Progress Update on Pre-Application Review Analysis of Coolant Void Reactivity and Related Neutronic Phenomena in ACR-700

This report summarizes progress through September 3, 2003, on the pre-application activities for the independent analysis of coolant void reactivity (CVR) and related neutronic phenomena in the ACR-700.

The NRC analysis objectives can be stated as follows:

(1) Applying rigorous nuclear analysis methods to models of the ACR-700 core lattice, core, and associated benchmarks;

(2) Provide a detailed independent analysis of the ACR-700 CVR and related neutronic phenomena;

(3) Analyze the sensitivities of the CVR and related phenomena to simplifying modeling assumptions and to variations and uncertainties in core configurations and operating parameters;

(4) Compare the detailed neutronic phenomena governing the CVR and related effects in ACR-700 to those governing the measured quantities in experimental benchmark configurations used by AECL for assessing computational biases and uncertainties in the prediction of CVR in ACR-700.

Based on the resulting analysis, the staff will provide, preliminary conclusions and observations on the nominal values of CVR in ACR-700, associated neutronic modeling needs and issues, the applicability and adequacy of the experimental benchmark database used for validating computed predictions of CVR, and the evaluation and treatment of CVR computational biases and uncertainties.

The NRC's efforts to meet these objectives fall under the seven activities discussed below.

1. Acquiring Necessary ACR-700 Nuclear Design Information

The independent analysis of CVR and related neutronic phenomena in ACR-700 requires detailed nuclear design and operational information well beyond what AECL otherwise provided through its early interactions with the NRC staff. To identify and acquire the necessary information, the staff drafted an initial set of requests for additional information (RAIs) in January 2003.

The initial draft set of RAIs was subsequently edited to address internal comments. An advance draft of the set of 12 RAIs was e-mailed to AECL on March 10, 2003. Through follow-up discussions, the set of RAIs was ultimately revised to request only the more limited preliminary design information that AECL can provide during the pre-application phase. The revised and finalized RAI set was then formally transmitted to AECL on May 13, 2003.

The RAI response package from AECL submitted on June 15, 2003, provides nuclear design and operational details only for the equilibrium ACR-700 core as it is presently designed. AECL indicates that details of the equilibrium core design may still change and that no designs have yet been developed for the initial fuel loadings and transitional cores. Our independent analyses during the pre-application phase will therefore consider only the equilibrium core design as represented in AECL's RAI responses and subsequent submittals.

The RAI response provides AECL's predicted nuclide compositions of irradiated equilibrium reload fuel at only three selected burnup levels: nearly fresh, mid burnup, and average discharge burnup. No information is provided on the predicted axial burnup variations near the bundle ends or on the radial or azimuthal variations of irradiated fuel compositions within the fuel pins (e.g., the rim effect). Effects of local operating variables (e.g., coolant temperature and density) and associated modeling assumptions are not discussed. Core fuel exposure maps are likewise not provided. The lack of more detailed information on nuclide compositions with burnup will tend to limit the scope of our analyses during the pre-application phase.

At this time, it is not clear when AECL plans to provide requested detailed information on the experimental validation benchmarks to be used for assessing the computational biases and uncertainties in the results from their predictive core physics models. It is also not clear when AECL will tell us how specific tests and measurements on the first ACR-700 cores will be used for confirming or further assessing the accuracy in their predictions of CVR and related phenomena.

2. Acquiring Codes for Pre-Application Analysis of ACR-700 Neutronics

The staff's initial pre-application calculations of CVR and related neutronic phenomena in ACR-700 make extensive use of a general Monte Carlo code for neutron and photon transport (MCNP) and a commercial code developed, maintained, and marketed by the ANSWERS Software Service of Serco Assurance Corporation headquartered in Winfrith, England (MONK).

Note that AECL also makes use of MCNP as a higher-order method to help qualify the more approximate methods and models used in their IST design and safety analysis tool set, WIMS-IST, DRAGON-IST, and RFSP-IST.

The staff's own uses of MCNP and MONK are for the initial independent analysis of CVR and related ACR neutronic phenomena and for developing design-specific physical insights for the NRC's ACR neutronics PIRT (phenomena identification and ranking tables) exercise.

