Workscope Descriptions

SEPARATIONS AND WASTE FORMS

(FEDERAL POC – JIM BRESEE & TECHNICAL POC – TERRY TODD)

Separations and Waste Forms (FC-1) – The separations and waste forms campaign develops the next generation of fuel cycle and waste management technologies that enable a sustainable fuel cycle, with minimal processing, waste generation, and potential for material diversion. Today's technology challenges include the economical recovery of transuranic elements for recycle/transmutation; and minimizing waste generation (including both high level and low level waste). Priority research efforts revolve around achieving near-zero radioactive off-gas emissions; developing a simplified, single-step recovery of transuranic elements; and significantly lessening the process wastes. Exploratory paths include developing fundamental understanding of separation processes and waste form thermodynamics; understanding the underlying separation driving forces; exploiting thermodynamic properties to effect separations; elucidating microstructural waste form corrosion mechanisms; and developing improved sampling and process monitoring technologies. The results of this R&D should contribute to development of a predictive capability for separation and waste form performance over a broad range of operational conditions and novel separations technologies. Key university research needs for this activity include:

- Experimental collection of fundamental data to characterize and quantify chemical processes of aqueous or electrochemical separation, validation of modeling approaches as well as to develop a better understanding of electrochemical separation methods;
- Develop a fundamental understanding of interfacial electrochemistry of actinides and fission product elements important in the fuel treatment process;
- Development of novel transformational separation technologies that have the potential of significantly reducing cost of processing fuel while reducing proliferation risk and waste generation;
- Development of alternative waste forms that have the potential of significantly increased waste loading (of fission products) and durability over borosilicate glass;
- Investigation of novel volatilization methods for complete or partial recycle of used fuel components. Approaches could include oxidation/reduction methods, reactive gas reagents, or any combination of approaches to segregate used fuel components for recycle or disposal.

ADVANCED FUELS

(FEDERAL POC – FRANK GOLDNER & TECHNICAL POC – KEMAL PASAMEHMETOGLU)

Advanced Fuels (FC-2) – The advanced fuels program conducts research and development of innovative next generation LWR and transmutation fuel systems. The major areas of research include, for example, enhancing the accident tolerance of fuels and materials, improving the fuel system's ability to achieve significantly higher fuel and plant performance, and developing innovations that provide for major increases in burn-up and performance. The advanced fuels program is interested in advanced nuclear fuel and materials technologies that are robust, have high performance capability and are more tolerant to accident conditions than traditional fuel systems. Research and development in the areas of fabrication, characterization, and performance of advanced fuel, materials, and target systems are within the scope of this program element. Key university research needs for this activity include:

• Advanced fabrication technology and research with potential for decreasing fabrication process

losses while increasing fuel quality and consistency;

- Fabrication process models, such as compaction and sintering models, fuel materials studies, and associated technology development that supports increased understanding of fuels performance;
- Supporting the development of predictive, physics-based fuels performance models at a microstructural level by developing and conducting separate effects tests to provide the required fundamental physical and chemical data;
- Development of in-pile instrumentation, novel characterization techniques and innovative out of pile testing that supports the goal of understanding the behavior of and predicting the performance of the nuclear fuel system at a microstructural level;
- Fuel related core materials tolerant to LWR beyond-design-basis events.

NUCLEAR MATERIALS SAFEGUARDING AND INSTRUMENTATION

(FEDERAL POC – DAN VEGA & TECHNICAL POC – MARK MULLEN)

Nuclear Materials Safeguarding and Instrumentation (FC-3) – This program element develops technologies and analysis tools to support next generation nuclear materials management and safeguards for future U.S. fuel cycles. This includes both extrinsic measures and safeguards over-laid on a nuclear energy system, as well as the intrinsic design features incorporated into system design. New technologies and approaches to in-facility accounting and safeguarding of nuclear materials will be pursued under this research area. This research topic will also pursue advanced measurement techniques that could complement the ongoing measurement program. In particular, fission multiplicity and fission neutron spectrum measurements as a function of incident neutron energy have been identified as important data in recent sensitivity analyses. Key university research needs for this activity include:

- New and improved detector systems and sensor materials that can be used to increase the accuracy, reliability, and efficiency of nuclear materials quantification and tracking from the perspective of the operator or state-level regulator. Such systems could include new neutron coincidence/anti-coincidence counting, spectroscopic analysis, chemical, calorimetric, or other non-nuclear methods, as well as any other novel methods with potential MC&A benefits;
- Methods for data integration and analysis, include cutting-edge work in multi-variant statistical techniques for process monitoring, risk assessment, plant-wide modeling & simulation directed at the accounting challenges of high-interest fuel cycle processes, including advanced separations processes;
- High-fidelity nuclear data measurements and associated technology that benefit MC&A effectiveness. Such proposals should include clear sensitivity analyses addressing the benefits of the evaluation of key nuclear parameters such as multiplicity, covariance data, and cross section refinement for isotopes of interest to the nuclear fuel cycle.

USED NUCLEAR FUEL DISPOSITION

(FEDERAL POC – SYED BOKHARI & TECHNICAL POC – PETER SWIFT)

Used Nuclear Fuel Disposition (FC-4) – The used fuel disposition technical area develops technologies for storing, transporting, and disposing of used nuclear fuel and assessing performance of the waste forms in the associated storage and disposal environments. Key university research needs for the storage and transportation portion of this activity include:

• Innovative approaches to evaluating degradation and aging phenomena of fuel, cladding,

containers, and storage facilities including vertical over packs, horizontal bunkers and pads, relevant to extended interim storage;

- Development of superior concrete that could be used for extended storage;
- Materials research that would facilitate transportation of used nuclear fuel;
- Advanced modeling approaches for radiological consequence analyses of disruptive scenarios relevant to storage transportation;
- Data relevant to risk-informed cask qualification and the storage and transportation behavior of high-burnup and advanced fuels;
- Development of techniques to monitor and managing the aging of dry storage systems.

Assessments of waste form and disposal options start with the degradation of waste forms and consequent mobilization of radionuclides, reactive transport through the near field environment (waste package and engineered barriers), and transport into and through the geosphere. Research needs support the development of modeling tools or data relevant to permanent disposal of used nuclear fuel and high-level radioactive waste in a variety of generic disposal concepts, including mined repositories in clay/shale, salt, and crystalline rock, and deep boreholes in crystalline rocks.

Key university research needs for the disposal portion of this activity include:

- Improved understanding of the degradation processes (i.e., corrosion and leaching) for used nuclear fuel and waste forms that could be generated in advanced nuclear fuel cycles (i.e., glass, ceramic, metallic) in aqueous environments leading to the development of improved models to represent these degradation processes;
- Improved understanding of the degradation processes for engineered barrier materials (i.e., waste containers/packages, buffers, seals) and radionuclide transport processes through these materials leading to the development of improved models to represent these processes;
- Improved understanding of coupled thermal-mechanical-hydrologic-chemical processes in the near-field of relevant disposal model environments, leading to the development of improved models to represent these processes;
- Improved understanding of hydrologic and radionuclide transport processes in the geosphere of relevant disposal model environments, leading to the development of improved models to represent these processes;
- Systematic experiments under controlled conditions to obtain data regarding material properties, degradation processes, and radionuclide transport processes;
- Development of methods to upscale atomistic descriptions into continuum-scale models of barrier degradation and radionuclide transport processes;
- Aqueous speciation and surface sorption at temperatures and geochemical conditions relevant to the disposal environments being considered;
- Radiation and thermal effects on used fuel, waste forms, and engineered barrier materials.
- Consideration of how specific waste forms may perform in different disposal environments using theoretical approaches, models, and/or experiments, with quantitative evaluations of how the long-term performance of waste forms can be matched to different geologic media and disposal concepts.

