

# **NUCLEAR SCIENCE AND TECHNOLOGY**

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*Director's R&D Fund*

## Innovative Safety Technologies for Generation IV Reactor Designs

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The objective of this project was to develop new analysis tools and capabilities that will enable ORNL to be a significant contributor in emerging programs to develop advanced fission reactors and, specifically, to extend our ability to design advanced reactor systems that have enhanced safety features while simultaneously improving system reliability and economics. The project focused on three related but distinct aspects of nuclear plant safety: probabilistic risk assessment (PRA), reactivity control, and component surveillance and diagnostics. In all three cases, the new capabilities were demonstrated for a specific advanced reactor concept, the International Reactor Innovative and Secure (IRIS), led by Westinghouse Electric Company. New capabilities generated from the project include the development of a graphical-based software tool for performing PRA studies on concept-level reactor designs, the assembling of a state-of-the-art reactor physics analysis system for studying reactivity control in light water reactors, and the development of an architectural framework for advanced diagnostics and monitoring systems. Demonstrations of these tools for IRIS include the 100-fold decrease in estimated core damage frequency by proper selection of safety system components, the design of an IRIS core that uses erbium as a burnable poison to greatly reduce the level of soluble boron for reactivity control, and an integrated demonstration of advanced software simulation models and prototypic wireless communication hardware to detect and isolate faults in a helical coil steam generator.

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### Introduction

A resurgence of the nuclear energy industry in the U.S. and its growth worldwide is being driven by three major factors: an increasing demand for electricity, an increasing concern regarding the global warming effects of fossil fuels, and a new urgency to replace our dependence on foreign supplies of energy with domestic resources. The ability of the nuclear power industry to meet these expectations will depend substantially on our ability to build new plants that have increased safety and reliability relative to existing plants, while also remaining economically competitive with alternative energy sources. Increased nuclear plant safety places a greater demand on creative design solutions and advanced technology. The objective of this project is to develop new analysis tools and capabilities that will enable ORNL to design advanced reactor systems that have enhanced safety features and improved system reliability and economics. This was accomplished by addressing three aspects of plant safety: (1) the novel application of probabilistic risk assessment (PRA) methodologies to concept-level trade-off studies, (2) the development of advanced computational methodologies for the study of innovative alternatives to reactor reactivity control, and (3) the development of an innovative approach for in situ surveillance and diagnostics

to ensure plant integrity during extended periods of operation. In all cases, new capabilities were demonstrated using a specific advanced reactor concept: the International Reactor Innovative and Secure (IRIS) concept,<sup>1</sup> which is a leading advanced reactor concept that has a “safety by design” philosophy and special design characteristics that make it especially attractive for deployment in developing countries.

### Technical Approach and Results

The following sections describe the technical approach for each of the three major tasks in this project. Also described are results from the application and demonstration of the new tools and methodologies to the IRIS design.

#### *Task 1: Probabilistic Risk Assessment*

Current PRA analyses are performed primarily to demonstrate the safety of the plant and are typically performed when the design is approximately 50% complete and also 90–100% complete. It is difficult and costly at these points in the design process to make changes to the design, and changes are done only if significant vulnerabilities in the design are demonstrated by the PRA. A much better approach is to perform PRAs throughout

the design process, especially in the formative stages when individual components and systems are being selected. This allows for safety and reliability to be incorporated into the design from the very outset. Task 1 of this project was to develop an easy-to-use software tool that can facilitate the selection of nuclear plant components based on their impact on the predicted probability of system failure, core damage, radiological release, etc.

The overall architecture of a new concept-level PRA tool was defined, and a working version of the *VisualBasic* driver/overlay program was constructed. Considerable planning had to be invested to determine how the event trees and fault trees are combined in order to allow the user to not only evaluate different system design options but also to select alternatives to the underlying probabilistic models and component data. Extensive use was made of data from the PRA of Westinghouse's AP-600 certified reactor design.<sup>2</sup> The one-button architecture was designed to evaluate combinations of design and event options through sets of fault tree modules in a dynamic PRA. Changing the design is easily performed by picking a design alternative from a drop-down menu. The new program, designated RBOT (Reliability-Based Optimization Tool), automatically inserts the correct fault tree module(s) into the PRA model in *FaultTree+*,<sup>3</sup> relinks the correct support systems, and recalculates the parameters of interest.

Data structures were defined that permit the accumulation of design alternatives and resulting failure probabilities, which facilitates the ability of the code to perform reliability-based design optimization.