Insights emerging from the staff's initial analysis and PIRT efforts will be used to guide the establishment of an independent tool for analyzing ACR-700 power transients. This tool will be based on the Purdue Advanced Reactor Core Simulator (PARCS) nodal-diffusion-theory spatial kinetics code coupled with the TRACE system thermal hydraulics code. The essential step of preparing (i.e., collapsing, smearing, and parameterizing) the few-group nodal data to be used in the staff's PARCS model of ACR-700 will be done using the NRC's SCALE/TRITON lattice physics analysis sequence in combination with the recently updated SCALE/AMPX generic multi-group nuclear data libraries. Our development and testing of the resulting ACR-700 audit analysis tools and models will be completed during the design certification review phase.

MCNP is an open-source code developed and maintained at Los Alamos National Laboratory (LANL) under sponsorship of the U.S. Department of Energy. MCNP's source code and executable are freely available to all NRC staff under the terms of RES's sponsorship and use of the Radiation Safety Information Code Center (RSICC, http://www-rsicc.ornl.gov/rsicc.html) at Oak Ridge National Laboratory (ORNL).

Both MCNP and MONK are widely used to provide k-effective eigenvalue solutions to the static Boltzmann equation for neutron transport. Both codes allow exact modeling of complex three-dimensional geometries and use similarly rigorous continuous-energy treatments of neutron kinematics. A particularly useful feature of MONK is the code's ability to read input fields comprised of user-named variables and user-defined mathematical formulas. This input feature is used in this study to simplify input quality control and to automate the serial execution of parametric and sensitivity study cases. MONK's numeric printout of the variable and formula-computed input fields is also used to help check corresponding numeric inputs to equivalent MCNP models.

While MONK simulates neutron transport only, MCNP has the added capability of simulating combined neutron-and-gamma-ray transport problems in the eigenvalue mode. This MCNP capability was recently expanded to include photoneutron production, which in all heavy-water-moderated reactors such as ACR-700 contributes a significant source of delayed neutrons. While delayed photoneutrons will significantly affect the time evolution of many ACR reactivity transients (i.e., transients that we will ultimately simulate using the PARCS spatial kinetics code coupled to TRACE), photoneutrons are not expected to greatly affect the values of CVR in ACR-700, which is the focus of this study.

After using MCNP4C for our preliminary modeling work, we adopted MCNP5 as soon as it was released by RSICC in late May 2003. RES MONK eigenvalue calculations use the MONK8b code version released in December 2001. The staff's analysis work also makes occasional use of the Python object-oriented scripting language in conjunction with the Gnuplot plotting software for the analysis and visualization of code-computed results. Python, Gnuplot, and related peripheral software were acquired as free downloads from the Web. We are using Windows XP Pentium-4 laptop PCs for all MONK and MCNP calculations and for all postprocessing, analysis, and plotting of the code-computed results.

3. Acquiring Cross Section Data for Pre-Application Analysis of ACR-700 Neutronics

Data Libraries for MCNP

The MCNP code's treatment of cross section data through the energy domain is based on linear interpolation of specially formatted pointwise nuclear data. All existing pointwise data libraries for MCNP have been processed from files of evaluated nuclear data using specialized modules of LANL's NJOY code. This NJOY processing is done for specified nuclide temperatures on a hyper-fine neutron energy grid that varies from one nuclide and nuclide temperature to the next. Depending on the number of resolved resonances and the accuracy level selected in NJOY, the MCNP neutron data files for a given nuclide and temperature can have anywhere from a few hundred energy points to over 100,000 energy points. Because we have no qualified NJOY code users on the NRC staff, we will rely on outside NJOY users (e.g., at LANL or ORNL) to fill our eventual needs for updated or supplemental MCNP nuclear data for specific nuclides and temperatures.

The MCNP data libraries acquired to-date from RSICC cover a large but not comprehensive selection of neutronically significant nuclides at one or more temperatures. These libraries have been derived from the evaluated cross section data contained in Releases 2 and 6 of the Evaluated Nuclear Data File, Volume B, Version VI (ENDF/B-VI). The so-called ENDF66 library (derived from ENDF/B-VI, Release 6) that was recently released with MCNP5 is the first public-domain MCNP data library to include the 1993 corrections to ENDF/B-VI's $S(\alpha,\beta)$ bound thermal scattering data for common neutron moderating materials (e.g., light water, heavy water, zirconium hydride, beryllium oxide, graphite). It is noted that AECL has produced and uses its own proprietary MCNP library which is significantly more comprehensive than the MCNP libraries available through RSICC. AECL states that their proprietary library contains all ENDF/B-VI nuclides evaluated at several temperatures.

