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Reactor Core Simulations in Canada

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This review will address the current simulation flow-chart currently used for reactor-physics simulations in the Canadian industry. The neutron behaviour in heavy-water moderated power reactors is quite different from that in other power reactors, thus the core physics approximations are somewhat different. Some codes used are particular to the context of heavy-water reactors, and the paper focuses on this aspect. The paper also shows simulations involving new design features of the Advanced CANDU Reactor™ (ACR™), and provides insight into future development, expected in the coming years.

KEYWORDS: code development, validation and verification, core simulations, heavy-water reactor, reactor physics.

1. Introduction

In this paper, we will review the methodologies and codes that are used in Canada to achieve accurate numerical simulations of reactor cores. The extensive experience gained from the operating CANDU® reactors has been used for the design of new reactors, such as the Advanced CANDU Reactor (ACR-700)™. In these new core designs, the basic features of CANDU reactors have been kept (separate low-pressure, low-temperature heavy-water moderator; on-power refuelling). However, to achieve a much-reduced capital-cost target, and at the same time make the void-reactivity coefficient negative, the ACR has evolved from the original CANDU design to include other features (CANFLEX® slightly enriched uranium-oxide fuel bundles, dysprosium burnable absorber in the central fuel element, light-water coolant, much smaller lattice pitch). Engineering studies for the new ACR design rely on a modern set of computer codes, and require validation of the codes against experimental data.

This paper focuses on specific validation results important to CANDU cores: reactivity-device inter-calibration, prediction of fuel exit burnup, etc. In section 2, we describe the code suite available and currently used to perform core simulations. Section 3 addresses the accuracy of reactor physics simulations for CANDU reactor design and operation; this section will also present new design features and how the standard code suite analyzes these design features. Section 4 is devoted to a discussion of newer code developments, interfaces and packages needed to maintain state-of-the-art nuclear engineering practices. Finally, in the last section, we draw conclusions.

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2. Software currently used in Canada

2.1 Industry Standard Toolset (IST)

Reactor-physics calculations for CANDU reactors consist of three stages:

- Calculation of lattice properties for the basic “bare” CANDU cell, which includes fuel bundle, coolant, pressure tube, gas gap and calandria tube, and the appropriate amount of moderator, but which excludes any interstitial reactivity device;
- Calculation of “incremental” cross sections of reactivity devices, which represent the effect of such devices, and which are added to the basic lattice cross sections in a modelled volume around the reactivity device;
- Modelling of the entire reactor core in three dimensions, and calculation of the core-wide flux and power distributions.

Computer codes to perform these calculations were developed specifically for CANDU reactors from the earliest days. These codes contributed to the excellent design and performance of the operating CANDU reactors, from Ontario’s multi-unit stations at Pickering and much larger Bruce and Darlington reactors to the single-unit CANDU-6 reactors in Québec, New Brunswick, Argentina, Korea, Romania and the latest proud addition to the family, the two CANDU-6 reactors in Qinshan, China.

POWDERPUFS-V [1], a semi-empirical lattice code based on the results of research-reactor measurements for natural-uranium-fuelled, heavy-water-moderated lattices, was used until the last few years for lattice calculations for all CANDU reactors. While POWDERPUFS-V has served CANDU designers and operators extremely well over the years, its empirical basis, the lack of its foundation in formal neutron-transport theory, and its applicability to natural-uranium-fuelled cores only, have led to it being supplanted in the last few years by **WIMS-AECL** for safety analysis and for the design of the ACR and of Advanced Fuel Cycles for CANDU.

