

Physics Codes and Methods for CANDU Reactor

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Abstract

This paper presents an overview of the physics codes and methods that are in current use at AECL for physics design and analysis of CANDU[®] reactors. The 3 levels of calculations - lattice-cell, “supercell” and finite-core - are discussed, with references to the computer codes used in each step. The theoretical formulation and representation of the physical processes at each level of the analysis and the solution methods used are also explained.

1. Introduction

The physics of CANDU (CANada Deuterium Uranium) reactors is based on extensive measurements of physical parameters in heavy-water-moderated lattices typical of CANDU reactor design. It is also based on design calculations using theoretical methods tested against these measurements. The calculational tools developed, in the form of computer codes, are based on numerical models that recognize specific features of CANDU neutronics. These computer codes are also kept under constant scrutiny and review, to ensure the accuracy of their predictions.

This paper presents an overview of the physics codes and methods that are currently used at AECL for physics design and safety analysis of CANDU reactors. In the design stage, the primary analysis objectives are:

- a.* To model the steady-state core and to determine the global flux and power distributions, without accounting for the detailed variations caused by channel refuelling. The essentially daily on-power refuelling operations superimpose power ripples on top of an otherwise constant power shape;
- b.* To determine the core response to various perturbations such as changes in temperature or other lattice conditions;

- c.* To establish the configuration and neutronic characteristics of control and shutdown devices, which will ensure that they meet their functional requirements;
- d.* To study behaviour of the core in both slow and fast transients, such as xenon transients originating from normal operational maneuvers or postulated accidents, e.g. a large loss of coolant. The analysis of hypothetical accidents is performed in support of safety analyses, to characterize the reactor's dynamic response, accounting for delayed-neutron effects and the action of the fast-acting shutdown systems.

Physics calculations are also performed in support of normal reactor operation. The objectives in these specific applications are:

- a.* To track the reactor operation history in terms of power production, channel refuellings, fuel-bundle movements, in-core power and burnup distributions, and discharge burnup;
- b.* To ensure that the peak channel power and bundle power comply with the licensing limits;
- c.* To establish the maximum channel-power peaking factor due to refuelling ripples;
- d.* To facilitate the judicious choice of fuel channels scheduled for refuelling.

There are three levels or steps of calculations in the analyses performed to achieve these objectives:

1. The CANDU core consists of a lattice of fuel channels arranged in a square array of fixed spacing (the "lattice pitch"). Each lattice cell, consisting of a fuel bundle, the coolant, pressure and calandria tubes, and moderator is therefore a basic unit in building a reactor core model, with its neutronics characteristics represented by a set of "homogenized nuclear reaction cross sections" determined from lattice-cell calculations. The first step is therefore to determine these homogenized lattice-cell properties, which are dependent primarily on the isotopic composition of the fuel.
2. In a reactor-core model, a mesh structure is set up in Cartesian geometry to delineate the lattice cells and the interstitial reactivity devices. The reactivity devices are modelled by modifications ("incremental cross sections") to the basic-lattice properties in the mesh regions in the immediate vicinity of the devices. These modifications represent the effect of the presence of the devices as changes in the various reaction cross sections, and are determined in "supercell" calculations. A supercell model is a subregion of the reactor, consisting typically of 2 neighbouring basic-lattice cells with a device in the interstitial position; the supercell is used to calculate the device incremental cross sections.
3. The core model is then assembled according to the lattice arrangement, the device positions, and the fuel composition in various basic-lattice cells, with appropriate nuclear cross sections (incorporating device incremental cross sections) assigned to the various mesh regions in the model. The mathematical equation governing the neutron

transport is solved numerically to give the flux and power distributions. In static calculations, delayed neutrons are not explicitly represented, although their effect is included since the concentrations of delayed-neutron precursors being proportional to the neutron flux. In transient calculations, the concentrations of delayed-neutron precursors are explicitly accounted for as separate variables in the equations being solved.

With regard to the calculation methods that are used to determine the spatial and spectral distribution of the neutrons, different levels of approximations in the neutron-balance formulation are used in the basic-lattice cell and in the whole core. The degree of sophistication of the mathematical formulation and the solution method are commensurate with the accuracy requirements of the specific calculation. For typical lattice-cell and supercell calculations, the multigroup integral-transport equation is solved, using the collision-probability method. For finite-core simulations, the neutron-diffusion equation is solved, in its time-independent form for steady-state problems or its time-dependent form for transients. Experience has shown that there is no advantage in performing finite-core analysis of the heavy-water-moderated CANDU in more than 2 energy groups. The use of 2 energy groups has made it possible to model the core accurately in 3 dimensions.