To demonstrate the power of the new tool, RBOT was used to assess the sensitivity of the predicted IRIS core damage frequency to design choices for the valves in the automatic depressurization system (ADS) and the emergency heat removal system (EHRS). Choices included using either air-operated valves (AOV) or motor-operated valves (MOV), whether to configure the system with the valves initially open or closed, the number of valve trains, and the capacity of the relief valves. Eleven component choices in the ADS and EHRS generate a total of 160 unique design choices. Using RBOT, we were able to easily evaluate the impact of the 11 component choices, which resulted in a selection of preferred components that was not intuitive. Specifically, although AOVs have higher reliability than MOVs, when used in an integrated system, they resulted in a higher core damage frequency (CDF). This is because the common cause failure for air-operated systems is higher than for electrically driven systems. Figure 1 compares the failure probability for AOVs and MOVs when treated individually or within an integrated system. It was determined that for the EHRS, using two valve trains with one AOV and one MOV provided a 42% higher reliability and a 23% reduction in CDF. Using this

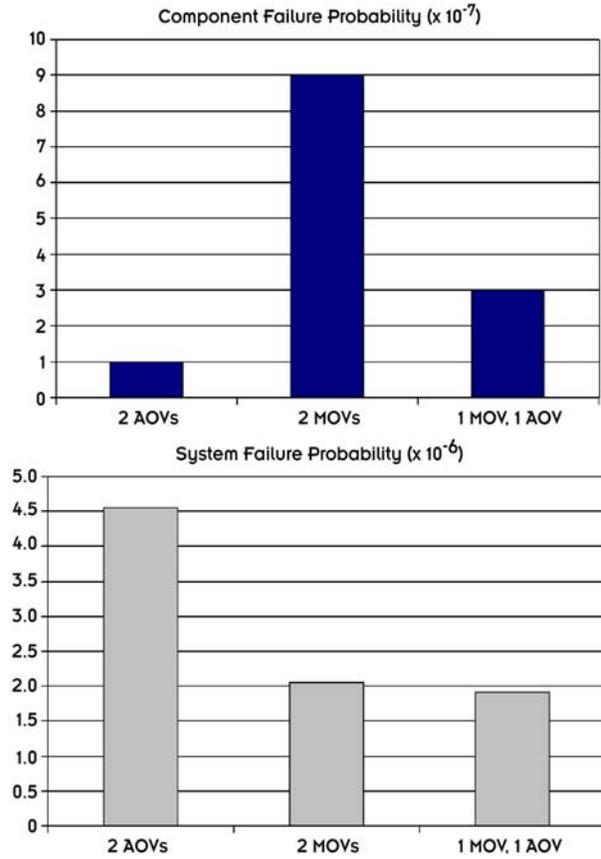


Fig. 1. Failure probabilities for combinations of air-operated valves (AOV) and motor-operated valves (MOV) taken as isolated components or integrated into the emergency heat removal system.

input and other results from our application of RBOT, the IRIS PRA specialists were able to reduce preliminary estimates of the CDF by nearly two orders of magnitude from  $1 \times 10^{-6}$  to  $2 \times 10^{-8}$  incidences per reactor-year.

### Task 2: Reactivity Control Options

For the analysis of reactivity control options, a state-of-the-art core analysis methodology was assembled and validated against IRIS-specific benchmark problems. For pin and assembly level analysis, the HELIOS code<sup>4</sup> was selected, which is a highly configurable collision probability code. The NESTLE nodal diffusion code<sup>5</sup> was used for basic core analysis and the study of reactor transients. A code linking the HELIOS lattice code with the NESTLE code was developed for this project and tested with several single-assembly benchmarks. An evaluation was made of different versions of the FORMOSA core loading optimization code<sup>6</sup> to determine which version was the best suited for IRIS analysis. Standard versions of FORMOSA exist for pressurized water reactors (PWR) and for boiling water reactors (BWR), but the innovative IRIS design incorporates some

features of both. The FORMOSA-P code was selected and adapted for this project and used to perform general core design analysis, minimization of power peaking, maximization of core lifetime, and analysis of two-batch core designs. Four IRIS-specific benchmarks were analyzed, and results compared with results from other IRIS team members: two pin cell benchmarks, one assembly benchmark, and a whole core benchmark. Benchmark results showed good agreement with the consensus results.

Using the newly assembled analysis package, we studied the feasibility of using distributed burnable poisons (BP) in the fuel pins as an alternative to relying on soluble boron in the coolant as a means of compensating for the excess reactivity that must be included in the fuel. Eliminating the need for soluble boron not only improves the safety of the core by eliminating the potential for a positive void reactivity coefficient and eliminates the potential for a boron dilution accident but also significantly improves the economics of the plant by eliminating boron chemistry systems. Several BPs in various homogeneous and heterogeneous arrangements were considered, including gadolinium (Gd), erbium (Er), and zirconium-diboride ( $ZrB_2$ ). Preliminary design studies were performed for a standard  $17 \times 17$  fuel assembly by varying the Er and Gd content and pin distribution to obtain an “ideal” reactivity profile, that is, an infinite multiplication factor ( $k_{inf}$ ) of 1.0 throughout the fuel burn-up cycle. Figure 2 shows the burnup-dependent profiles for several distributions of Er in an IRIS assembly. Although an acceptable profile could be achieved, it required that the BP be loaded into 32 pins at an unacceptably high weight percent (>20%). The result of this preliminary analysis indicates that Er is the preferred BP since it can be distributed more evenly throughout the core and results in lower power peaking factors. Currently, the IRIS design retains soluble boron due to other considerations; however, the use of Er as a burnable poison permits a reduced boron concentration in the coolant, which improves the safety performance of the core.