In fact, in the last several years the Canadian nuclear industry has established an Industry Standard Toolset (IST) of computer programs, which are the basis of the common tools used by the industry for safety analysis, including computer codes for each of the three stages of reactor-physics calculations listed above. The industry is also migrating toward the use of these codes for routine station operations. The reactor-physics computer codes in the IST are:

- **WIMS-IST** [2]: a 2-D lattice-cell code (a version of WIMS-AECL) used for transport calculations and cross-section condensation in CANDU cells; this code provides the homogenized cell cross sections for any type of fuel;
- **DRAGON-IST** [3,4]: a 2-D/3-D cell and supercell code used for transport calculations and for the computation in 3D of the incremental cross sections for CANDU reactivity devices, which are perpendicular to the fuel channels;
- **RFSP-IST** [5]: a reactor code for CANDU full-core 3-D static and dynamic analysis, currently in 2 energy groups. RFSP-IST contains a diffusion-theory solver, but it can also perform flux-mapping calculations. For core-follow applications, it is run at the operating stations 2 or 3 times per week, and the results it provides for the 3-D flux, power, and burnup distributions are used by the fuelling engineer to schedule the channels that are to be refuelled on-power in the next few days. RFSP-IST is also used in design and safety-analysis applications. For kinetics analysis, the *CERBERUS module of RFSP-IST can also be coupled to a thermalhydraulics code, such as CATHENA [6].

2.2 Other recent code developments and hybrid studies

New software and/or methods are also needed to assist and broaden the scope of day-to-day simulations. There are new developments, both at AECL and at École Polytechnique, associated with the reactor-physics tools, to increase accuracy or implement new calculation methods, namely:

- **WIMS-AECL**: building new cross-section libraries, refinement of the self-shielding treatment as well as the geometric modelling;
- **DRAGON-EPM**: inclusion of the 3-D characteristics solver with anisotropic scattering [7], extension in the geometry treatment, improvement in the self-shielding treatment, calculation of discontinuity factors; open-source downloads at http://www2.polymtl.ca/nucl/
- **NDF-EPM**: new multigroup reactor code for reactor-transient analysis including nodal methods, discontinuity factors and a full P_1 solver;
- **RFSP-IST**: new methods being studied for implementation are the use of discontinuity factors, a micro-depletion method for history-based local-parameter calculations, and a multigroup solver. Discontinuity factors at cell edges have been in use in the LWR industry and have increased the accuracy of diffusion calculations; their usefulness in calculations for the ACR will be investigated. The micro-depletion methodology allows history-based local-parameter calculations, i.e., calculations that take into account the different local conditions (such as coolant density, fuel temperature, absolute power level, etc.) at various locations in the core, as well as the history of these parameters throughout the reactor's operating history. In the micro-depletion methodology, the depletion equations are solved for each fuel bundle individually within RFSP-IST, using local lattice conditions, thus providing consistency between cell properties and full-core results. The multigroup solver will be useful for comparing reference 2-group results of ACR calculations or advanced fuel cycles.

In addition to the applications of IST codes, greater and greater use is being made of Monte Carlo analysis: **MCNP 4C** [8] is being used for special applications in both lattice and full-core calculations, and for benchmarking of other codes. We will now show the accuracy of this code suite in the context of CANDU reactors.

3. Reactor Physics Simulations Using the Industry Standard Toolset

This section provides some examples of the validation of the reactor physics toolset with data from power-reactor measurements, as well as the use of this toolset for ACR analysis. Much of the validation was documented in Reference 9. The validation includes core-tracking calculations, time-average calculations, and time-dependent kinetics calculations. The accuracy of the nominal core-state flux shape calculations has been demonstrated through core-follow simulations, and the accuracy of the delayed-neutron kinetics modelling has been demonstrated through shutdown-system-test simulations. Validation of flux-shape calculations by comparison with in-core detector readings (vanadium detectors and reactor overpower [ROP] protection-system detectors) has been extensive.

3.1 Core-Follow Simulations

The application of RFSP-IST to core-follow simulations was tested at an early stage of development using the two-energy-group WIMS-IST/RFSP-IST methodology. A one-year period of operating history of the CANDU 6 reactor at Pt. Lepreau was tracked. The accuracy of the flux-shape calculations performed was demonstrated by comparing computed and measured fluxes at the 102 inc-core vanadium detectors. The standard deviation of differences between the computed and measured fluxes at each snapshot simulation was around 3%. The excess reactivity, representing a small bias in the computed k_{eff} from criticality, was stable and experienced no divergent trend. The predicted maximum channel and bundle powers were consistent with those previously obtained using the conventional PPV/RFSP methodology. The consistency of these parameters (excess reactivity and vanadium fluxes comparisons) shows the code stability and convergence for routine core-follow.

