rating of « high » is given to this issue under the assumption that it is conditional upon oxidant actually getting to the Inner PyC layer after having passed over and through a lot of reactive material. Though it is possible for the oxidant to do this, it may not be especially likely. IF, indeed, oxidant reaches the PyC surface it can react exothermically – thereby increasing the driving force for fission product vaporization – reactions will remove layer material and facilitate transport of fission products across the layer – and it will affect the volatility of the fission products – accentuating the vapor pressures of some fission products and reducing the vapor pressures of others.	Rationale: There is quite a lot of information about the interactions of air with carbon analogous to the carbon that makes up the inner PyC layer though none, apparently, for the specific material. At low temperatures the attack on carbon can be localized rather than uniform. The reactions can be catalyzed. There is much less information of the reactions of nitrogen from air that has been depleted of its oxygen by reactions prior to reaching the inner PyC layer. Certainly, one can hypothesize the reactions of nitrogen to form cyanogens and this would certainly affect temperatures in the particle, remove material from the layer and affect the volatility of radionuclides through the formation of vapor phase cyanides which could be viewed as pseudo halides Continued next column	Closure Criterion: (continued from previous column) The situation at higher temperatures is much the same as above though the potential for reaction of the layer with nitrogen increases. Also, at higher temperatures the reactions should become more homogeneous so that they work primarily to thinning the layer rather than to enhancing the facility of gas phase mass transport across the layer.

Additional Discussion

Life Cycle Phase	Factor, Characteristic or Phenomenon	Definition
Accident With Subsequent Air Intrusion	Inner PyC Layer: Chemical attack by air Catalysis	Modification of the reaction rate by fission products or impurities

Importance Rank and Rationale	Knowledge Level and Rationale	Remedy for Inadequate Knowledge/Issue Closure Criteria
Rank: H	Level: 3	Remedy: Models of graphit oxidation will have to account for catalysis and a more comprehensive base of data on catalytic agents will have to become available
Rationale: there is information suggesting that the rates of reaction of oxidant with graphite can be catalyzed and this catalysis can lead to preferential attack on the layer – perhaps enhancing gas phase mass transport across the layer	Rationale: It is known that some materials such as Cs and Fe will catalyze the oxidation of carbon. The effects of these catalytic materials or the catalytic effectiveness of other fission products on the reactions of the specific material are not reported in literature that I have seen.	Closure Criterion:
	Catalysis is less of an issue at higher temperatures where the reactions rates are inherently more rapid – eventually becoming limited only by the availability of oxidant. It is not that we know more about catalytic reactions at high temperature, it is that we need to know less that leads to relative scoring of the two temperature regimes.	

Additional Discussion

Life Cycle Phase	Factor, Characteristic or Phenomenon	Definition
Accident With Subsequent Air Intrusion	Inner PyC Layer: Chemical attack by air	Changes in chemical form resulting from oxidizing or reducing fission products
	Changes in chemical form of fission products	

Importance Rank and Rationale	Knowledge Level and Rationale	Remedy for Inadequate Knowledge/Issue Closure Criteria
Rank: H	Level: 5	Remedy:The data bases used to calculate fission product speciation need to be reliable or at least known. Codification of the data base to be used for NRC would be beneficial. There also needs to be an examination of the literature and even molecular calculations concerning the likely importance of vapor phase nitrides and cyanides.
Rationale: It is well established that the ambient oxygen potential can strongly affect the volatility of many fission products – enhancing the vapor pressures of some such as Ru, Mo and Te, and depressing the vapor pressure of others such as Ba, Sr, Ce, and La. Of additional interest for this particular location is the enhancement of the vapor pressures of fission products caused by an ambient partial pressure of nitrogen or the products of nitrogen reactions with carbon.	Rationale: We have the technical capability to assess the effects of oxygen potential on the vapor pressures of fission products as long as we confine or interest to oxides and elemental forms of the fission products. We don t have much of a data base to assess the effect of nitride formation and the formation of pseudo halides like cyanides on the vapor pressures of fission products. Modern methods of molecular orbital calculations have advanced to the point that it ought to be possible to explore computationally for stable species of these types that have not been systematically investigated experimentally	Closure Criterion:

Additional Discussion

Life Cycle Phase	Factor, Characteristic or Phenomenon	Definition
Accident With Subsequent Air Intrusion	Inner PyC Layer: Chemical attack by air Changes in graphite properties	Changes in diffusivity, porosity, adsorptivity, etc.