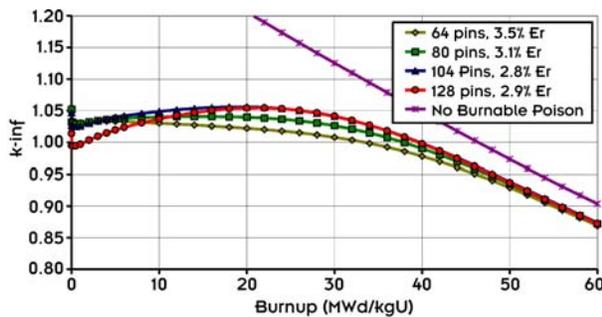


Fig. 2. Infinite multiplication factor for a  $17 \times 17$  pin fuel assembly with different distributions of erbium burnable poison.

### Task 3: In Situ Monitoring and Diagnostics

The third major task involved three related studies: (1) developing an architectural framework for an advanced diagnostics and monitoring system, (2) exploring in situ diagnostic techniques capable of automatically checking the integrity of critical sensors and reactor components, and (3) performing an integrated demonstration of a control system with fault detection. A conceptual architectural framework for control and communications was developed and adapted to IRIS. The supervisory control structure is hierarchical with a recursive nature among the vertical levels. Each node in the hierarchy (except for the terminal nodes at the base) is a separate supervisory module. Each module makes decisions appropriate for its level in the hierarchy and passes the decision and necessary supporting data to the modules above. The hierarchical structure is depicted in Fig. 3. Plant-wide use of secure, wireless data communication and the use of “open systems” (i.e., nonproprietary communication standards) were emphasized and recommended. The use of wireless systems where feasible will significantly reduce both capital and maintenance costs.

Steady-state and dynamic models of a helical coil steam generator (HCSG)<sup>7</sup> were developed to generate simulated “measurement” data for both normal and off-normal conditions. Using subspace identification techniques, a ninth-order linear state space model of the HCSG was developed for the dynamic simulation of full power operation. The model was able to predict the steam generator pressure, the cold leg temperature, the steam outlet temperature, the saturated boiling length, and the sub-cooled length with acceptable accuracy. A robust dynamic parity space approach was then developed to design residual generators for fault detection and isolation (FDI). Using the residuals from multiple FDI variables, the methodology was able to reliably detect and isolate

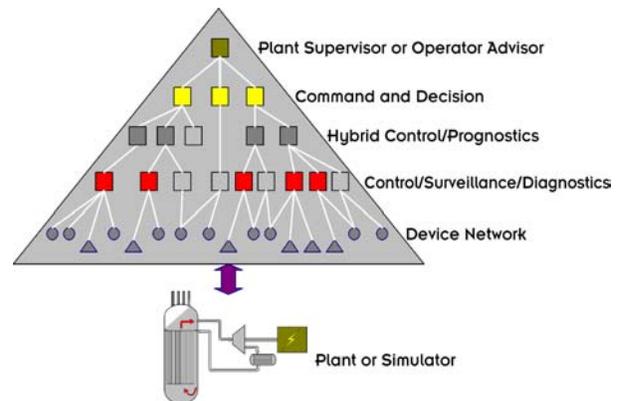


Fig. 3. Schematic of a hierarchical control system with progressive layers of decision-making functions.

the simulated fault of a steam temperature sensor during steady state or transient operation of the HCSG.

As a final demonstration of the new methodology, an experiment was performed, with the dynamic model of the HCSG running on one computer connected to a wireless transmitter and the FDI module running on a second computer connected to a wireless receiver. Temporary faults in the steam temperature sensor were injected into the simulation, and in all cases, the FDI module was able to identify the fault within 10 sec and also recognize the return to normal conditions.

### Summary and Conclusions

The project was highly successful both in terms of technical accomplishment and in attracting interest in follow-on work for ORNL. With many universities, laboratories, and vendors now exploring a wide range of advanced reactor concepts, the availability of the concept-level PRA tool developed by this project will be highly valuable for producing safe, reliable, and cost-effective plant designs. In addition to positively impacting the design of the IRIS safety systems, we have received interest from the U.S. Nuclear Regulatory Commission and from Westinghouse for potential sponsorship of its further development. The assembling of a powerful reactor core analysis package was directly beneficial to the evolving design of the IRIS core and has positioned ORNL well to participate in the design of other advanced reactor systems. Finally, the development and demonstration of new in situ plant monitoring and diagnostics methods will help to

facilitate plant designs with longer fuel cycle and maintenance cycle times without compromising plant safety and has positioned ORNL as the lead organization within the IRIS consortium for plant control. Additionally, our active participation in the IRIS team has led to DOE-funded collaborations with other consortium members.