FUEL CYCLE OPTION ANALYSIS

(FEDERAL POC – BRADLEY WILLIAMS & TECHNICAL POC – TEMITAIWO)

Fuel Cycle Option Analysis (*FC-5*) – The Fuel Cycle Options campaign performs analysis and evaluates integrated fuel cycle systems with the purpose of identifying and exploring sustainable nuclear fuel cycles that are candidates for future deployment. Results of these studies and R&D activities must be effectively disseminated to program stakeholders and the public in an accurate, open, and simple manner. Initial efforts will support development of the understanding of what needs to be communicated and why, the audiences to reach, how best to communicate the messages, and the evaluation approach to measure effective communication. Of prime importance is the development of effective methods to communicate the potential benefits of alternative nuclear fuel cycle options and associated enabling technologies that could be developed in the future. Key university research needs for this activity include:

- Identify and develop the essential features and messages for effective communication of the fuel cycle program and its achievements;
- Develop any tools, processes, and products to improve communication of the progress and results of the program and campaigns;
- Interact with the public, stakeholders and other customers external to the program to develop understanding of communication needs and approaches;
- Develop methods to evaluate the effectiveness of program communications;
- Understanding the societal and public viewpoints associated with nuclear power and advanced nuclear fuel cycles.

MISSION SUPPORTING TRANSFORMATIVE RESEARCH

FUEL CYCLE R&D

(FEDERAL POC - BRADLEY WILLIAMS & TECHNICAL POC - MIKE GOFF)

Fuel Cycle R&D (MS-FC) – Game-changing, innovative ideas will play an important role in developing revolutionary fuel cycle concepts of the future. Developing and defining these concepts can support the Fuel Cycle Research and Development (FCR&D) Program's mission to research, develop, and demonstrate alternatives to the current U.S. commercial fuel cycle to enable the safe, secure, economic, and sustainable expansion of nuclear energy while minimizing proliferation and terrorism risks. While proposals relevant to all fuel cycle R&D areas are sought, there is particular program interest in developing accident tolerant light water reactor fuel designs and concepts; and in analyzing extended dry storage of used nuclear fuel, including the subsequent transportation of used fuel (with particular interest on high burn up fuel). Project proposals should include a description of the concept, an analysis of technology risks and feasibility, and a technology roadmap describing how this concept can be further developed.

SMALL MODULAR REACTORS

(FEDERAL POC - TIM BEVILLE & TECHNICAL POC - DAN INGERSOLL)

Advanced Concepts (SMR-1) – SMR concepts offer the opportunity to expand nuclear energy to a broader range of customers and energy-intensive applications, including base-load electricity for remote communities or dedicated facilities, dispatchable electricity to stabilize local grids with high renewable fractions, process heat applications, etc. The more diverse customer base imposes new or enhanced requirements such as extreme reliability or power agility. Innovative concepts are sought that are designed from the outset to provide increased levels of safety and robustness and new functionalities while also maintaining or improving the operational and economic performance. The concepts may utilize advanced technologies or innovative engineering but should be viable for eventual commercial deployment. The scope of the proposed project should include: a thorough viability assessment of the advanced concept, a detailed technology gap analysis, and a comprehensive technology development roadmap.

Advanced Technologies and Analysis Methods (SMR-2) – Advanced technologies can enable new SMR concepts and designs to achieve even greater levels of safety and resilience, flexibility of use, sustainability and construction or operational affordability. For example, improved materials can provide additional core integrity in severe accident situations and advanced sensors and instrumentation can provide better knowledge of plant health during normal and upset conditions. Also, SMRs differ from large plants in their fundamental design features, which may require or benefit from new analysis methods to quantitatively characterize the performance and risk factors associated with SMRs. For example, modeling and simulation methods must accurately predict: radionuclide inventory and component integrity for non-traditional materials and components, different source term release and dispersion paths, extended refueling and maintenance cycles, and greater use of intrinsic safety and security features. Innovative technologies and analysis methods for extending and modeling unique SMR performance and safety factors are encouraged.

NEXT GENERATION NUCLEAR PLANT

The NGNP is a high temperature helium-cooled, graphite moderated reactor with a core outlet temperature between 750 and 850°C. These reactors are well suited for the co-generation of process heat and electricity and for the production of hydrogen from water for industrial applications in the chemical and petrochemical sectors. NGNP is a part of the Office of Nuclear Energy's gas-cooled very high temperature reactor technologies research and development (R&D) program that has a long term goal of achieving outlet temperatures of 950°C. The NGNP R&D program is organized into the areas of: (a) materials, (b) fuels, (c) computational methodologies, and (d) heat transport, energy conversion, hydrogen and nuclear heat applications.