None of the MCNP data libraries available from RSICC include neutron data for dysprosium (Dy). For modeling the dysprosia burnable poison used in the ACR-700 fuel design, we therefore needed to acquire supplemental MCNP data for the five neutronically significant Dy isotopes. These data were provided to us in December 2002 by ORNL. At no cost to NRC, ORNL ran NJOY on evaluated data from Release 6 of ENDF/B-VI to create MCNP libraries for Dy-160, Dy161, Dy-162, Dy-163, and Dy-164 at the following temperatures: 300 K, 500 K, 700 K, 900 K, and 1100 K. However, even with this addition of Dy data, a few small yet potentially non-negligible gaps still remain in the MCNP cross section data necessary for completing an independent analysis of CVR and related neutronic phenomena in ACR-700. Such gaps exist for several weakly to moderately absorbing fission product nuclides at representative fuel temperatures. To fill these and other minor gaps in the available MCNP libraries, we have planned a small task at ORNL starting in early FY'04. This task would benefit our MCNP analyses for all reactor types and fuel cycles (e.g., including LWRs, MOX, HTGRs, spent fuel burnup credit, etc.).

Data Libraries for MONK

The MONK code uses either (a) quasi-pointwise nuclear data libraries evaluated at room temperature on a fixed hyper-fine grid of 13,189 energy groups, or (b) multi-group data libraries evaluated for variable temperatures on a fixed grid of 167 energy groups by employing a special subgroup method (i.e., akin to multi-band methods) for automatic treatment of problem-specific resonance self-shielding. The cross section libraries used by MONK are generally those provided by the ANSWERS Software Service as part of the code user license agreement. These MONK libraries have been processed from evaluated nuclear data files using appropriate NJOY modules in combination with proprietary data processing routines developed by ANSWERS.

MONK's three quasi-pointwise data libraries at room-temperature are derived respectively from Release 6 of ENDF/B-VI, Release 2.2 of the Joint European File (JEF2.2), and Release 3.2 of the Japan Evaluated Nuclear Data Libraries (JENDL3.2). MONK's 167-group library at variable temperatures is derived from JEF2.2 and is identical to the library used by ANSWERS for their commercial version of the WIMS code, WIMS8.

A key motivation for using MONK in this context lies in the unique capability it provides for checking results computed with data libraries derived from the U.S. data evaluations (ENDF/B-VI) against those computed with otherwise identical data libraries derived from the European and Japanese data evaluations (JEF2.2 and JENDL3.2). It is noted that AECL analyses mainly use data derived from ENDF/B-VI. Furthermore, selected MCNP results can be directly cross-checked against MONK results, albeit with the restriction that MONK's quasi-pointwise libraries are presently available at room-temperature only. A further restriction arises from the lack of $S(\alpha,\beta)$ bound thermal scattering data for heavy water in MONK's quasi-pointwise libraries. The procedure for MONK-MCNP cross checking under these restrictions therefore entails running equivalent room-temperature cases in which both codes approximate thermal scattering in heavy water by using the simple free-gas kernels for deuterium and oxygen. This provisional approximation neglects the upscatter-enhancing effects resulting from the D2O molecular bonds and the intermolecular forces present in condensed matter, thereby leading to a softer neutron energy spectrum.

Much as the case with MCNP, we found that none of the standard libraries available for MONK include data for dysprosium. Fortunately, when ANSWERS was informed of our need for Dy data, they immediately agreed to provide supplemental Dy cross section data for use with all of the standard MONK libraries. These supplemental data were provided at no cost to NRC in November 2002.