The average exit burnup is another key feature of core-follow related to the fuelling rate, and thence to the fuelling cost and the economy of power generation. The burnup calculation in the Time-Average module of RFSP-IST was validated against Pt.-Lepreau data from one year of operation. Most of the refuellings performed in this period used an eight-bundle-shift scheme; the total number of bundles discharged was 5486 over the period. The computed average exit burnup was then compared to the actual burnup achieved at site over that time period. The following results were obtained:

- The time-average bundle feed rate was 15.34 bundles/FPD, which compared very well with the "measured" fuelling rate for the 12-month operating history, 15.24 bundles/FPD.
- Vanadium-detector fluxes from the time-average calculations reproduced very well the year-average vanadium measurements. The average difference over the 102 detectors was about -0.18 %, with a standard deviation of 3.1%, consistent with the results obtained in other core-follow simulations.

3.2 Static Reactivity-Device Modelling

The modelling of CANDU reactivity devices in RFSP-IST, using device incremental cross sections generated through 3-D neutron–transport calculations with the DRAGON-IST code, has been successfully validated against ZED-2 experiments and against device-calibration tests in power reactors. We present here, as an example, the comparison of predicted reactivity worth of light-water liquid zone-controllers (LZC) in Pickering-A Unit 4 with measurements performed during Phase-B commissioning, with fresh fuel and at low reactor power. Tables 1 and 2 give results with all adjuster rods inserted in-core and out-of-core respectively. The average simulation error and standard deviation are –4.2 ± 5.9% in the configuration with all adjusters inserted, and –6.3 ± 2.6% with the adjusters withdrawn. The methodology was also validated for other devices: adjuster rods in Pickering-A Unit 4, and shutoff rods (SOR) and mechanical-control absorbers (MCA) in Darlington NGS-A Unit 4.

3.3 Validation of Kinetics Calculations

The accuracy of the full-two-group kinetics formalism in the *CERBERUS module of RFSP-IST has been demonstrated using flux/power run-down data from a shutdown-system-1 (SDS1 ≡ cadmium shutoff rods) test in the Pt.-Lepreau reactor, which was performed from an initial power of 75% full power. The fluxes were measured by fast in-core platinum detectors and by out-of-core ion chambers. The level of agreement obtained is illustrated here with two examples: the measured and calculated log-rate signals for an ion chamber (Figure 1) and the measured and calculated fluxes at an in-core detector, actually associated with the liquid-poison-injection shutdown system 2 (Figure 2).

3.4 New design features for the ACR

The ACR design has evolved from the original CANDU: new design features include the use of slightly enriched uranium fuel in the CANFLEX fuel bundle, dysprosium burnable absorber mixed with natural uranium in the central element of the fuel bundle, light-water coolant, and smaller lattice pitch. We now give some IST results pertinent to this new reactor core. Figure 3 compares the natural-uranium CANDU and ACR lattices in terms of the lattice pitch (LP), the pressure-tube (PT_{OR}) and calandria-tube (CT_{OR}) outer radii, and the moderator-to-fuel volume ratio (VM/VF). The small ACR lattice results in a highly compact core, with significant savings in D_2O cost. The reference ACR-700 design [10] produces 731 MWe from 284 fuel channels in a 5.20-metre-diameter calandria By comparison, the current CANDU 6 has 380 fuel channels in a 7.6-metre-diameter calandria and produces 728 MWe.

The ACR-700 incorporates many advanced features that enhance reactor licensing. One of the most significant differences between the ACR-700 and the current CANDU reactors is that the ACR-700 is designed to have negative full-core coolant-void reactivity (CVR) under nominal operating conditions. This slightly negative CVR eliminates the power pulse during a postulated Loss-of-Coolant-Accident (LOCA) that is present in current CANDU reactors. A full-core LOCA simulation was performed with the *CERBERUS (kinetics) module of RFSP-IST with lattice properties at different locations in core calculated with the WIMS grid-based (local-parameter) methodology. Figure 4 shows the power transient for a postulated full-core LOCA scenario where 99% of the coolant in the core is voided within two seconds. Because of the negative CVR, reactor power decreases automatically upon LOCA, even without the intervention of the safety systems.