Another method of analysis, often used for core tracking, is off-line flux mapping. This uses the readings of 102 vanadium flux detectors which are present in the CANDU 6 core. The primary use of these detectors is for on-line flux mapping by the reactor regulating system (RRS) to calibrate zone-control detectors to region-wise average fluxes; but in off-line flux mapping they allow calculations to reflect as accurately as possible the measured spatial flux distribution.

The Monte Carlo method is also used in special applications, such as the calculation of the axial flux peaking near the bundle junctions and in the design of small research reactors. It will not be discussed further here.

The rest of this paper will review the three levels of physics calculations, the computer codes used, the solution methods, and the capability and accuracy of the codes.

2. Lattice-cell Calculation Methods

Since the early days of CANDU prototypes, there has been a need for a fast and reasonably accurate cell code for survey and design purposes. The POWDERPUFS-V (PPV) code^[1] was developed to meet these requirements. The cell is treated in a very simple manner. The following approach is used.

- a.* The lattice cell divided into 3 main regions: a fuel-and-coolant region, an annulus (pressure-tube, gap and calandria-tube) region, and a moderator region.

- b.* The conventional 4-factor formula with 2-energy-group leakage is used for the neutron balance.
- c.* The nuclear cross sections for the heavy isotopes are based on the Westcott convention, in which the neutron spectrum consists of a Maxwellian distribution and a 1/E “tail”. These cross sections are characterized by two spectral parameters: the epithermal-to-thermal ratio and the neutron temperature. For other materials, constant input or simple recipes with correction terms for spectral effect are used.
- d.* Resonance integrals are determined in a semi-empirical manner fitted to experimental results.
- e.* Fast fission is taken into account only in ^{238}U , and is lumped into the thermal fission cross section.
- f.* Saturating fission products, characterized by high absorption cross sections, are explicitly tracked. Other, non-saturating, fission products are represented by 3 pseudo-fission-product groups, each with an effective absorption cross section.

The PPV program has the following capabilities:

- a.* It calculates the 4-factor parameters and the infinite and effective multiplication factors, the diffusion coefficients, the conversion ratio, and isotopic compositions as functions of fuel irradiation.
- b.* It produces 2-group homogenized-cell lattice properties for use in full-core calculations.
- c.* It can be used to calculate the reactivity effect of a “perturbation” (instantaneous change) in selected lattice parameters. This calculation is essential in predicting various reactivity coefficients and other important quantities such as the reactivity change on loss of coolant.

The PPV code has a unique “reaction-rate-average” capability, which performs a lattice cell calculation using the nuclear properties obtained by reaction-rate-weighted averaging over a range of fuel irradiation, typically from zero to exit irradiation. This option allows the determination of the nuclear characteristics similar to that of a whole core in which the fuel bundles have various stages of irradiation as is typical in a CANDU reactor.

In recent years, there has been a need to employ a lattice code based on fundamental physics principles and on a more rigorous representation of the physical processes. The need arises especially when advanced fuel-bundle designs and advanced fuel cycles are considered. The WIMS-AECL code ^[2] has been designated for use in the design and analysis of next-generation CANDU reactors. WIMS-AECL evolved from the general-purpose multigroup transport lattice-code WIMS-D4 ^[3], and has the following specific features for CANDU applications:

- a. It performs multigroup neutron-transport calculations in 2 dimensions, with explicit representation of the fuel-element cluster. The collision-probability solution of the integral form of the neutron transport equation is adopted as the standard method.
- b. It accounts for resonance shielding effects that depend on fuel composition and geometry.
- c. The nuclear data utilized in WIMS-AECL is stored in libraries external to the code. Typically, 89-energy-group ENDF/B-V or -VI libraries are used.
- d. The neutron source from scattering is assumed isotropic. The in-group scattering cross sections are transported-corrected.
- e. The radial and axial directional diffusion coefficients are based on the standard Benoist theory accounting for streaming effects.
- f. The code has a search capability for energy-group-independent critical buckling, and the homogenized-cell critical spectrum can be obtained with a variety of leakage treatments.

3. Supercell Calculation Methods

Several types of reactivity devices are used in the CANDU core. These devices are placed perpendicular to the fuel channels, and their presence influences the flux level in nearby fuel channels. The separation of the device and the fuel is typically about a few transport mean free paths. The spectral effect on the fuel due to the presence of a nearby device is not expected to be significant. This assumption allows certain simplifications in the supercell methodology used to model the devices.