Focused materials research projects have already been initiated that focused on the development of graphite, ceramics, composites and high temperature structural materials, fundamental mechanisms of creep, creep-fatigue, dynamic strain aging, stress relaxation, and environmentally assisted crack growth in component alloys and pressure vessel steels. Ongoing research is studying graphite for fuel blocks and core structures, detecting small cracks in graphite, advanced carbon fiber carbon composite (CFC), silicon

carbide fiber composite (SiC/SiC), composites and ceramics for gas-cooled reactor ceramic components, and improved Non-Destructive Examination (NDE) techniques for predicting lifetimes for CFC, SiC/SiC, and composites. No materials-related proposals are sought at this time.

Fuel development and qualification activities are focused on producing robust fuel particles that can retain fission products during normal and accident conditions and have very low failure rates, as demonstrated by irradiation and accident safety testing programs. Tristructural-isotropic (TRISO) fuel designs for current pebble bed and prismatic gas-cooled reactors are based on historical designs that build upon large experimental fuel performance databases and historical fabrication methods, and ensure robust performance and fission product retention. The NGNP Advanced Gas Reactor TRISO Fuels program has developed novel TRISO fuel particle designs, fabrication methods, characterization techniques, and initiated research to evaluate radiation source term and fission product transport effects. No TRISO fuels-related proposals are sought at this time.

Proposals are being sought for the Computational Methodologies and Heat Transport, Energy Conversion, Hydrogen and Nuclear Heat Application areas that do not duplicate completed or currently funded NEUP grants and programmatic research activities:

Computational Methodologies (NGNP-1) –

(FEDERAL POC – STEVE REEVES & TECHNICAL POC – HANS GOUGAR)

The computational methodologies R&D is focused on providing practical tools to analyze the reactor core neutronics/thermal-hydraulics, performance, and reactor gas-coolant helium thermal fluids behavior during normal operations, transient and accident scenarios, and safety evaluations for gas-cooled reactors and scaled experimental design. Research efforts have been initiated and/or completed in the areas of neutronics, thermal-hydraulics, and multiphysics, in terms of time-dependent coupled fuel/neutronic/thermal fluids modeling, reactor kinetics effects, and mechanical-neutronic-thermal fluid interactions during graphite dimensional changes under irradiation with thermal and neutronic feedback. Gas-cooled reactor plant simulation and safety analysis methods development has been initiated for uncertainty and sensitivity analysis for statistical importance ranking. Methodologies for determining credible fission product transport mechanisms that support the mechanistic source term approach for gas-cooled reactors under normal operating conditions, off-normal events, and accident conditions, including both air and/or moisture ingress events are under development.

Proposals related to gas-cooled reactors that have a special emphasis on experimental validation and uncertainty and sensitivity analysis to benchmark computer simulation methods are particularly encouraged. Proposals are particularly sought in the areas of: (a) Steam Ingress Flow and Chemistry, (b) Seismic Interactions Analysis of the reactor vessel, inlet/outlet vessel and steam generator/turbo-machinery, in a below-grade silo containment/confinement building structure, (c) impact of externally-initiated events and accident scenarios (e.g., seismic, flooding) on safety and risk analyses, and (d) methods that integrate externally initiated events (e.g. earthquake, flooding) and core/reactor dynamics and structures vibrations (e.g. graphite reflector and prismatic block movement). Proposals are sought that focus on conducting integral benchmark experiments for fission product/source term transport and dispersion, using non-radioactive surrogates, that investigate fission product release phenomena (i.e., aerosols, metallic and gaseous species plate-out, dust transport) inside the reactor vessel, turbomachinery, piping systems during severe accident conditions, including benchmarks with historical gas-reactor tests (COMEDIE, KUFA, etc.), which could be used to benchmark computational fission

product/source term methods/algorithms compatible with NRC's MELCOR code methodology.

Heat Transport, Energy Conversion, Hydrogen, and Nuclear Heat Applications (NGNP-2) – (Federal POC – Carl Sink & Technical POC – MW "Mike" Patterson)

The Heat Transport, Energy Conversion, Hydrogen and Nuclear Heat Applications area focuses on the development of approaches to coupling gas-cooled reactors with the wide variety of process heat applications (co-generation, coal-to-liquids, chemical feedstocks).