At the same time, ANSWERS also volunteered to extend the existing transport and depletion capabilities in WIMS8 to include Dy activation and depletion. This WIMS8 extension was completed and provided to NRC in March 2003. However, due to the continuing shortage of nuclear analysis staff in NRC, we presently have no plans to apply WIMS8 user license to ACR-700 or other advanced reactors. WIMS8 was acquired by NRR, originally in the context of the LWR MOX program, to provide an established lattice physics depletion capability to be used pending the completion of ongoing RES efforts with ORNL, BNL, and Purdue to develop and test the new TRITON-B6 lattice physics analysis sequence of the SCALE code system. While WIMS8 is obviously related to WIMS-IST (i.e., WIMS stands for Winfrith Improved Multigroup Scheme), AECL states that the respective codes and data libraries have evolved separately since the early 1980s.

4. ACR Cell and Super-Cell Calculations and Analysis

Throughout this study, we use AECL's definition of coolant void reactivity, which can be expressed as CVR={k(voided)-k(cooled)}/{k(voided)*k(cooled)} = 1/k(cooled)-1/k(voided), where k is the neutron multiplication factor.

The staff's analyses use static neutronics models of increasing detail and complexity to evaluate the predicted CVR as it is affected by modeling assumptions and by operating conditions and core configurations. These models progress from simple cell calculations of a repeating two-dimensional core lattice of identical fuel channels, to super-cell calculations of a repeating three-dimensional core lattice comprised of several neighboring fuel channels with transverse reactivity devices, and finally to full three-dimensional models of the ACR-700 core. This modeling progression corresponds conceptually to the sequences of models used by AECL for fuel lattice physics, reactivity device lattice physics, and full-core physics analysis, respectively. Our analyses will ultimately include selected cases with independent calculations of the nuclide compositions in irradiated fuel.

While awaiting the RAI responses from AECL, we were able to develop and test some preliminary "strawman" models of a simplified ACR lattice cell. We started by modeling a simple test case consisting of an infinite lattice cell with cold, unirradiated equilibrium-reload fuel in the presence of cold, unpressurized coolant and moderator. The estimated dimensions and compositions used in the strawman model were based on partial information gleaned from AECL handouts and from caliper measurements we made on the loaned ACR channel mockup. With these initial test models, both MCNP and MONK computed a CVR that was strongly positive (i.e., >2 dollars). These unexpected results from our preliminary models highlighted the need for accurate ACR design information and models while also providing an early indication of the sensitivity of CVR to variations in the core lattice and its modeling.

Other activities initiated before we received the RAI responses included the preliminary development and testing of Python-Gnuplot scripts for use in extracting, post-processing, and plotting the MCNP- and MONK-computed energy spectra of neutron fluxes and nuclide reaction rates. We plan to further develop and use these post-processing analysis capabilities to present the NRC ACR-700 PIRT participants with independent insights into the detailed phenomenology of ACR-700 core neutronics and the CVR.

In late June 2003, we revised the simple strawman cell models to reflect some of the design and operating information provided in AECL's first RAI response package. With these revised cell models, the CVR for a code-to-code test case with coolant and moderator at room temperature (293 ^{o}C) and nominal operating densities described above was calculated by MCNP and by MONK, with its three different quasi-pointwise libraries, as very slightly positive, with values ranging from +0.0019 (± 0.0005) to 0.0008 (± 0.0005). [Disclaimer: The CVR computed with this simple test model of an infinite lattice of fresh equilibrium-reload fuel is not intended to closely approximate the CVR of any real configuration of the ACR-700 core. First, because neither MCNP nor MONK provide for buckling corrections, all such lattice cells and super-cells modeled with MCNP and MONK inherently neglect the CVR-reducing effects of neutron leakage. More importantly, the neutronics of a modeled core or core lattice of fresh equilibrium-reload fuel clearly bears little resemblance to any of the initial, transitional, or equilibrium core configurations of ACR-700.]

In July 2003, the staff extended the MONK model of the simplified ACR lattice cell to investigate two fundamental lattice modeling issues. The first issue concerns the potential need to consider systematic variations of neutron flux, fission power, and burnup as a function of the azimuthal position of fuel pins within the ACR fuel bundle. Specifically, we postulated that, in relation to conventional CANDU lattices, the reduced amount of moderator between fuel channels in ACR could give rise to more significant azimuthal power and burnup variations within bundles. Such variations cannot be treated by AECL's approximate WIMS-IST cell models, which use the simplifying approximation of a white boundary condition applied to an equivalent (i.e., mass conserving) circular cell boundary instead of the more accurate use of specular reflective (or periodic) boundary conditions applied to the square boundary surfaces of the true lattice cell. Our MONK results, using accurate square cell boundaries with specular reflection, have revealed azimuthal variations so slight (<2%) that they are difficult to resolve with a Monte Carlo model.