The primary purpose of supercell calculations is to generate incremental cross sections that are superimposed onto the basic-cell cross sections in a reactor core model, reflecting the changes in various reaction rates that are due to the presence of the reactivity device. The supercell consists of a subregion of the core - measuring typically 2 lattice pitches by 1 lattice pitch by 1 bundle length - with the reactivity device at the centre and perpendicular to the fuel channel. The conventional supercell calculations have been performed with the diffusion-theory-based MULTICELL code^[4], designed to be compatible with the Westcott-based PPV lattice cross-sections. MULTICELL seeks the flux solution in the moderator region only. The fuel channel and the device are represented as “virtual regions” in the model, with predetermined boundary conditions (current-to-flux ratios) imposed at their surfaces. The current-to-flux ratios are established either from a transport calculation using WIMS-AECL, or from theoretical considerations of the neutron capture, scattering and escape probabilities, with the assumption of a cosine angular distribution for the incident neutrons. MULTICELL allows only Cartesian geometry, and the cylindrical fuel channels and devices are represented as square regions in the model, with the surface area conserved.

Improvements to the MULTICELL method have recently been made to allow a full 2-group diffusion treatment of the supercell, with the fuel channels and devices explicitly

represented. These improvements are made possible by relating the strong-absorber (fuel-channel and device) properties to the reaction rates predicted by using a simplified WIMS-AECL model through a superhomogenization (SPH) technique^[5].

A more rigorous transport-theory treatment of the supercell can be performed using the DRAGON code^[6]. DRAGON is a lattice-cell code as well as a supercell code. It incorporates a neutron-balance formulation based on the integral transport equation, solved by the collision-probability method. It allows mixed cylindrical and Cartesian geometries, with further annular and sector subdivisions possible in the cylindrical region. Thus, the actual geometry of the fuel channel and of the device can be accurately reproduced in the model. A full 89-energy-group flux solution with a detailed mesh discretization is, in theory, possible, but is very demanding in terms of computer-hardware resources and computation time. A reduced number of energy groups with a fine mesh structure usually provides a completely adequate solution.

4. Core Calculation Methods

The most frequently used method to obtain global flux distribution is the solution of the finite-difference form of the 2-group diffusion equation. This is the basic method used in the RFSP (Reactor Fuelling Simulation Program) code^[7], which is the major computer program in use at AECL for design and analysis of CANDU reactor cores. It has been under continuous development since the 1970s, in response to the need of more refined and accurate representations of the core.

In addition to the neutron-diffusion solution, a flux-mapping method is also available in RFSP. This reconstructs the core flux distribution by taking into account the measured flux values at in-core flux-detector locations. This is the fundamental method used at Point Lepreau and some other stations for tracking the reactor operation history.

The RFSP code structure is modular. Each module is designed to perform a specific function or task. The modules share information and data through a direct-access file, which contains the details of the reactor model and key calculation results.

4.1 Static Core Simulations - Diffusion Calculations

The core-flux solution is based on an assumed fuel burnup distribution and corresponding lattice cross sections. The burnup distribution can be established in different ways, depending on the type of calculation being performed.

a. Time-Average Calculations (*TIME-AVER module)

In this type of calculation, the long-term average core flux and power distributions are sought. The lattice cross sections at any position in core (i.e., any fuel bundle) are

evaluated by averaging over the residence time of the fuel at that position. The fuelling scheme is explicitly taken into account. This type of calculation is used primarily to design the target core power distribution, to test various refuelling schemes, to identify refuelling rates for different regions of the core, and to establish the location and design nuclear properties of the reactivity devices. A detailed description of the time-average calculations is presented in Reference 8.

b. Instantaneous-Core-State Snapshot Calculations (*SIMULATE module)

For certain applications, the instantaneous snapshot of the fuel burnup distribution is “exactly” known, and the lattice cross sections can be readily assembled. Then the code can be used to solve for the instantaneous or snapshot flux and power distributions. A good example is the main application of RFSP on site, to track the reactor operating history. In core tracking, snapshot are calculated at time intervals of 2-3 full-power-days (FPD), and channel refuellings are taken into account as they occur. The bundle irradiation history is tracked together with the flux and power histories. The effect of the spatial distribution of ^{135}Xe on the lattice properties is usually included in the calculation.

c. Random Channel-Age Snapshot Calculations (*INSTANTAN module)