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## Advanced High-Temperature Test Loop for Materials Compatibility in Advanced High-Temperature Reactors

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A primary hurdle for use of molten salts in advanced high-temperature reactors (~1000°C) is materials performance. To this end, materials/molten-salt compatibility was evaluated in a thermal-convection loop and redox potentials of buffers to further reduce corrosion were determined.

The neutronics results show that very attractive salt and buffer systems exist, which have acceptable responses to the most common nuclear stability perturbations. The electrochemical results indicated that there are suitable redox buffers (Yb, V) that can be used to minimize corrosion at very high temperatures. Further, a stable reference electrode has been identified. In the presence of very low impurities in this Group IA-halide salt (FLiNaK), corrosion of Hastelloy-N was minor. However, molybdenum fluoride, which has an extremely low solubility in this salt, was transported around the loop. A mechanism based on the change in coordination with temperature is proposed.

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### Introduction

The desire to increase the operating temperatures of Advanced high-temperature reactors (AHTRs) to achieve greater efficiencies gives rise to the need for materials systems that possess good compatibility with external air and the internal environment of the reactor and/or heat exchangers. Molten fluoride salts, because of their low vapor pressures at high temperatures, are candidates for use in these AHTRs. Materials compatibility in molten fluoride salts is dependent on the salt constituents being more stable than the fluorides of the structural containment material. In addition, mass transfer due to thermal gradients must be evaluated. This project was designed to assess system compatibility at high temperatures under dynamic flow conditions and to conduct preliminary experiments.

### Technical Approach

Evaluation of materials for use in AHTRs and/or heat exchangers is a complex activity that involves many factors. In addition to materials mechanical properties and external oxidation resistance, neutronic viability and molten salt/materials compatibility must be considered. The technical approach screens candidate materials and salt systems for application to AHTRs, evaluates their chemical and neutronic viability, and establishes prototypic system compatibility at high temperatures under the flow conditions developed in a thermal-convection loop.

### Thermodynamic Screening and Buffer Chemistry

Screening of likely candidates was performed based upon (a) their properties at high temperatures, (b) their likely resistance to corrosion (based upon thermodynamic projections), and (c) their neutronic properties. A requirement for material compatibility is that fluorides of the salt constituents be more stable than fluorides of the containment materials. Thus, alkali metals (e.g., Li) are the preferred cations for salt constituents, and the more noble metals (e.g., Ni) are the preferred container constituents. As a consequence, the experimental part of this project was focused on “FLiNaK,” LiF-NaF-KF” (46.5-11.5-42 mol %) as a prototypical coolant salt. It is also known that the thermodynamic potential for corrosion can be minimized by maintaining the salt in a net reducing condition by use of an oxidation-reduction (“redox”) buffer. Hence, buffer elements, which were studied by cyclic voltammetry (CV), were added as a fluoride (VF<sub>3</sub>, EuF<sub>3</sub>, UF<sub>4</sub>, YbF<sub>3</sub>) at concentrations between 10<sup>-2</sup> M and 10<sup>-3</sup> M. Before use, they were purified by flowing F<sub>2</sub> in a closed loop that included a NaF bed to retain HF. These buffers were not employed in the thermal convection loop test.

A three-electrode system was used for the CV determinations. The working and counter electrodes were made of iridium wire 1 mm in diameter welded to 3.175 mm stainless steel rods. The iridium wire was immersed approximately 25 mm into the molten salt. The reference electrode was adapted from a design by Kontoyannis.<sup>1</sup> The electrode consists of a graphite cylinder

(12.7-mm diameter) that was drilled (6.35-mm internal diameter), leaving a flat membrane at the bottom (1 mm thick) and 3.17-mm-thick walls. The top of the graphite electrode was threaded to accommodate a boron nitride cap. The cap had a threaded hole in the center to accommodate the nickel electrode, which consisted of a thin nickel rod (1.59 mm in diameter) connected to a stainless steel rod (3.175 mm in diameter). The cavity inside the graphite electrode was filled with  $\text{NiF}_2$  (0.1 M) dissolved in FLiNaK. Further details are presented elsewhere.<sup>2</sup>

### Neutronic Screening

A preliminary neutronic screening of the proposed redox buffers was performed. The neutronic models at ORNL for the modular high-temperature gas-cooled reactor were modified for use with a molten salt coolant (in place of the conventional helium coolant). For this screening analysis, adequate neutron cross-section libraries exist to evaluate the spectral range of interest for the redox buffers considered and for all other salt constituents. In addition to evaluation of new buffers, the neutronic performance of an alternate to the well-established FLiBe salt system (2LiF-BeF<sub>2</sub>) was evaluated. “FLiNaRb” (LiF-NaF-RbF: 45-10-45 mole%, 430°C m.p.) has some very attractive features. It promises very significant neutronic improvements over the most common competitor to FLiBe, “FLiNaK” (LiF-NaF-KF: 46.5-11.5-42 mole%, 454°C m.p.). Because it does not contain Be, it is a relatively nonhazardous chemical.