The second modeling issue that we analyzed in July is an extension of the first, in that it evaluates the potential effects on bundle azimuthal power distribution that would arise from the expected sagging of the pressure tube within the calandria tube. To properly investigate this modeling issue, we had to change the boundary conditions on the top and bottom boundary surfaces of the square lattice cell from mirror-reflective to mutually periodic, thereby keeping the modeled direction of sagging consistently downward. Again, even for the extreme case of sagging into near contact with the calandria tube, the azimuthal variation of pin powers was found to be very slight (<2%). Work to cross check these MONK model results against results from equivalent MCNP models is now underway.

The staff's present work in this area also includes: (a) revising our models of the simple ACR lattice cell to address hot operating temperatures and pressures as well as the three irradiated fuel compositions provided in AECL's RAI response package, (b) preliminary development and testing of a super-cell model with multiple channels and transverse reactivity devices, and (c) preliminary development of a simplified full-core model. We are now in the process of compiling a summary table of completed and planned models and modeling cases. The resulting table will be included in future progress updates.

5. ACR Fuel Depletion Calculations and Analysis

As noted above, our initial calculations make use of the irradiated ACR fuel compositions as predicted by AECL at three selected burnup points.

NRC plan to contract ORNL in early FY'04 to perform our first independent calculations of ACR irradiated fuel compositions. The ORNL calculations will use GP-TALLY, a recently developed code that combines a rigorous MCNP-based flux solver with a nuclide transmutation solver based on a specially updated version of the ORIGEN code. Scoping and parametric modeling studies with GP-TALLY will provide a basis for evaluating and qualifying the more approximate methods that SCALE/Triton will later use for producing the nodal data tables needed by our future PARCS models of ACR-700.

6. ACR-700 Full-Core Calculations and Analysis

We are presently in the early experimental stages of developing simple full-core ACR-700 models with MCNP and MONK. Given the shortage of nuclear analysis staff, our plans in this area include collaborating with ORNL on the completion and application of more detailed and accurate MCNP models of the ACR-700 equilibrium core. Such models will be used to investigate full-core modeling issues in evaluating the effects of neutron leakage and localized core phenomena on CVR. Schedules for completing work in this area during the pre-application versus design certification review phases are subject to FY'04 contract funding priorities and uncertainties.

7. CVR-Related Benchmark Calculations and Analysis for ACR-700

At this time, it is not clear when AECL plans to provide requested detailed information on the experimental validation benchmarks to be used for assessing the computational biases and uncertainties in the results from their predictive core physics models. It is also not clear when AECL will tell us how specific tests and measurements on the first ACR-700 cores will be used for confirming or further assessing the accuracy in their predictions of CVR and related phenomena.

Noting the small nominal value of the ACR-700 designer's targeted negative CVR, we anticipate that the assessment of prediction bias uncertainties will weigh heavily in our considerations of AECL Focus Topics 3 and 9 (i.e., pertaining to neutronics validation data base and negative CVR, respectively). For example, in the case of sparse validation data or validation based on questionable or marginally representative benchmark measurements, one might ultimately conclude that the derived uncertainties in the prediction bias are potentially larger than the small nominal value of the predicted negative CVR.

Assuming that sufficient and timely information is provided by AECL, full-core models will also be developed for some of the benchmark experiments that AECL is using to validate and bias-adjust the computed CVR in ACR-700. Working in collaboration with related efforts at ORNL, the staff will use these models to evaluate the applicability of selected benchmarks in terms of phenomenology and associated sensitivities and uncertainties.

Pre-application activities to support final recommendations on the benchmark evaluation and treatment of ACR void reactivity bias uncertainties will be completed during the design certification review phase. The NRC will provide a report summarizing the insights gained from our pre-application review and analysis activities in this area no later than July 30, 2004.