Importance Rank and Rationale	Knowledge Level and Rationale	Remedy for Inadequate Knowledge/Issue Closure Criteria
Rank: H	Level: 1	Remedy:Models of PyC layer oxidation will have to recognize the possibility of localized attack that increases the porosity or permeability of the material. Mechanistic models or even bounding models of mass transport across the inner PyC layer will have to recognize that the porosity and permeability of the material is time dependent when there is oxidation taking place.
Rationale: Again given that oxidant can reach the inner PyC layer this is a high importance issue especially at low temperatures. Oxidant does not attack carbon homogenously. There is preferential attack at energetic sites and the concentrations of energetic sites are points where catalysts reside and in cracks and pores. Attack on surfaces in cracks and pores will enhance vapor phase mass transport of fission products across the layer.	Rationale: There appears to be little information on the localized attack on PyC by oxidants and its effects on the effective permeability of the material to gases	Closure Criterion:
	Localized attack becomes less important at elevated temperatures where reactions become faster.	

Additional Discussion

Life Cycle Phase	Factor, Characteristic or Phenomenon	Definition
Accident With Subsequent Air Intrusion	Inner PyC Layer: Chemical attack by air	Release of graphite FP inventory
	Holdup reversal	

Importance Rank and Rationale	Knowledge Level and Rationale	Remedy for Inadequate Knowledge/Issue Closure Criteria
Rank: L	Level: 2	Remedy: no remedy needed
Rationale: It is known that fission products can adsorb on energetic sites in graphite. It is also known that chemical reactions with these sites can release the adsorbed material. What is not evident is whether the adsorption of fission products on energetic sites in the inner PyC layer can involve sufficient amounts of fission products to be risk significant.	Rationale: We don't have information for quantifying the holdup of fission products on the energetic sites created by irradiation or by cracking in the inner PyC layer. What holdup does occur will be reversed at the rate of oxidation reaction.	Closure Criterion:
	Holdup by adsorption is much less important at high temperatures because the vapor pressures of the interesting fission products are so high.	

Additional Discussion

Life Cycle Phase	Factor, Characteristic or Phenomenon	Definition
Accident With Subsequent Air Intrusion	Inner PyC Layer: Chemical attack by air Temperature distribution	Impact of graphite oxidation on temperature distribution through material

Importance Rank and Rationale	Knowledge Level and Rationale	Remedy for Inadequate Knowledge/Issue Closure Criteria
Rank: H	Level: 3	RemedyAny fission product ttransport model will require goo, local temperature descriptions including the effects of chemical reactions on these temperatures
Rationale: If oxidant can get to the inner PyC layer, its reactions will be exothermic and will affect temperature distributions. As noted above these temperature distributions affect both the volatilities of the fission products and their transport across the layer	Rationale: We know enough in principle to calculate the effects of chemical reactions on the temperature distributions if we know the kinetics of reaction. Certainly we know the heats of reaction with pristine material and these heats need to modified to account for the additional energy coming from the reaction of defects introduced by irradiation. A key to the calculation of temperature distributions is the thermal conductivity of the porous, defected and possibly cracked material.	Closure Criterion:
	The situation at higher temperatures is much the same as above except radiation heat transfer becomes more of an issue and the ambient atmosphere of CO will participate in the radiation heat transfer.	