### Materials Evaluation

As outlined earlier, alkali metals (e.g., Li) are some of the preferred cations for fluoride salt constituents, and the more noble metals (e.g., Ni) are the preferred container constituents. Thus, the materials evaluation work focused on FLiNaK as the molten salt and Hastelloy-N as the material of containment. In addition, this alkali halide mixture permits a most sensitive investigation of thermal-gradient, mass-transfer effect, because of the greater solubility of the structural material fluorides in this IA-halide (FLiNaK) than in salts containing IIA-halides (FLiBe). Hastelloy-N is a nickel-based material that was originally designed for use in the Molten Salt Reactor Experiment, and as a result, there is a large data base of materials properties.

Because of the significant role impurities in the salt can play in the corrosion behavior of the material/salt system, extreme care was taken in the manufacturing, purification, and handling of the salts. After preparing a mixture of reagent-grade components to produce the LiF-NaF-KF (46.5-11.5-42 mol %) composition, moisture, hydroxides, and sulfates were removed by sparging with a mix of HF/H<sub>2</sub> at 600°C.

A thermal convection loop was used to evaluate materials compatibility issues of the FLiNaK/Hastelloy-N system. The temperature gradient and flow field in a loop are necessary to determine the importance of a mass-transfer effect. A Hastelloy-N loop, shown in Fig. 1, was used. The construction of this loop, which contained 32 Hastelloy-N specimens in each of the hot and cold legs, is detailed elsewhere.<sup>3</sup> The Hastelloy-N thermal convection loop was connected to salt supplies and equipped with clam-shell heaters on the hot leg and calorods on the cold leg, thermocouples, pressure gauges, a helium gas supply and associated gas purification system, and an array of alarms. Freeze valves at the bottom of the loop maintained the salt in the loop during testing. Analytical ports and instrumentation (Fig. 2) consisted of a double ball valve (DBV) arrangement for removing salt samples and electrodes in the surge tank for CV measurements.

Prior to the start of testing, the Hastelloy N loop was cleaned of residual oxides in two steps. First, the loop was flushed and then filled with argon/4% hydrogen, held at 850°C for 2 h, and then allowed to cool under argon/4% hydrogen environment. Secondly, the loop and one of the salt supplies (a “flush” salt) was heated to 550°C and the salt pushed into the loop by pressurizing the salt supply vessel with helium. The loop was then heated to 650°C

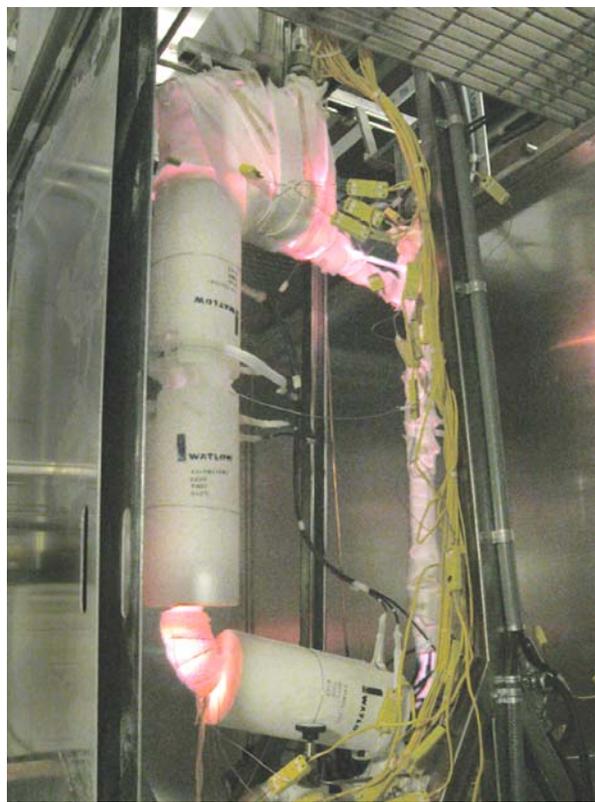


Fig. 1. Loop showing clamshell heaters (left), surge tank (top), and thermocouples. Salt supplies are at the bottom of the loop (not shown).



Fig. 2. Assembly at top of surge tank showing double ball valve for salt sampling and three electrodes for cyclic voltammetry.

and maintained at temperature overnight. The next day, the “flush” salt was allowed to flow back into its salt supply vessel.

Following the above procedure, the loop was then filled with the working salt from the second salt supply vessel. The working temperature of 800°C at the top of the hot leg was established, power to the cold leg calrods turned off, and flow established. The system was operated for 3048 h.

Periodically, electrochemical analyses were performed on the salt using three-electrode, cyclic voltammetry. When not in use, the nickel reference electrode was pulled into the void space above the loop surge tank. Following these measurements, salt samples were collected by submerging a small nickel crucible into the melt through the DBV arrangement (Fig. 2) and withdrawing the sampler into the DBV system under a helium atmosphere. The samples were analyzed for cation content.