Proposals are only sought in these areas: (a) dynamic simulation and control of Reactor-driven Process Heat Plants, including interactions of multiple modules and (b) simulation and analyses for the use of interactive and prognostic "intelligent control" systems and advanced instrumentation and control methods (e.g. adaptive controllers, "fuzzy logic", neural networks, genetic algorithms, etc.) to handle combined interactions between the heat transport, energy conversion plant and the reactor systems (core, reactor systems, turbo-machinery, steam generator, compressors) and balance-of-plant systems, during plant upsets, off-normal events, and accident conditions. No Hydrogen-related proposals are sought at this time.

LIGHT WATER REACTOR SUSTAINABILITY

Advanced Mitigation Strategies (LWRS-1) –

(FEDERAL POC - RICH REISTER & TECHNICAL POC - JEREMY BUSBY)

Advanced mitigation strategies and techniques. Extended operating periods may reduce operating limits and safety margins of key components and systems. While component replacement is one option to overcome materials degradation, other methods (e.g. thermal annealing or water chemistry modification) may also be developed and utilized to ensure safe, long-term operation. Validation and/or development of techniques to reduce, mitigate, or overcome materials degradation of key LWR components are sought. Mitigation strategies for pressure vessel steels, core internals, weldments, or concrete are encouraged. Universities engaging in this effort will be expected to produce concepts, supporting data and/or model predictions demonstrating the viability of mitigation strategies for key LWR components.

Risk-Informed Safety Margin Characterization (LWRS-2) -

(FEDERAL POC - RICH REISTER & TECHNICAL POC - ROBERT YOUNGBLOOD)

R&D should address the Risk-Informed Safety Margin Characterization (RISMC) methodology. Areas of high priority include advanced modeling and simulation methods to support the development, verification, and validation of next-generation system safety codes that enable the nuclear power industry to perform analysis of a nuclear power plant's transients and accidents. An especially important need in this analysis is a very clear understanding of the real uncertainties in the analysis. This requires not just propagation of parameter uncertainty via sampling techniques, but also meaningful quantification of the underlying distributions, addressing not only epistemic uncertainty but also variability in phenomena, including variability in component behavior (variability in stroke times, pump head curves, heat transfer coefficients, and so on). Universities performing this research will be expected to produce results that integrate multiple mechanistic processes. Also of interest are advanced approaches to coarse-grained single-phase and two-phase thermal-hydraulics modeling and experimental validation, including coupling of models of different resolutions, for example, between one dimensional system thermal-hydraulics and

three dimensional Computational Fluid Dynamics-type models, and treatment of dynamic flow regimes.

Instrumentation and Control (LWRS-3) -

(FEDERAL POC - RICH REISTER & TECHNICAL POC - BRUCE HALLBERT)

Digital instrumentation and control technologies for highly integrated control and display, improved monitoring and reliability. Research is needed to improve upon available methods for online monitoring of active and passive components to reduce demands for unnecessary surveillance, testing, and inspection and to minimize forced outages and to provide monitoring of physical performance of critical structures, systems, and components (SSCs). In addition, methods are needed to analyze the reliability of integrated hardware/software technologies that comprise digital systems. Research should investigate NDE technologies to characterize the performance of physical systems in order to monitor and manage the effects of aging on SSCs. High priority research areas include the following: 1) methods and technologies that can be deployed for monitoring nuclear plant systems, structures, and components, and that can be demonstrated in test bed environments representative of nuclear plant applications; and 2) methods for analyzing the dynamic reliability of digital systems, including hardware and software systems based on formal methods that can be demonstrated on systems that are proposed or representative of systems proposed for nuclear plant control and automation. This research is expected to support the development of methods and technologies to support digital instrumentation and control integration for monitoring and control as well as for noting areas of improved reliability and areas requiring further information and research. Universities performing this research will be expected to produce results that integrate multiple mechanistic processes.