Additional Discussion

Life Cycle Phase	Factor, Characteristic or Phenomenon	Definition
Accident With Subsequent Air Intrusion	Buffer Layer Gas phase diffusion	Diffusion of gaseous fission products through layer (Knudsen and bulk diffusion through pore structure, and pressure driven permeation through structure)

Importance Rank and Rationale	Knowledge Level and Rationale	Remedy for Inadequate Knowledge/Issue Closure Criteria
Rank: H	Level: 4	Remedy a fairly sophisticated model of the layer porosity will be needed as will a very sophisticated model of mass transport across the layer:
Rationale: Gas phase mass transport across this layer will be the dominant transport mechanism for volatile fission products because the temperatures are high and because the material is quite porous.	Rationale Given the nature of the porosity in the layer it should be possible to calculate the gas phase mass transport quite well. We can estimate the diffusion coefficients for most vapor species. The analysis probably cannot treat the diffusion as Fickian. A multicomponent model will have to be considered because there will be a flow of CO across the layer that may be, in fact, pressure driven rather than diffusion. Diffusion may have to be augmented by consideration of thermal diffusion because of the large temperature gradient and the mixture of molecular weights of the gaseous species. Other complexities in the analysis include lack of spherical symmetry of the layer and the variations in the layer thickness	Closure Criterion:

Additional Discussion

Life Cycle Phase	Factor, Characteristic or Phenomenon	Definition
Accident With Subsequent Air Intrusion	Buffer Layer Condensed phase diffusion	Inter-grannular diffusion and/or intra-grannular solid-state diffusion

Importance Rank and Rationale	Knowledge Level and Rationale	Remedy for Inadequate Knowledge/Issue Closure Criteria
Rank: L	Level: 1	Remedy:no remedy needed
Rationale: Fission products that reach the interface between the buffer carbon and the fuel kernel will have all escaped the kernel as some sort of a vapor species through the interconnected pore network in the urania. (The flux of fission products from the fuel via intragrannular diffusion is really quite small at temperatures that are well below the urania melting point) It does not seem likely that significant transport of even species with very modest vapor pressures would switch to a condensed phase process upon encountering the highly porous buffer region.	Rationale: Don't have definitive condensed phase diffusion coefficients for the material Condensed phase mass transport rather than vapor phase mass transport is even less likely to be dominant at higher temperatures and the condensed phase diffusion coefficients are even less known at elevated temperatures	Closure Criterion:

Additional Discussion

Life Cycle Phase	Factor, Characteristic or Phenomenon	Definition
Accident With Subsequent Air Intrusion	Buffer Layer Response to kernel swelling	Mechanical reaction of the layer to the growth of the kernel via swelling

Importance Rank and Rationale	Knowledge Level and Rationale	Remedy for Inadequate Knowledge/Issue Closure Criteria
Rank: M	Level: 4	Remedy:Because integrity of the layer is not critical, it may not be necessary to develop a very detailed understanding of the mechanical properties of the buffer layer. It may not even be present in future incarnations of coated particle fuel pellets
Rationale: cracking and otherwise opening pathways for gas phase mass transport as a result of mechanical interactions could facilitate fission product transport across the buffer region, but the region is already quite porous so the incremental effects of cracking on gas phase mass transport are not likely to be as dramatic as cracking of the more compact structural barriers in the coated particle fuel.	RationaleWe have been shown some evidence that in the current inadequate fuels mechanical interactions can rupture the buffer layer. We have not been shown any indication that this process can be predicted in a quantitative way. There are data on the mechanical properties of materials analogous to materials in the buffer region, but these data may not be applicable to the thin layer that can bond to either the kernel or to the bounding PyC layer	Closure Criterion:

Additional Discussion

Life Cycle Phase	Factor, Characteristic or Phenomenon	Definition
Accident With Subsequent Air Intrusion	Buffer Layer Maximum fuel gaseous fission product uptake	Maximum loading of fission products that can deposit from the gas phase onto surfaces of materials surrounding the fuel kernel