## Results and Accomplishments

### Thermodynamic Screening and Buffer Chemistry

Table 1 shows the preliminary standard electrode potentials for the following redox couples: Yb(III)/Yb(II), U(IV)/U(III), V(III)/V(II), and Eu(III)/Eu(II) in FLiNaK at 610°C. The behaviors of Eu and Yb appeared to be simple and reversible. The behavior of vanadium was more complex and irreversible and needs further analysis. The irreversible behavior of the U(IV)/U(III) system in FLiNaK was briefly evaluated, and the results are similar to those of Clayton.<sup>4</sup> Ytterbium and vanadium are suitable redox buffers for minimizing containment corrosion at high temperatures.

**Table 1. Standard electrode potential in FLiNaK at 610°C with Ni/NiF<sub>2</sub> reference electrode**

Redox couple	E <sub>o</sub> (V)
Yb(III)/Yb(II)	-1.45
U(IV)/U(II)	-1.2
V(III)/V(II)	-0.9
Eu(III)/Eu(II)	-0.64

### Neutronic Screening

A computational model for an Advanced High Temperature Reactor was defined, and critical nuclear parameters (voiding coefficients, temperature feedback) for the candidate molten salt coolants were calculated. In Table 2, coolant salts with attractive physical properties that are also nontoxic and do not generate tritium are presented. The buffer systems with low void coefficients are presented in Table 3. Natural vanadium and enriched ytterbium show a zero void coefficient. Calculation of the time-dependent fuel temperatures (and Doppler feedback)

**Table 2. Coolant void reactivity coefficient using 1 mol % natural vanadium (ΔK/K for whole core 100% voiding)**

Compounds	Composition	Void %
<i>Alkali-Fluorides (IA)</i>		
LiF-NaF-RbF	(45-10-45) (0.01 at % Li6)	0.3
LiF-NaF-KF	(11.5-46.5-42) (0.01 at % Li6)	0.5
LiF-RbF	(43-57) (0.01 at % Li6)	0.2
<i>Alkali + Alkaline Earth Fluorides (IA + IIA)</i>		
LiF-BeF <sub>2</sub>	(66-34) (0.01 at % Li6)	-0.1
NaF-BeF <sub>2</sub>	(57-43)	0.0
<i>Alkali + Zirconium fluorides (IA + Zr)</i>		
NaF-ZrF <sub>4</sub>	(50-50)	0.0
LiF-NaF-ZrF <sub>4</sub>	(42-29-29) (0.01 at % Li6)	0.1
RbF-NaF-ZrF <sub>4</sub>	(40-23-37)	0.2
RbF-NaF-ZrF <sub>4</sub>	(50-8-42)	0.2

**Table 3. Coolant void reactivity coefficient with 1 mol % buffer**

$(\Delta K/K \text{ for whole core } 100\% \text{ voiding})$		
Buffer	Enrichment	Void %
Vanadium	Natural	0.0
Thulium	Natural	5.0
Ytterbium	Natural	0.7
Ytterbium	100 wt % Yb172	0.0
Ytterbium	100 wt % Yb176	0.0
Samarium	Natural	28.5
Samarium	100 wt % Sm144	0.0
Samarium	100 wt % Sm148	0.05
Samarium	100 wt % Sm154	0.1
Samarium	100 wt % Sm153	5.8
Europium	Natural	25.5

after an accidental voiding of the coolant needs to be completed to determine if the desired negative void coefficient can be obtained.

### Materials Evaluation

Results of the 3048-h thermal convection loop test are presented in Fig. 3. As in previous work,<sup>5</sup> the Hastelloy-N specimens (surface area of 10.8 cm<sup>2</sup>) at higher temperature lost weight and those at lower temperatures gained weight. However, the weight changes were significantly smaller than those previously observed. As shown in Fig. 4, the cross-section of a specimen at 815°C (highest temperature and weight loss) exhibits a very shallow depth of attack and no voids. In contrast, a specimen that was 566°C and gained weight (Fig. 4) exhibits a deposit on the surface. As shown in Fig. 5, there is a deposit on the surface of the maximum-weight-loss specimen, which is significantly thinner than that on the specimen that gained weight. Further examinations revealed that there were deposits on all specimens, with the amount deposited increasing with decreasing

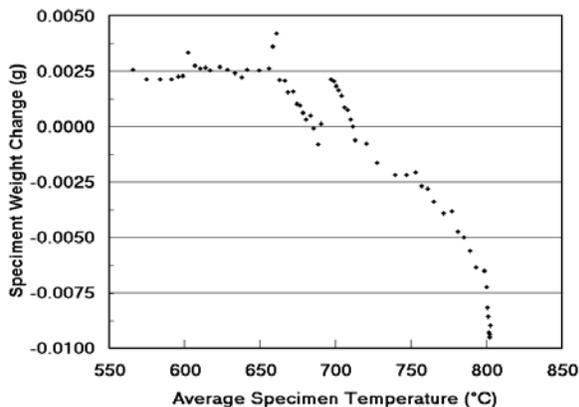


Fig. 3. Weight change as a function of temperature. Highest and lowest temperatures are in the hot and cold leg, respectively.