The INSTANTAN module is used to model a random fuel-burnup distribution, corresponding to a hypothetical snapshot in the reactor operating history, without doing lengthy simulations of a period of operation. The fuel-burnup distribution is constructed based on a random distribution of channel “ages”. The channel age is defined as the fraction of cycle time that has elapsed since the channel was last visited. Because of continuous refuelling, the channel ages range approximately uniformly between 0 and 1; a value of 0 corresponds to a channel at the beginning of its cycle, i.e., one that has just been refuelled, while a value of 1 corresponds to a channel at the end of its cycle, i.e., one that is about to be refuelled. A “patterned” age distribution, defined over a small subregion of the core, and repeated cyclically to cover the entire core, can also be specified.

4.2 Static Core Simulations Mapping Calculations (*FLUXMAP module)

Flux-mapping calculations take advantage of in-core flux measurements from 102 spatially distributed vanadium detectors, to compute the instantaneous flux distribution. The flux measurements are least-squares fitted to a linear expansion in a set of basis functions, which are the eigenfunction solutions to the diffusion equation. These basis functions (typically numbering 15, and called harmonic modes) are pre-calculated and orthogonalized. The eigenfunction with the lowest eigenvalue (highest value of k_{eff}) is the fundamental mode. Best results are obtained when the fundamental mode is selected to be a recent core-state snapshot; in this case the “synthesized” mapping solution provides the best agreement with the measured fluxes. Typically, the differences between the

mapped and measured fluxes at the detector locations have a standard deviation of less than $\pm 2\%$.

This type of flux-mapping calculation is often used in core-follow, in conjunction with diffusion-method calculations, which provide the fundamental mode. The computed maximum channel and bundle powers are used to monitor compliance with the licensing limits.

4.3 Quasi-Static Calculations

When time steps are taken in a series of static core simulations, a number of physical processes can be modelled in a quasi-static manner. These include:

- a.* Changes in fuel composition in each bundle position due to fuel burnup and refuelling. The fuel burnup is advanced over the time interval using a value of flux level averaged over the time step.
- b.* Xenon and iodine and other saturating fission product transients. The “fission-product driver” option in the *SIMULATE module explicitly tracks the concentrations of saturating fission products and their contribution to the basic-lattice properties as the flux/power level changes at each bundle position.
- c.* Bulk reactivity control, which automatically adjusts the average water fill in the zone-controller compartments to maintain criticality or reduce or raise power, as required.
- d.* Spatial control, which automatically adjusts the water fill in the individual zone-controller compartments to maintain a desired distribution of zone fluxes.

The modelling of some of these processes is automatic, while the modelling of others is optional. Fuel-burnup advance is automatic in core-tracking simulations. The fission-product-tracking option is used when there is a significant change in power level or significant spatial redistribution of power due to device movements. Site-recorded zone water fills corresponding to the time of a core snapshot being simulated can also be specified in the input, instead of being established from bulk and spatial controls.

4.4 Lattice-Cell-Properties Representation

In all diffusion-calculation applications discussed above, the lattice-cell properties form the basis of the core simulations. Different levels of details and approximations can be used to represent these properties:

- a.* The “uniform-parameter” method provides basic-lattice cross sections dependent on irradiation (burnup) only. The lattice properties are tabulated as “fuel tables”, with irradiation as the only independent parameter. The fuel tables are computed with the

assumption of core-average values for all other lattice parameters, such as fuel temperature, coolant density and flux (power) level.

- b. “Local-parameter” methods provide lattice properties that are derived with respect to the local value of certain parameters, such as fuel temperature, coolant density and flux (power) level.
- c. The “history-based local-parameter” method ^[9] is used especially in core-tracking or operational transient simulations. At each time step, an individual lattice-cell calculation is performed within RFSP for each bundle, to update the lattice properties over the incremental burnup step, using the appropriate local values of flux level, fuel temperature, and coolant density, and any other “local parameter” desired. In this way, the evolution of the nuclear properties of each individual fuel bundle is tracked more accurately.

4.5 Time-Dependent Calculations (*CERBERUS module)

A spatial-kinetics capability for transient analysis is provided by the *CERBERUS module of RFSP. The most typical application is in the calculation of the power transient following a hypothetical loss-of-coolant accident, and the evaluation of shutdown-system performance in terminating a power excursion.