Importance Rank and Rationale	Knowledge Level and Rationale	Remedy for Inadequate Knowledge/Issue Closure Criteria
Rank: L	Level: 3	Remedy no remedy needed:
Rationale: It is likely that some fission products will deposit in the buffer region at least temporarily and this effect has to be considered in developing the modeling of the fission product transport. But it does not appear likely that the fraction of the released fission product inventory that can deposit in this region will be sufficiently large to be of risk significance	Rationale We know deposition can take place. We don't have quantitative information on the density of active sites for deposition or adsorption desorption isotherms for the fission products	Closure Criterion:
	Adsorption on active sites become even less important at elevated temperatures first because the vapor pressures at such elevated temperatures are so high and second because at elevated temperatures active adsorption sites are being thermally annealed. So it is not that we know more about the situation at high temperatures, it is that relatively we need to know less.	

Additional Discussion

Life Cycle Phase	Factor, Characteristic or Phenomenon	Definition
Accident With Subsequent Air Intrusion	Buffer Layer Layer oxidation	Reaction of pyrolytic graphite with oxygen released from the kernel

Importance Rank and Rationale	Knowledge Level and Rationale	Remedy for Inadequate Knowledge/Issue Closure Criteria
Rank: H	Level: 2	Remedy Easily one of the most important characteristics to understand for coated particle fuels is the reaction of carbon with the urania fuel. This may well be a heterogeneous reaction of gas phase oxidant with carbon. It may also involve a homogeneous direct reaction of two solid materials especially under conditions of irradiation. The reaction will be dependent on the ambient CO pressure. In fact leakage of the CO from the coated particle fuel may well dictate the extent of reaction
Rationale: The 'uptake' is really the reaction of oxygen from the fuel reacting with carbon in the buffer layer to form CO that pressurizes and possibly ruptures the compact barriers with the fuel particle such as the PyC layer and the SiC layer. Rupture of these layers will allow the venting of the vapor phase fission products within the particle and provide a facile pathway for the gas phase mass transport of fission products out of the fuel particle as the accident progresses. The reaction could also damage the crystal structure of urania at the surface of the kernel – converting it into UCO and eventually UCx. The crystallographic changes are sufficiently large that fission products within grains of the surface fuel will be expelled and ready to vaporize without mass transport limitations that affect release of fission products from grain surfaces within the fuel kernel.	Rationale Reactions of carbon with urania are thermodynamically possible at sufficiently low CO partial pressures even at low temperatures. They do appear to be slow. Irradiation of the carbon may create energetic sites that are more reactive than might be expected based on tests with unirradiated materials. Still the empirical evidence is that the reactions are slow in absence of some sort of catalyst. Always a concern is that the fission product species may act as catalysts under circumstances not so far encountered in the studies of coated particle fuels	Closure Criterion:
	Reactions of carbon with urania definitely occur at more elevated temperatures. I am not aware of definitive rate data for the reactions	

Life Cycle Phase	Factor, Characteristic or Phenomenon	Definition
Accident With Subsequent Air Intrusion	Buffer Layer Thermal gradient	Change in temperature with distance

Importance Rank and Rationale	Knowledge Level and Rationale	Remedy for Inadequate Knowledge/Issue Closure Criteria
Rank: H	Level: 4	Remedy: Modeling of fission product transport in the coated particle fuels will require that there be a detailed model of the local temperatures and temperature gradients. To do this for the buffer layer will first require that the porosity of the layer be characterized and then some heat transfer modeling be done to develop expressions for the thermal conductivity of the material.
Rationale: Thermal gradients across the buffer layer – which could be substantial in magnitude – will affect the fission product release both by chemical diffusion of vapors and by thermal diffusion of vapors	Rationale: In principle we can calculate the mass transport across the layers given the temperature distributions. Calculations of the thermal distributions are made complicated by the poor knowledge of the material thermal conductivity and the effects of radiation defects and pores or cracks on the thermal conductivity. It is unlikely that simple corrections of material thermal conductivity using things like the Loeb correction will be adequate since the layer is so thin the bulk averaging inherent in the Loeb correction and similar corrections simply will underestimate the effects of porosity. Something much more sophisticated will have to be done.	Closure Criterion:
	The situation is largely the same at elevated temperatures except that radiation heat transfer within the layer becomes more of an issue. It is not simple to calculate because the ambient CO cannot be taken as transparent to the radiation.	