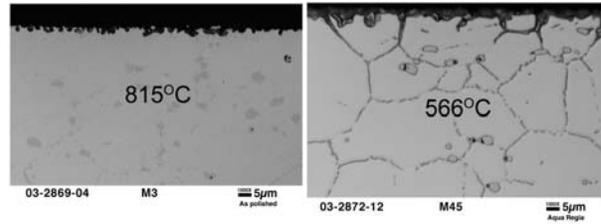


Fig. 4. Specimen at 815°C lost weight and showed a shallow depth of attack whereas the specimen at 566°C gained weight and showed a layer on its surface.

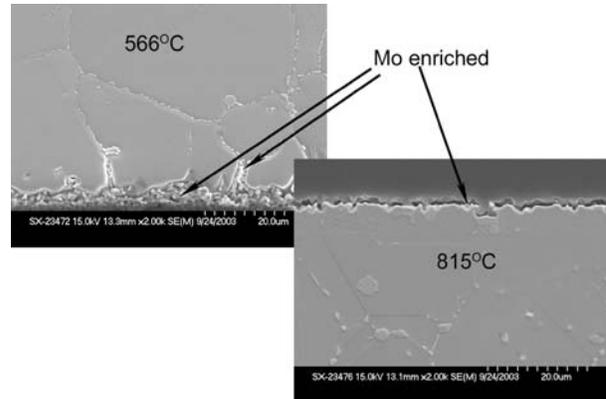


Fig. 5. SEM photo shows a very thin layer on the surface of the specimen that lost weight at 815°C. This layer is much thinner than that on the specimen at 566°C. These layers are enriched in molybdenum.

temperature. These layers are significantly higher in molybdenum content than the base material. There is also transport of the molybdenum along the grain boundaries (Fig. 5). In keeping with the absence of voids and no enhancement of chromium in the deposited layer, the chromium content in the salt was low and over the lifetime of the test averaged 167 ppm as compared to less than 40 ppm in the as-prepared salt. The molybdenum content of the salt averaged less than 60 ppm, as compared to less than 40 ppm in the as-prepared salt. These results clearly demonstrate that corrosion can be significantly reduced by reducing the impurity levels in the salt. Also, these results raise the prospect of a mechanism of molybdenum transport based on the unusual properties of some lower valence molybdenum compounds at the different temperatures, which would allow the molybdenum to disproportionate and deposit at all temperatures in the test loop. This proposed mechanism, somewhat supported by the delay before the CV scans showed a minor change in behavior (Fig. 6), needs further investigation.

### Summary and Conclusions

The results from this project removed two of the fundamental barriers to pursuit of very-high-temperature

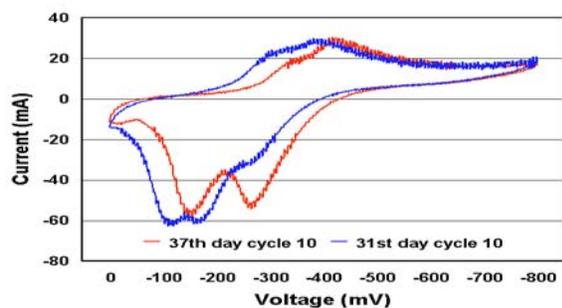


Fig. 6. Cyclic voltammetry data showing splitting of the peaks with increasing time. This is indicative of a slow increase of a species in solution.

molten salt coolants. The neutronics results showed that attractive salt and buffer systems that have acceptable responses to the most common nuclear stability perturbations exist. The electrochemical results indicate that there are very suitable redox buffers (Yb, V) that can be used to minimize corrosion at very high temperatures. Further, a stable nickel reference electrode has been identified. In the presence of very-low-salt impurities in this Group IA-halide salt (FLiNaK), which has a greater solubility for the fluorides of structural materials than Group IIA-halides, containment corrosion was very minor. However, molybdenum fluoride, which has an extremely low solubility in this salt, was transported around the loop. A mechanism based on the change in coordination with temperature is proposed. Additional studies are necessary in order to confirm the mechanism and to understand the effect on the long-term behavior of containment material.