Advanced LWR Nuclear Fuel (LWRS-4) –

(FEDERAL POC - RICH REISTER & TECHNICAL POC - GEORGE GRIFFITH)

The Light Water Reactor Sustainability program is conducting research and development on the use of silicon carbide ceramic matrix composite nuclear fuel cladding. The goal is to provide improved economic performance and a greater resistance to accident conditions than could be achieved with current zirconium based claddings. Areas of particular interest are the development of radiation resistant silicon carbide ceramic matrix composites, novel fabrication methods, and unique end plug to cladding tube connecting methods.

ADVANCED REACTOR CONCEPTS (ARC)

Advanced Reactors Concept Development (ARC-1) – (Federal POC – Brian Robinson & Technical POC – Robert Hill)

Development of new reactor concepts that use advanced technologies or innovative engineering is sought. The goals of the advanced reactor system should be to provide electricity at the same cost or lower than light water reactors with improved safety and system performance. This category could include the incorporation of advanced systems and components into existing reactor concepts or the inclusion of innovative design alternatives (e.g., new fuel type, coolant modifications, fuel handling strategy, etc.). Components within this scope include, but are not limited to innovative design for containment, seismic, fuel handling, pumps, safety systems, and instrumentation for both operations and maintenance. The scope of the proposed project should include a thorough viability and applicability assessment of the proposed reactor system, advanced systems and/or components, a detailed technology gap analysis, and a

comprehensive technology development roadmap.

Advanced Energy Conversion (ARC-2) -

(FEDERAL POC - BRIAN ROBINSON & TECHNICAL POC - JIM SIENICKI)

Development of new energy conversion systems that use advanced technologies or innovative engineering is sought. Supercritical CO₂ shows promise as a working fluid suitable for fast and thermal reactors because of its compatibility with materials and thermodynamic properties. Basic R&D is needed in turbomachinery performance and loss mechanisms. System optimization requires a detailed modeling of the system components and their response to steady-state and off-normal conditions. The university participants could contribute detailed Computational Fluid Dynamics (CFD) modeling of key components, such as the main compressor, for comparison to one-dimensional system level models and experimental data from ongoing small-scale testing. Alternately, contributions could be made to the development of plant dynamics models and control strategies, including the investigation of alternative cycle layouts (e.g., having turbomachinery on multiple shafts). The efficiency of different power conversion cycles is degraded by leaks at component interfaces. R&D is needed to develop models and/or test beds to predict the performance of seals (labyrinth, dry liftoff seal, brush, etc.) and bearings. Another topic could be projects that explore coupling of the reactor heat source with diverse process heat applications (cogeneration, coal-to-liquids, chemical feedstocks) and/or other energy products with an emphasis on novel approaches that can greatly improve the ease of coupling, the operability of the combined system, and the ultimate economics. The scope of the proposed project should include a thorough viability assessment of the advanced energy conversion system, a detailed technology gap analysis, and a comprehensive technology development roadmap.

Advanced Structural Materials (ARC-3) -

(FEDERAL POC – BRIAN ROBINSON & TECHNICAL POC – JEREMY BUSBY)

Development of new materials for advanced reactor systems is being sought for high temperature liquid metal, high temperature molten salt, and other advanced reactor applications. There are several key needs to support this effort.

- The microstructure stability of advanced structural materials must be validated at elevated temperatures and extended lifetimes under irradiation, elevated temperature and/or exposure to coolants. Novel test techniques and approaches to provide long-term performance data on key candidate-alloys and materials are sought. Such tests must be closely coordinated with advanced alloy development efforts in the supporting program.
- Semi-empirical modeling of material aging and irradiation degradation mechanisms need to be developed to predict neutron damage and temperature effects on bulk/macrostructural mechanical properties, including yield strength, creep, fatigue, ductility, etc. Such a model provides a near-term tool for future experiments by allowing interpolation and deeper understanding of the physical data and, in addition, provide a tool for designers to explore different operating conditions while having at least some understanding of the effects on materials performance, but is not expected to be atomic level detail. Such a model should be based on sound materials science and mechanistic understanding.