Another significant feature of the ACR-700 is a naturally flat thermal-flux distribution across the core. Figure 5 shows the radial thermal neutron flux distributions in the ACR-700 and the CANDU 6, as calculated with RFSP-IST. The flux-flattening effect of the adjuster rods is clearly seen in the CANDU 6. No adjuster rods are required in the ACR, because of the flat flux distribution. The stability of the flat radial thermal flux distribution in the ACR can be attributed to the peak in the reflector region, where large numbers of fast neutrons incident from the core region are moderated to the thermal range. This inherently flat and stable radial flux shape through the reactor core region enables the ACR-700 to operate with a very high radial power form factor (average to peak channel power ratio) of 0.95, requiring only small adjustments in the fuelling rates between the inner and outer core regions.

4. New tools for better core design and simulations

The validation of the reactor-physics Industry Standard Toolset has progressed to an advanced stage. A few gaps identified in the validation program are currently being addressed. The majority of the functionalities required of the code suite have been tested and shown to give reasonable results when compared with site measurement data. This ensures that the design and operation software used for CANDU reactor physics simulation is accurate. The migration to the WIMS-IST/DRAGON-IST/RFSP-IST methodology for safety analysis is complete, and utilities are considering the use of the toolset for day-to-day fuel management analysis.

Current industry projects now aim at extending the software packages into scalable tools with even more advanced computational methods, compatible with modern computer resources, and to increase the productivity of code users by providing clear and well-documented interfaces between codes.

4.1 Changes in the IST code suite

Enhancements being made to the code toolset were outlined in Section 2.2. Re-engineering IST codes is not an easy task. These codes consist of hundreds of thousands of FORTRAN-77 lines, and they have undergone extensive validation. Frozen versions of the codes are covered by strict quality-assurance procedures, and changing the coding (creating and issuing new versions) requires careful planning, change control and strict version control, verification and validation, and good documentation. In the future, work may tend towards providing enhanced versions of some codes: modular code structures may or will migrate to the newer FORTRAN-95 standard or other object-oriented coding, allowing most computational modules to be kept almost as they are, but providing a modern way of encapsulating data structures. Corrective and adaptive maintenance on the enhanced software will be made easier in the ever-changing environment of modern computers, enabling the use of improved computing environments (clusters and dedicated high-performance computing machines). Finally, newer developers will be able to harness and extend IST software without being bored by memory leaks, bad pointers and all unattractive features of low-level programming languages.

4.2 Other pertinent software tools

It is now desirable or even necessary to add pertinent graphical user interfaces (GUI) and modern visualization tools for analyzing 3D results of core simulations. Code development in these areas is of primary importance for next-generation CANDU nuclear engineers. A prototype of a portable and user-friendly interface tool, using modern client/server software construction with XML data exchange, can be found on the D2G2 project home page at http://www.d2g2.polymtl.ca/.

The coupling of codes is more and more necessary for fine-grain studies involving physics code-to-code interactions. Code users now require that software pieces be interfaced with one another, as well as with thermalhydraulics codes, in order to perform extensive simulations. The Canadian nuclear industry is currently involved in various studies on hybrid calculations schemes that are necessary for new core design.

5. Conclusion

The IST code suite and other related software developed in Canada have matured into industrial applications, offering reliable tools for designing and operating CANDU reactors. An important challenge is now to extend the package on key points where accuracy can still be improved: better cross-section data, finer transport calculations, etc. Another issue is to provide users with tools to harness the tremendous output data that simulations can produce.