The time-dependent diffusion equation with delayed-neutron terms is solved, using the Improved Quasi-static method ^[10]. The flux is assumed to be a product of an amplitude term, dependent on time only, and a shape function, dependent on both space and time. Separate, but coupled. Equations are written for the shape function, the amplitude term, and the delayed-neutron precursors. The factorization allows the frequency of the shape-function calculations to be greatly reduced. Shape calculations are performed at an interval over which there is significant change in flux shape due to device movements or other perturbations; the time interval is typically of the order of 50-100 milliseconds. The more rapidly changing amplitude is solved with the point-kinetics-like amplitude equation, over smaller time steps. The solution scheme iterates between the coupled flux-shape and amplitude solutions at each shape-calculation time step, to ensure cross-consistency.

The kinetics calculations are usually also coupled to thermalhydraulics calculations performed outside of RFSP, which provide data on the changes in thermalhydraulic quantities such as coolant density and temperature, and fuel temperature as well. The power transient computed by *CERBERUS at each time step is also fed to the thermalhydraulics calculations.

The capability for modelling the action of the reactor regulating system (RRS) in the CANDU 6 reactor has also been implemented, and coupled to the neutronics calculation^[11]. This capability allows the simulation of transients where reactivity devices are manipulated by the RRS in response to reactivity perturbations.

5. Validation of Codes and Methods

The physics codes and methods are continuously being validated against measurements. Some measurements are performed in the ZED-2 research reactor (zero-energy experimental assembly) at the Chalk River Laboratories, while others are carried out in power reactors during the commissioning phase or during operation. These measurements include:

- a. Integral experiments in the ZED-2 reactor to obtain lattice material bucklings, reactivity coefficients, and reactivity worth of devices;
- b. Reactivity of individual and group of devices against moderator poison in power reactors at cold conditions, at either fresh-fuel or equilibrium-fuelling irradiated-fuel conditions;
- c. Global flux distributions measured for various reactor configurations under either cold, zero-power or at-power conditions;
- d. Integral measurements of feedback reactivity due to changes in temperature and/or power level; and
- e. Flux-transient measurements with in-core instrumentation following shutdown-system actuation.

Validation of all three levels of physics calculations has been extensively documented. The validation of the core-simulation results implicitly covers also the lattice-cell and supercell calculations, and involves the accuracy of the spatial flux distribution, which is one of the key end-products of the chain of calculations. Sample results of code validation against measurement data from the 1992 Point Lepreau restart commissioning physics tests ^[12,13] are presented here for illustration.

Table 1 shows the standard deviation of the differences between the measured and computed flux “response” to various perturbed-core configurations at the 102 vanadium detector locations. “Response” is defined as the ratio of flux at a given location in the perturbed core to the flux at the same location in the nominal-configuration core. The relative accuracy of the various calculational methods is shown, including the results from pre-simulations performed with assumed core conditions before the actual tests were performed.

Figures 1a and 1b show comparisons of the flux response in horizontal and vertical directions, respectively, for a perturbed-core configuration. The flux shape was highly distorted by the 50%-insertion of two mechanical-control-absorber (MCA) rods and the withdrawal of adjuster bank 1. The measurements, obtained using a travelling flux detector (TFD) scanning along selected detector assemblies locations, are compared with RFSP computed results using the uniform-parameter diffusion method as well as the flux-mapping method.

Figure 2 compares results of a *CERBERUS simulation of a reactor trip to the measured response of shutdown-system in-core detectors. The reactor shutdown was initiated by a manual trip of shutdown system No. 1 (SDS1), and the power decreased to decay-power values in less than 2 s. The detector dynamic response and the electronic-circuitry signal processing were modelled. Note that the calculation results predict a power run-down rate slightly slower than the measured rate, which is on the conservative side from a safety-analysis perspective.

The above sample validation results demonstrate the accuracy of the chain of codes in situations where the flux shape is highly distorted or the flux shape is rapidly changing. In summary, a high level of confidence in the physics codes and methods has been culminated through continuous validation against actual operation data and operation experience.