Additional Discussion

Life Cycle Phase	Factor, Characteristic or Phenomenon	Definition
Accident With Subsequent Air Intrusion	Buffer Layer Irradiation and thermal shrinkage of buffer	Dimension changes in the buffer layer or changes in its porosity produced by irradiation or by exposure to elevated temperatures

Importance Rank and Rationale	Knowledge Level and Rationale	Remedy for Inadequate Knowledge/Issue Closure Criteria
Rank: L	Level: 5	Remedy: The only real issue that must be borne in mind is whether the dimensional changes are sufficient to cause rupture and then this is of concern only if holdup of fission products in the buffer layer is actually credited in the transport process.
Rationale: The effects are small enough that they will probably be safely neglected in the modeling of fission product transport. Of course, if the changes open pathways for gas phase mass transport of fission products they facilitate this transport as discussed above.	Rationale: We know that the buffer layer material will grow as a result of radiation-induced defects in the material. Thermal expansion during accident transients will affect the material. While w e don't have data for the specific material, we do have data for analogous materials	Closure Criterion:

Additional Discussion

Life Cycle Phase	Factor, Characteristic or Phenomenon	Definition
Accident With Subsequent Air Intrusion	Buffer Layer: Chemical attack by air Kinetics	Rate of reaction per unit surface area as a function of temperature and partial pressure of air

Importance Rank and Rationale	Knowledge Level and Rationale	Remedy for Inadequate Knowledge/Issue Closure Criteria
Rank: L	Level: 2	Remedy: no remedy really needed.
Rationale: It really begins to stretch the imagination of how oxidant intruding from outside the core could penetrate to the buffer layer rather than react with other carbon materials along the pathway. Besides, if oxidant is this far it has reached the fuel kernel and the game is up. Oxidation of fuel will initiate massive release of fission products. It does not seem useful to give great attention to the oxidation of the buffer layer from external gases. The more important issue is reaction of the buffer with oxygen from the fuel kernel and this has been discussed above.	Rationale Detailed reaction kinetic data for the specific material are not available and probably are not really needed. If models are really needed it may be adequate to assume reaction proceeds at the rate of mass transport of oxidant to the buffer region which cannot be very fast even if the other parts of the fuel particle have been completely ruptured.	Closure Criterion:

Additional Discussion

Life Cycle Phase	Factor, Characteristic or Phenomenon	Definition
Accident With Subsequent Air Intrusion	Buffer Layer: Chemical attack by air Catalysis	Modification of the reaction rate by fission products or impurities

Importance Rank and Rationale	Knowledge Level and Rationale	Remedy for Inadequate Knowledge/Issue Closure Criteria
Rank: L	Level: 4	Remedy no remedy needed:
Rationale: See discussion above. The reactions just are not likely to be important for this layer	Rationale: reactions of carbon with oxidants are catalyzed and fission products can be catalysts. This may more important for oxidants coming from the fuel kernel rather than intruding oxidants like air and water vapor.	Closure Criterion:
	Catalysis is just less important at very high temperatures where the rates of reactions especially of gases are intrinsically high.	