Acknowledgements

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Table 1 - Liquid-Zone-Controller Reactivity Worth with Adjusters "In-Core"

Boron (ppm)	Boron Reactivity Change (mk)	LZC Fill (%)	Calculated LZC Reactivity (mk)	Simulation Error (%)
9.850	0.00	88.4	0.00	-
9.906	0.39	74.3	0.42	+7.7
9.963	0.79	65.0	0.73	-7.6
10.019	1.18	56.1	1.05	-12.4
10.076	1.58	45.0	1.51	-4.4
10.132	1.97	38.5	1.82	-7.6
10.189	2.36	29.3	2.28	-4.2
10.245	2.75	21.0	2.73	-0.7
Average				-4.2 ± 5.9 %

Table 2 - Liquid-Zone-Controller Reactivity Worth with Adjusters "Out-of-Core"

Boron (ppm)	Boron Reactivity Change (mk)	LZC Fill (%)	Calculated LZC Reactivity (mk)	Simulation Error (%)
11.261	0.00	91.4	0.00	-
11.317	0.39	79.4	0.36	-7.7
11.374	0.79	68.4	0.71	-10.1
11.430	1.18	56.8	1.12	-5.1
11.487	1.57	48.4	1.44	-8.3
11.543	1.97	38.5	1.85	-6.1
11.599	2.36	30.0	2.24	-5.1
11.656	2.75	19.9	2.71	-1.5
Average				-6.3 ± 2.6 %

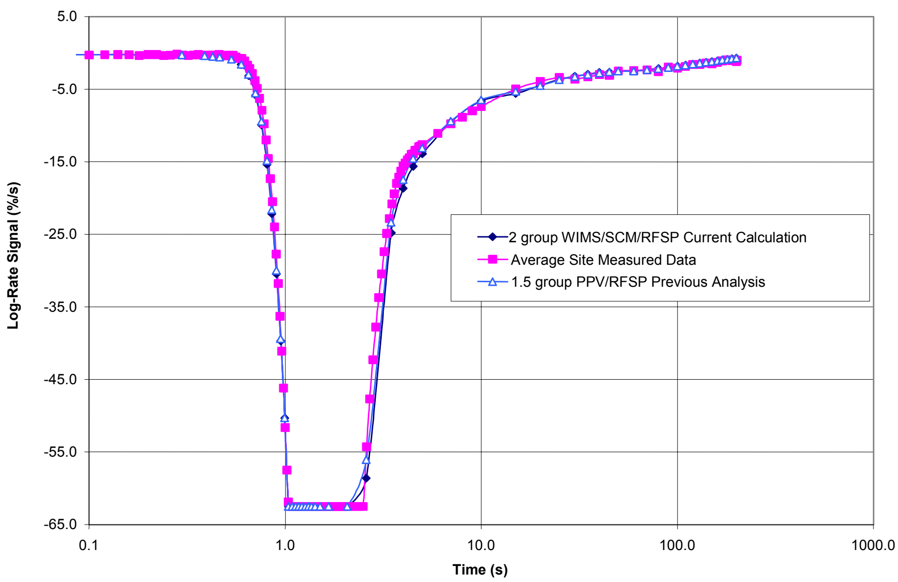

Fig. 1 Comparison Between Measured and Calculated "Log-Rate Signal: Ion Chamber H"