MISSION SUPPORTING TRANSFORMATIVE RESEARCH

REACTOR CONCEPTS RD&D

Reactor Concepts RD&D (MS-RC1) -

(FEDERAL POC - SAL GOLUB & TECHNICAL POC - ROBERT HILL)

Identification, investigation and development of revolutionary transformational advanced reactor system concepts having the potential to significantly improve performance in sustainability, safety, economics, performance, security or proliferation resistance. Such transformational advanced reactor concepts could include designs employing advanced coolants, fuel configurations and operational characteristics. Concepts could also include small modular reactors with unique capabilities to address operational missions other than the delivery of baseload electric power, such as industrial process heat or mobile reactors that can provide temporary power during emergency situations. The scope of the proposed project should include a thorough viability assessment of the concept, a detailed technology gap analysis and a comprehensive technology development roadmap that identifies research needed on key feasibility issues.

Space and Defense RD&D – Radioisotope Thermal Generator (RTG) Technologies (MS-RC2) – (Federal POC – Wade Carroll & Technical POC – Stephen Johnson)

Space and Defense Power Systems program has designed, developed, built and delivered radioisotope thermal generators (RTG) for space and terrestrial applications for over fifty years. These systems apply the decay heat from plutonium-238 to the hot side of thermoelectric couples to induce direct current electricity flow. Materials used in the early designs for these systems are increasingly difficult to obtain. Proposals that identify more readily available materials that can perform effectively in the extreme environment of atmospheric re-entry are encouraged. Proposals for breakthrough thermoelectric couples that produce electricity more efficiently than current designs are also encouraged.

- **Replacement Materials.** Develop alternate materials for the aeroshell module that protects radioisotope power system fuel during potential atmospheric reentry events. The material will need ablation resistance, thermal conductivity, and structural strength (compressive and tensile) that meet minimum performance requirements.
- Ultra high efficiency Thermoelectric couples. Develop a thermoelectric couple (N and P legs) with a hot side temperature of 1000 C. The couple should demonstrate efficiency between 20-30% with stable properties providing for a minimum operable life of 10 years.

PROGRAM SUPPORTING: NUCLEAR ENERGY ADVANCED MODELING AND SIMULATION (NEAMS)

ADVANCED MODELING AND SIMULATION

Structural materials (and nuclear fuels) for future generation nuclear reactors (NEAMS-1) – (Federal POC – Jim Peltz & Technical POC – Xin Sun)

Degradation of structural components (and fuels) under the harsh operating environment of a nuclear power plant are important challenges for future generation nuclear power plants, as well as for the current reactor fleet. Accurate assessment of structural component performance using integrated reactor performance and safety codes will require science-based, validated materials models incorporating mechanical properties, degradation kinetics, and chemical evolution of the material constituents under severe thermal, mechanical, and radiation loads, and propagate these materials behaviors into continuum level descriptions of structural response. The research needs are the development of validated materials models and methods that lead to accurate continuum simulations of materials response, with appropriate quantitative consideration of uncertainties at every scale.

- Predictive Models for Material Degradation at Different Scales. Aging and degradation mechanisms of different structural materials under various thermal and irradiation environments need to be better understood, quantified, and validated. Key university research needs in this area include (1) Development of atomistic chemical kinetics parameters and upscaling into meso-scale models; (2) Meso-scale models of microstructural and chemical evolution (e.g., phase field, Potts model, kinetic Monte Carlo and rate theory) with extraction of physical parameters for continuum scale materials models; and (3) Validated prediction of physical/mechanical property degradation, i.e., thermal conductivity, yield strength, ductility and fracture toughness, creep resistance, etc., to populate continuum scale constitutive models.
- Small-Scale Separate Effects Experiments for Model Validation. This element calls for the linkage between model development and small-scale experiments. Small scale separate effect experiments are necessary specifically targeted to validate models for different phenomena at various scales. These small scale experiments are intended for materials relevant to current and future generations of fuel, cladding and reactor vessels; and the properties of interest include but are not limited to: grain-level, directional dependent thermal conductivity and thermal expansion coefficient measurements with irradiation induced defects; grain boundary strength measurement with defect evolution; effective properties for mass and heat transport; directional dependent stress vs. strain curves for irradiated materials with pre-characterized defect distributions.
- **Methodology Development for Scale Bridging.** Multi-scale approaches (from atomic-level to meso-scale to continuum, and from picoseconds to years) are needed. New algorithms to achieve upscaling are a key component to the development of integrated reactor performance and safety codes.