The instrumented loop capability established on this project and the associated research findings provide several opportunities for follow-on funding. First and foremost, this work impacts the direction of the Department of Energy, Office of Nuclear Energy (DOE-NE), Generation IV Program especially, the Next Generation Nuclear Plant (NGNP) concept in which it is proposed that high-temperature (1000°C) heat be used to produce hydrogen. Fluoride salts are attractive as the heat transfer working fluids because of their low vapor pressures. The neutronics, buffers, and corrosion results of this work all support the desired outcomes of the NGNP concept. Hence, funding for the use of molten salts as heat transfer media and a molten-salt-cooled reactor concept will be pursued. A more detailed engineering evaluation of the entire concept, as well as the natural follow-on of extensive convection loop tests at even higher temperatures, will be proposed. Additional sources of support will be sought from programs that have stated an interest in fluid-fueled concepts. For fission concepts, this is the Advanced Accelerator Applications Program

(formerly Accelerator Transmutation of Waste Program) and DOE-NE. Fluid-fueled concepts are especially attractive for transmutation of minor actinides because of the difficulty in conventional fabrication of fuels from these intensely radioactive materials. Work in both thermal (fluoride) and fast (chloride) systems would be pursued. The interest in fast-spectrum devices is especially intense, so a focus on chloride systems that are inherently more corrosive would be a natural extension of this work. Operations at more reducing conditions could be proposed for minor actinide systems in chlorides and fluorides and may be the only hope for reliable containment of chloride salts. The work on corrosion in chloride systems would also have significant application to pyrochemical processing schemes. The Molten Salt Reactor Experiment coolant salt constituted with Li-7, FLiBe, is widely regarded as the premier tritium breeding salt for fusion applications. The fusion community has many of the same corrosion concerns as the proponents of molten salt cooled reactors and fluid-fueled concepts. The instrumented convection loop capability can establish the corrosion resistance in their model systems, and funding will be pursued in this area.

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## Breakthrough Multi-Megawatt Space Reactor Power System Design

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A Space Reactor Power System (SRPS) optimization tool is under development that uses evolutionary computational algorithms called genetic algorithms (GA) to optimize the design of SRPS subsystems for a nuclear electric propulsion (NEP) space vehicle. The tool is designed to work in conjunction with the Nuclear Electrical Vehicle Optimization Tool (NEVOT), which is being jointly developed by ORNL, Marshall Space Flight Center, and Arnold Engineering Development Center. The tool is being employed by ORNL to produce a pre-conceptual design for a multi-megawatt space reactor power system. Although the tool was developed for a space power application, the methodology can be applied to any multi-discipline, multi-objective optimization problem.

The objectives of this work are to (1) develop a breakthrough methodology for designing multi-discipline, multi-objective engineering systems, (2) to re-establish ORNL as a leading center for the design and development of multi-megawatt Rankine Space Reactor Power Systems (SRPS), and (3) to pilot the Tri-Lateral Alliance with Arnold Engineering Development Center and Marshall Space Flight Center.

The SRPS design optimization tool employs detailed subsystem design codes in conjunction with a genetic algorithm (GA) optimization tool to produce self-consistent, optimized, detailed SRPS designs. A series of design codes have been written to perform system evaluations after the important features of the system have been selected by the GA. The best solutions are found in the GA methodology by removing solutions with poor evaluations from a generation and repopulating the next generation with combinations or mutations of the better designs over many successive generations until only the best solutions remain.

The power of the methodology is that (1) the systems are created without sequential design information, which allows novel approaches to be investigated; (2) the algorithm does not require modification to search for the optimal solutions to different missions, constraints, or different definitions of fitness; (3) more sophisticated analyses, models, and approaches can be easily included into the methodology as they become available; and (4) the results are detailed, self-consistent designs of optimized integrated SRPS subsystems. These features make the SRPS optimization tool a flexible and powerful tool for performing subsystem trades studies and optimization for a broad range of design problems.

An integrated low-fidelity first-generation SRPS evaluation tool has been developed and is being used to facilitate the development of the NEVOT optimization tool at the Marshall Space Flight Center. A higher-fidelity second-generation SRPS evaluation module is being developed at ORNL, and initial results are expected during FY 2004. Second-generation design modules have either a sophisticated engineering design algorithm or a realistic physics evaluation of the subsystem. The liquid metal reactor module was derived from a modified version of the ALKASYS Design code.<sup>1</sup> The Rankine liquid metal power conversion module and the heat rejection module are derived from a set of programs developed to predict Nuclear Electric Propulsion subsystem performance and mass developed under NASA program RTOP 593-72. The potassium power conversion code<sup>2</sup> and the heat rejection code<sup>3</sup> were modified slightly to operate at lower power; however, they are largely unchanged. The shield and Brayton system power conversion design modules were written from first principles at ORNL. Integration software has been written to allow modules with different levels of sophistication to be selected for use in the evaluation, which permits the algorithm to scope down to better solutions with simple models before using the more computational-intensive second- and third-generation algorithms for fine tuning the designs.

The designs created are not derived through an iterative sequential design approach. They are evaluated after being created. By developing the tool without engrained sequential design logic, the GA algorithm has more flexibility to design and combine subsystems, which allows it to find new and unique design solutions. The algorithm does not have to be changed to search for the

optimal solutions to different problems or to emphasize a different set of optimization parameters. The result is a flexible and powerful tool for performing subsystem trade and optimization studies that can be applied to any multi-objective, multi-discipline science application.

In addition to developing a power design tool, this project will result in a state-of-the-art multi-megawatt SRPS design and new and improving relations with our Tri-lateral Alliance partners. It has already generated interest and attention from potential sponsors for follow-on funding including JPL and DOE.

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