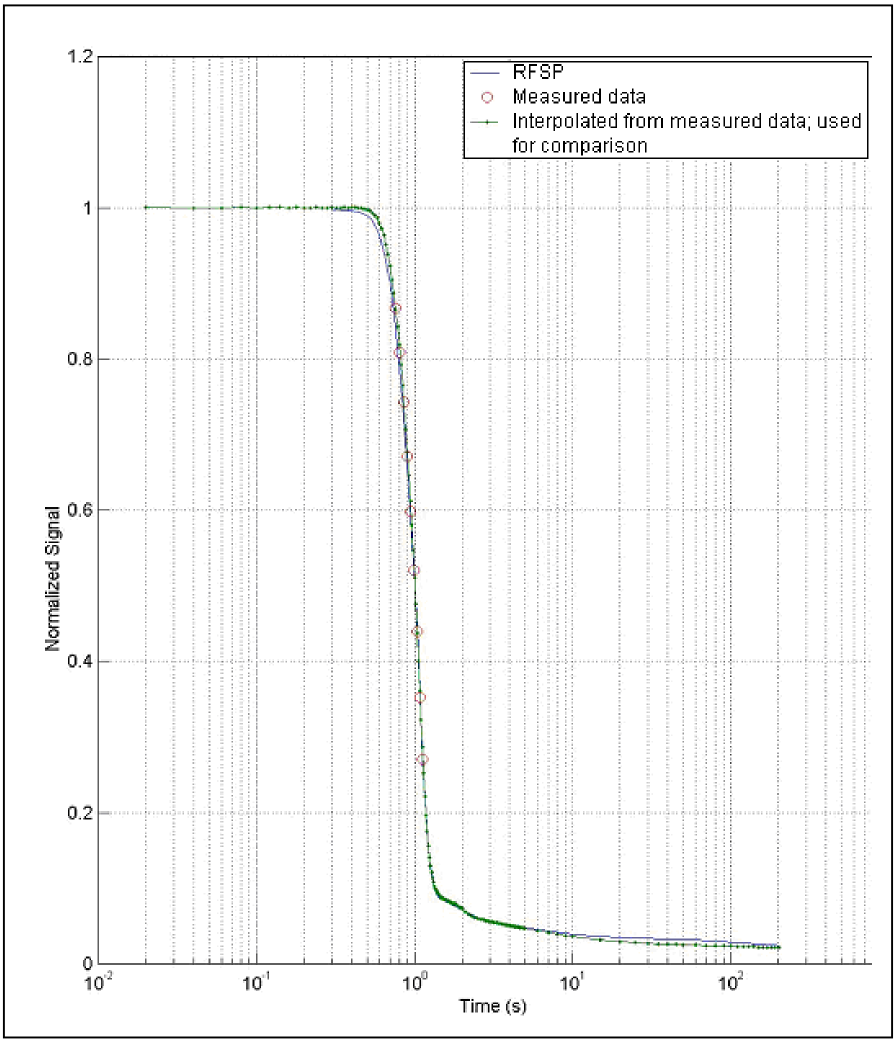

Fig. 2 Comparison Between Measured and RFSP-Calculated Signals: SDS2 Detector 5J

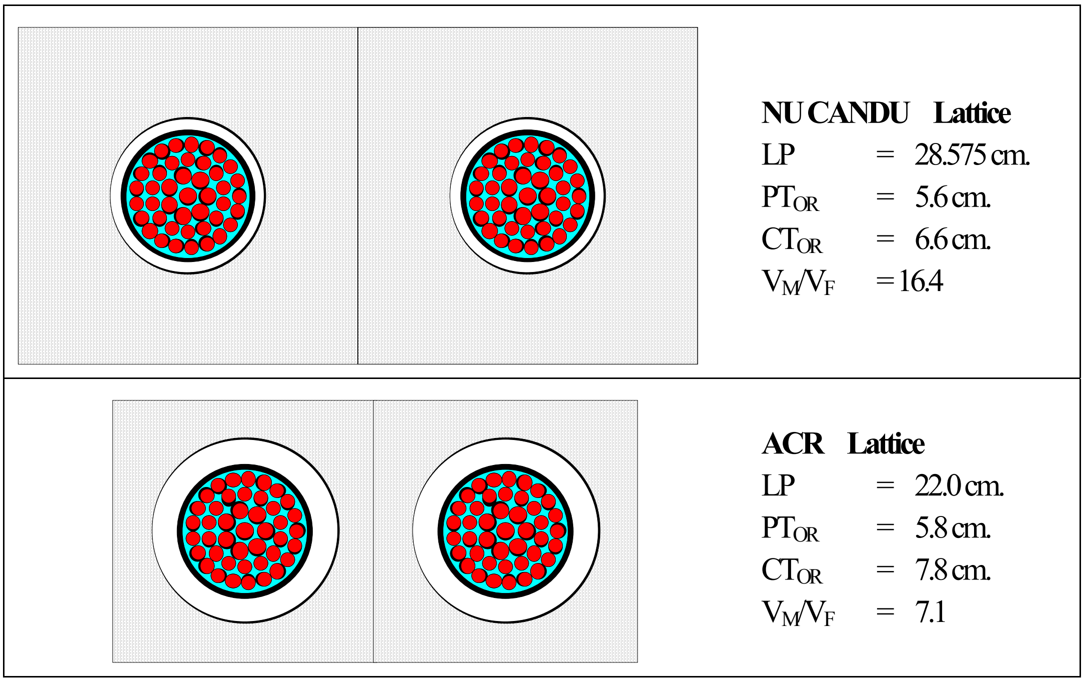

Fig. 3 ACR and NU CANDU Lattice-Cell Configurations