PROGRAM SUPPORTING: NUCLEAR ENERGY ADVANCED MODELING AND SIMULATION (NEAMS)

Model and method development to support current and future generation nuclear reactor performance and safety analyses (NEAMS-2) –

(FEDERAL POC – ROB VERSLUIS & TECHNICAL POC – DAVE POINTER)

Concepts have been identified for future generation nuclear power plants that take advantage of safety phenomenon that are inherent to the design and do not rely on active engineering systems in order to function. These phenomena include natural convection cooling, thermal-mechanical feedback, and passive decay heat removal. In the past, large base-technology programs existed in order to mature the components and technologies that would be deployed in future plant designs. Future design concepts will rely more heavily on modeling and simulations that can better predict core, systems, and plant performance, thus reducing the need for a large base-technology program. Research needs to support the needed predictive performance and safety analysis capabilities include:

- Methods to perform probabilistic safety assessment of component or system performance weighted over a broad spectrum of anticipated component or inherent feature failure conditions.
- Methods to perform sensitivity studies to evaluate variability and/or flow dominance regimes during the initiating phases of natural convection cooling and relevant experimental data to support validation of new methods.
- Predictive methods for simulation of two-phase boiling and/or flashing flows in complex geometry and relevant experimental data to support validation of new methods.
- Predictive methods for simulation of fluid-structure interaction in components with complex mechanical structure and thermal energy distributions, such as reactor fuel assemblies, and relevant experimental data to support validation of new methods.
- Upscaling methods to enable reduced order modeling of long term transients and fuel cycle performance informed by a limited number of high resolution quasi-steady case studies are needed.
- Water coolant chemistry models to support simulation of steam generating fouling and in core applications are needed.
- Modular structural mechanics codes to understand all aspects of pressure boundary integrity (piping, vessels, steam generators, nozzles etc.) are also needed.
- Expanded visualization techniques to assess system-wide coupling impacts so that the impact of perturbations in one part of a system can be viewed on a system-wide domain.
- Development of a coolant properties code library that contains highly-detailed correlations and uncertainty quantification data on coolant properties in liquid, vapor, and supercritical phases. This library could act as a reference for benchmark and validation purposes.
- Multi-scale integration methods to enable development of virtual reactor simulations using multiple levels of resolution to represent a single physics (e.g., neutronics, fluid dynamics, heat transfer, etc.) and relevant experimental data to support validation of new methods.
- Efficient, scalable mesh generation methods to provide accurate descriptions of realistic nuclear reactor component geometries for high-fidelity finite element or finite volume simulations.

PROGRAM SUPPORTING: NUCLEAR ENERGY ADVANCED MODELING AND SIMULATION (NEAMS)

Development of phenomena-based methodology for uncertainty quantification (NEAMS-3) – (Federal POC – Jim Peltz & Technical POC – Jim Stewart)

To promote quantitative confidence in the results, explicit consideration of verification of simulation codes, validation of models for an intended application, and quantitative assessment of physical and computational uncertainties (VVUQ) are expected elements of all computational and experimental work proposed under this call. In addition to this routine application of good computational practices, there are needs for targeted university research in methods for data analysis and VVUQ in support of:

- **Propagating uncertainties through inter-fidelity multiscale physics models—upscaling.** The uncertainty associated with model prediction of material behaviors need to be mathematically propagated through different scales. Systematic approaches are needed for managing uncertainties stemming simultaneously from abstraction into reduced (compact) models and in populating parameters in those reduced models. Conversely, methods are needed to propagate solution sensitivities downward, to identify inadequacies in constitutive model formulations and prioritize important sub-scale phenomena.
- Evaluating parameter sensitivities and uncertainties in tightly-coupled multi-physics models. Improved methods for efficient evaluation of sensitivities and uncertainties are needed for intra-fidelity simulations of highly coupled, non-linear multiphysics (e.g., thermal-chemical-mechanical) phenomena.
- **Interpretation of large experimental data sets**. Advanced modeling and computer simulation methods are needed to process and extract information from large data sets obtained from NDE measurements, and to establish the relationships between microstructural evolution and measured properties.