Additional Discussion

Life Cycle Phase	Factor, Characteristic or Phenomenon	Definition
Accident With Subsequent Air Intrusion	Buffer Layer: Chemical attack by air	Changes in chemical form resulting from oxidizing or reducing fission products
	Changes in chemical form of fission products	

Importance Rank and Rationale	Knowledge Level and Rationale	Remedy for Inadequate Knowledge/Issue Closure Criteria
Rank: L	Level: 6	Remedy: no remedy needed
Rationale: oxidant intrusion to this depth in the coated particle fuel structure is hard to believe. If it does occur the higher oxidant partial pressures will affect the speciation and consequently the vapor pressures of the fission products – enhancing some and depressing others.	Rationale: As discussed above for other layers there is some technical basis for at least estimating the effects of oxidants on the speciation and consequently the vapor pressures of fission products	Closure Criterion:

Additional Discussion

Life Cycle Phase	Factor, Characteristic or Phenomenon	Definition
Accident With Subsequent Air Intrusion	Buffer Layer: Chemical attack by air	Changes in diffusivity, porosity, adsorptivity, etc.
	Changes in graphite properties	

Importance Rank and Rationale	Knowledge Level and Rationale	Remedy for Inadequate Knowledge/Issue Closure Criteria
Rank: L	Level: 3	Remedy: no remedy needed
Rationale: again, it just is not apparent that oxidant is likely to intrude to the buffer layers	Rationale: see discussions above for the effects of oxidants on pathways for gas phase mass transport. Even if oxidant gets to this point and does react preferentially in local areas, the incremental effect on the facility of gas phase mass transport across the layer is likely to be very much less than it is for localized reactions in other layers that are more compact and less porous.	Closure Criterion:

Additional Discussion

Life Cycle Phase	Factor, Characteristic or Phenomenon	Definition
Accident With Subsequent Air Intrusion	Buffer Layer: Chemical attack by air	Release of graphite FP inventory
	Holdup reversal	

Importance Rank and Rationale	Knowledge Level and Rationale	Remedy for Inadequate Knowledge/Issue Closure Criteria
Rank: L	Level: 2	Remedy: no remedy needed
Rationale: Again, we just don't believe for most accident sequences that oxidant will penetrate to the buffer layer and if it does little details like the release of holdup inventory in the layer will hardly matter.	Rationale: Don't know the concentrations of the active sites for adsorption nor do we know the adsorption/desorption isotherms for the material with the radiation induced sites. It is not apparent however that in any case the fractional holdup could be risk significant.	Closure Criterion:
	There is likely to be little to release since active sites will thermally anneal at elevated temperatures and vapor pressures are so high that adsorption on defects that remain may be small.	

Additional Discussion

Life Cycle Phase	Factor, Characteristic or Phenomenon	Definition
Accident With Subsequent Air Intrusion	Buffer Layer: Chemical attack by air	Impact of graphite oxidation on temperature distribution through material
	Temperature distribution	

Importance Rank and Rationale	Knowledge Level and Rationale	Remedy for Inadequate Knowledge/Issue Closure Criteria
Rank: M	Level: 4	Remedy: Any modeling of fission product transport in the coated particle fuel will require a detailed model of the temperature distributions in the layers including the buffer layer.
Rationale: As noted above, it is unlikely that oxidant will penetrate to the buffer layer itself and so chemical reactions of oxidant with this layer will not distort temperature distributions. But to some small extent the temperature distributions in the buffer layer will be affected by the chemical reactions of intruding oxidant with other layers. The effect is not likely to be large since the buffer layer thermal conductivity will not be huge.	Rationale: The pertinent knowledge bases are those discussed in connection with reactions of other layers and the modeling of thermal conductivity in the buffer layer.	Closure Criterion:

Additional Discussion

Life Cycle Phase	Factor, Characteristic or Phenomenon	Definition
Accident With Subsequent Air Intrusion	Kernel Maximum fuel temperature	Maximum fuel temperature attained by the fuel kernel during the accident

Importance Rank and Rationale	Knowledge Level and Rationale	Remedy for Inadequate Knowledge/Issue Closure Criteria
Rank: H	Level: 6	Remedy:
Rationale: Temperature is well known to be one of the dominant variables controlling the release of fission products form urania kernels	Rationale: In principle, it should be possible to calculate the maximum kernel temperature fairly accurately. Even so, errors on the order of 50 degrees are possible. Definitive, defensible calculations for credible accidents have not yet appeared.	Closure Criterion:

Additional Discussion

Life Cycle Phase	Factor, Characteristic or Phenomenon	Definition
Accident With Subsequent Air Intrusion	Kernel	The time-dependent variation of fuel temperature with time
	Temperature vs. time transient conditions	

Importance Rank and Rationale	Knowledge Level and Rationale	Remedy for Inadequate Knowledge/Issue Closure Criteria
Rank: H	Level: 4	Remedy:
Rationale: Fission product release is a strong function of both time and temperature	Rationale: Though fairly reliable temperature histories are in principle possible to predict defensible calculations have not yet been produced. Most existing calculations are hopelessly optimistic about heat loss pathways.	Closure Criterion:

Additional Discussion

Life Cycle Phase	Factor, Characteristic or Phenomenon	Definition
Accident With Subsequent Air Intrusion	Kernel Energy Transport: Conduction within kernel	Flow of heat within a medium from a region of high temperature to a region of low temperature

Importance Rank and Rationale	Knowledge Level and Rationale	Remedy for Inadequate Knowledge/Issue Closure Criteria
Rank: M	Level: 3	Remedy:
Rationale: Conduction as well as decay heat generation determine the temperature history of the kernel during the event	Rationale: Conduction in moderately porous urania is known with some accuracy. But, the porosity of the urania kernels can become heroic during extended operations and the events of the accident could easily produce porosities and configurations of the kernels that are quite intractable for conduction calculations.	Closure Criterion:

Additional Discussion

Life Cycle Phase	Factor, Characteristic or Phenomenon	Definition
Accident With Subsequent Air Intrusion	Kernel	Chemical and physical state of fission products
	Thermodynamic state of fission products	

Importance Rank and Rationale	Knowledge Level and Rationale	Remedy for Inadequate Knowledge/Issue Closure Criteria
Rank: H	Level: 5	Remedy:
Rationale: Fission product release depends on the chemical activity of the fission products. Completely diluted in the urania matrix, the fission product activities could be quite low. But, when the segregate into separate phases such as uranate phases or metallic nodules, chemical activities can be driven up substantially – orders of magnitude.	Rationale: We have a useful understanding of chemical activities of fission products in urania fuel at moderate burnups. At the higher burnups expected for some gas reactor fuels, our knowledge and predictive capabilities begin to fail us	Closure Criterion:

Additional Discussion

Life Cycle Phase	Factor, Characteristic or Phenomenon	Definition
Accident With Subsequent Air Intrusion	Kernel Oxygen flux	Mass transport of oxygen per unit surface area per unit time

Importance Rank and Rationale	Knowledge Level and Rationale	Remedy for Inadequate Knowledge/Issue Closure Criteria
Rank: M	Level: 3	Remedy:
Rationale: Diffusion of fission products will occur simultaneously with the diffusion of oxygen from the kernels to the reactive graphite at the buffer-kernel interface. The release is far more a multicomponent process than we have encountered in the case of fission product release from conventional fuels. The gettering of oxygen by reaction with the carbon is not passivating as is the case with gettering of oxygen by reaction with zirconium in the case of conventional fuels. It is not evident, then, that the usual Fickian diffusion approximation can be made incaustiously to predict release from the kernels	Rationale: Release analysis recognizing the multicomponent nature of the transport within fuel grains have not been published. In multicomponent systems remarkable things can be predicted that appear counter-intuitive when viewed within the context of binary diffusion.	Closure Criterion:

Additional Discussion

Life Cycle Phase	Factor, Characteristic or Phenomenon	Definition
Accident With Subsequent Air Intrusion	Kernel Grain growth	Enlargement of grains as a result of diffusion

Importance Rank and Rationale	Knowledge Level and Rationale	Remedy for Inadequate Knowledge/Issue Closure Criteria
Rank: L	Level: 8	Remedy:
Rationale: Grain growth is largely unimportant because of the grain boundary pinning effects of fission products and especially separated phases of fission products	Rationale: It has not been essential to consider grain growth in models of fission product release from conventional reactor fuels, though some codes include such models.	Closure Criterion:

Additional Discussion

Life Cycle Phase	Factor, Characteristic or Phenomenon	Definition
Accident With Subsequent Air Intrusion	Kernel Buffer carbon-kernel interaction	Chemical reaction between carbon and the fuel (UO2 or UOC) to form UC2 and CO (gas)

Importance Rank and Rationale	Knowledge Level and Rationale	Remedy for Inadequate Knowledge/Issue Closure Criteria
Rank: H	Level: 3	Remedy:
Rationale: The reaction of the buffer with the kernel can be responsible for the pressurization perhaps to failure of the SiC layer. The reaction can also lead to fission product release as the reactive refinement of the urania progresses	Rationale: Details of the reaction process and even the phase relations in these systems are not known well.	Closure Criterion:

Additional Discussion

Life Cycle Phase	Factor, Characteristic or Phenomenon	Definition
Accident With Subsequent Air Intrusion	Kernel: Chemical attack by air Kinetics	Rate of reaction per unit surface area as a function of temperature and partial pressure of air

Importance Rank and Rationale	Knowledge Level and Rationale	Remedy for Inadequate Knowledge/Issue Closure Criteria
Rank: L	Level: 9	Remedy:
Rationale: Air attack on the kernel would produce catastrophic release of fission products. But, if the fuel particle was so damaged that air could reach the kernel, there would have already have been catastrophic release of fission products	Rationale: We have a growing knowledge of fission product release from fuel exposed to air. We also know that carbon will react with air well before it is possible for the air to reach the kernel.	Closure Criterion:

Additional Discussion

Life Cycle Phase	Factor, Characteristic or Phenomenon	Definition
Accident With Subsequent Air Intrusion	Kernel: Chemical attack by air Catalysis	Modification of the reaction rate by fission products or impurities

Importance Rank and Rationale	Knowledge Level and Rationale	Remedy for Inadequate Knowledge/Issue Closure Criteria
Rank: L	Level: 1	Remedy:
Rationale: Air attack is unimportant and there is not a lot of evidence that air attack on urania is catalyzed	Rationale: Not aware of information on catalysis of air attack on urania at temperatures that would lead to extensive fission product release	Closure Criterion:

<u>Additional Discussion</u>

Life Cycle Phase	Factor, Characteristic or Phenomenon	Definition
Accident With Subsequent Air Intrusion	Kernel: Chemical attack by air Changes in chemical form of fission products	Changes in chemical form resulting from oxidizing or reducing fission products

Importance Rank and Rationale	Knowledge Level and Rationale	Remedy for Inadequate Knowledge/Issue Closure Criteria
Rank: L	Level: 5	Remedy:
Rationale: Should air reach the fuel, it can cause changes to the volatility of fission products by changes in the chemical forms of these fission products. It is just not obvious that air will reach the kernels and if air does reach the kernels, core damage may be so extensive there will be few fission products left that can react with the air.	Rationale We certainly know of possible changes to the chemical forms of fission products exposed to air.	Closure Criterion:

Additional Discussion

Life Cycle Phase	Factor, Characteristic or Phenomenon	Definition
Accident With Subsequent Air Intrusion	Kernel: Chemical attack by air Changes in kernel properties	Changes in diffusivity, porosity, adsorptivity, etc.

Importance Rank and Rationale	Knowledge Level and Rationale	Remedy for Inadequate Knowledge/Issue Closure Criteria
Rank: L	Level: 8	Remedy:
Rationale: The changes in the thermophysical properties of urania when it is exposed to air are quite significant. But, as noted above, such changes are not likely to be of importance either because air cannot get to the urania or because the fission products have already been released once the air arrives.	Rationale: Huge amounts of information about the changes to urania exposed to air exist.	Closure Criterion:

Additional Discussion