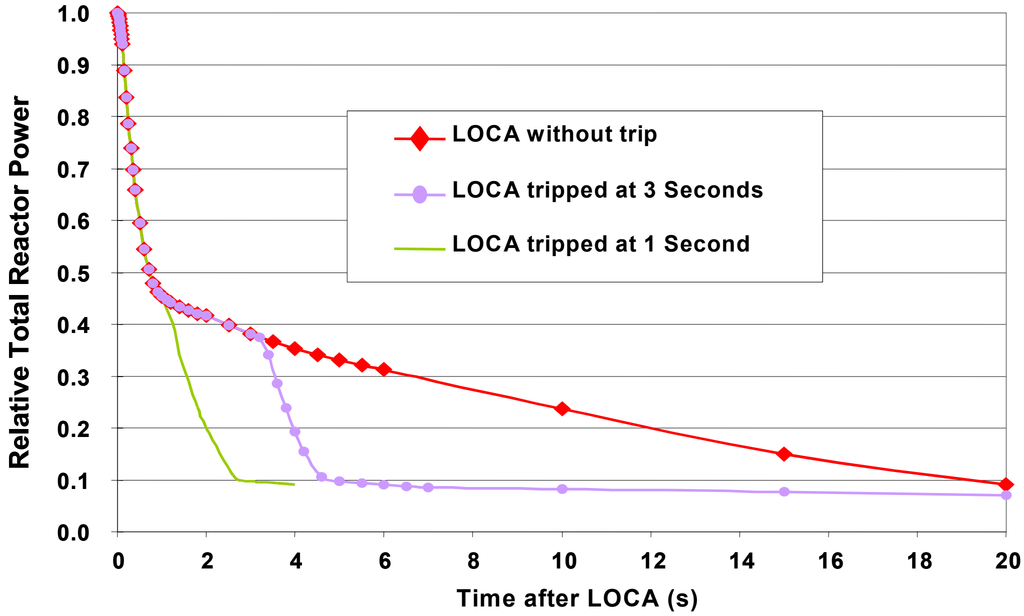

Fig. 4 Reactor Power Transient in ACR-700 After Full-Core LOCA

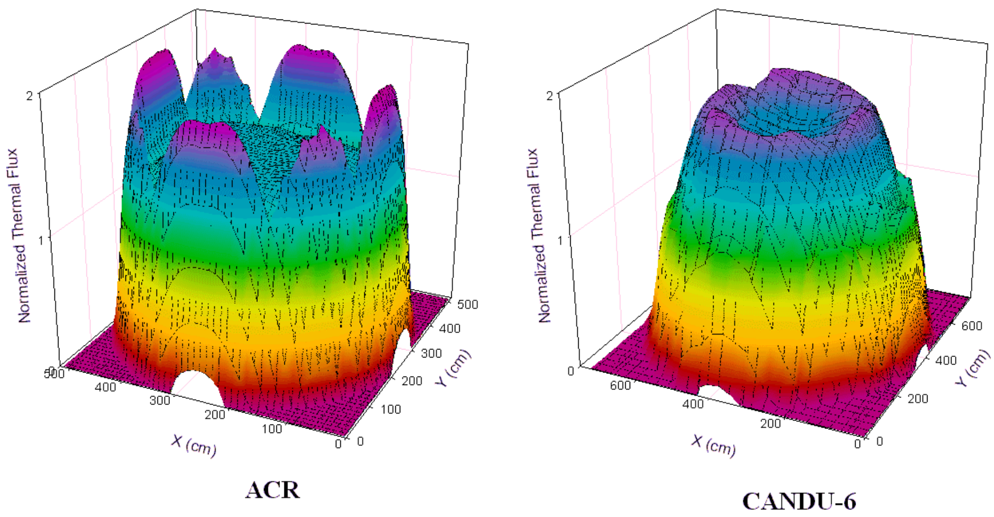

Fig. 5 Radial Thermal Flux Profiles in ACR-700 and CANDU-6