6. References

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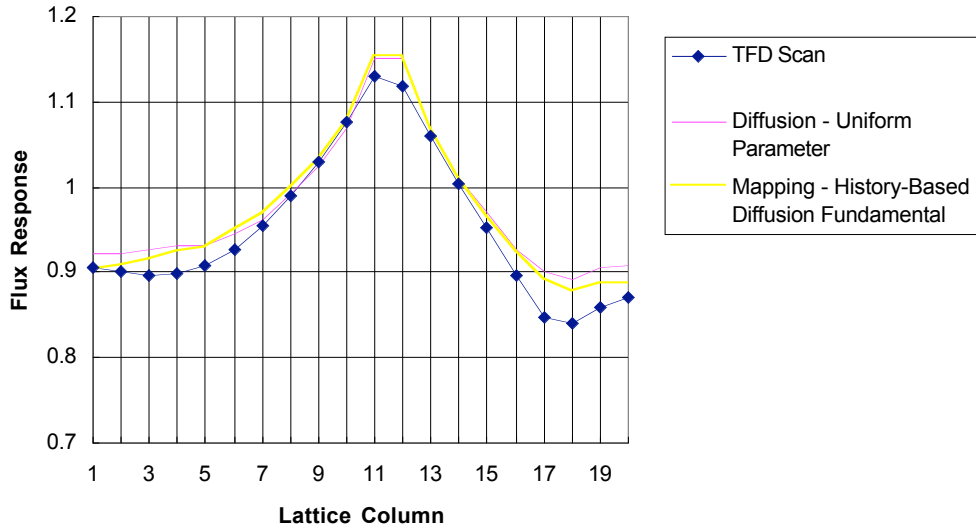
Table 1 Comparisons of Perturbation Response Measured by Vanadium Detectors and Computed by RFSP

Calculation Method	Perturbed-core Configuration (Standard Deviation of Difference at 102 Vanadium-Detector Locations)						Average Standard Deviation
	MCA Bank 1 50% Inserted; Adjuster Bank 1 Withdrawn	SOR Rod #19 50% Inserted	Zone #2 Drained	Adjuster Rod #18 Withdrawn	Adjuster Bank 1 Withdrawn	Adjuster Banks 1-4 Withdrawn	
*Diffusion (Pre-Simulation)	5.8%	2.7%	2.1%	2.0%	2.2%	3.1%	3.0%
Diffusion - Uniform Parameter	1.2%	1.4%	2.8%	2.6%	2.5%	1.5%	2.0%
Diffusion - History-Based	1.2%	1.3%	1.6%	2.3%	2.5%	1.8%	1.8%
**Flux Mapping	0.6%	0.7%	0.3%	0.3%	0.3%	0.3%	0.4%

* Pre-simulations were performed before the actual tests, using assumed core conditions and the uniform-parameter method.

** Flux-mapping calculations were done using the history-based diffusion-method solution as the fundamental mode.

**Figure 1a Flux Response Comparisons
RFSP vs. TFD Scan Along HFD #3
(MCA Bank 1 Half-In / AA Bank 1 Out)**



**Figure 1b Flux Response Comparisons
RFSP vs. TFD Scan Along VFD #16
(MCA Bank 1 Half-In / AA Bank 1 Out)**

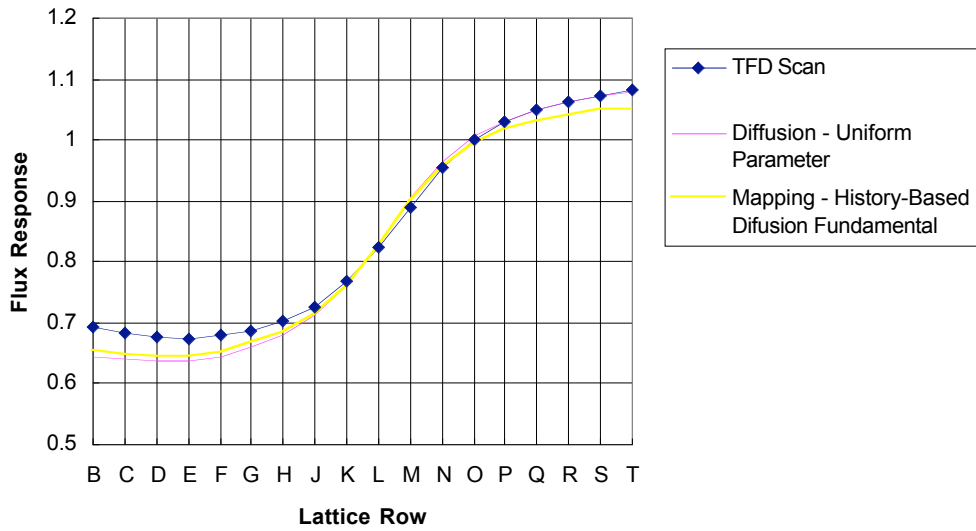


Figure 2 ROP Detector 4F Response in SDS1 Trip Test

