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Rapid Light Water Reactor Modeling for MCNP and Associated Boiling Water Reactor Library

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INTRODUCTION

As computational capability increases, modeling a full reactor burning each pin individually using the Monte Carlo transport code MCNP becomes more feasible, but generation of input files requires an automated process because a large number of cells and materials are necessary. An MCNP input file generator called, "LWRGen" was designed for Light Water Reactor (LWR) cores to facilitate rapid modeling of pressurized and boiling water reactors (PWRs and BWRs). LWRGen was designed using Bison and Flex, standard software that has been in use for over 30 years for parsing and lexical analysis, to read the input generation file, create the geometry, and populate the materials with a user specified enrichment of fresh fuel with input parameters allowing for both variable core and assembly sizes. The generator allows for pin-by-pin fidelity with unique materials for both radial and axial zoning, as well as setting the parameters for gap and clad radii, so that the fuel composition can be more accurately simulated over the fuel cycle. Guide tubes, control rods, and burnable poison rods with gadolinium have also been implemented to further increase the accuracy of the simulation for real designs. Reflectivity options allow for a single assembly with reflective boundaries for an infinite core, limited to 1/4th and 1/8th of the core for symmetric modeling, or for the entire core to be modeled. When generating a BWR Reactor, box walls and control blades have been implemented as well as axial zoning for the moderator density.

Using LWRGen to create the geometry and composition for BWR models, a new spent fuel library has also been created for the Next Generation Safeguards Initiative (NGSI) spent fuel NDA project by coupling MCNP to the isotope generation and depletion code CINDER90 using MonteBurns to perform Monte Carlo transport and burnup calculations¹⁻⁶. The BWR models expand the previous NGSI libraries for quantifying the plutonium mass in, and detecting the diversion of pins from, BWR spent nuclear fuel assemblies.

DESCRIPTION OF THE ACTUAL WORK

LWRGen was initially designed and implemented with C/C++ to generate full PWR cores with fresh fuel in each assembly. Options in the generation input file allow for variable assembly sizes and zoning of fuel into equal

volume axial and radial zones, each with their own material compositions, so that a desired fidelity may be achieved. Fuel composition is determined by specifying the density and enrichment values, which also includes the isotopes for ²³⁴U. Fuel pin geometry is generated by specifying the pellet radius, pin pitch and height; gap radius and height; and values for the cladding radius, top, and bottom. Guide tubes are generated by specifying their inner and outer radii, and placed within the assemblies by specifying their locations within an assembly fuel mapping grid. The assembly locations are then specified in the core mapping grid, and the inner core radius is then determined from the outer most fuel pin unless the user inputs a specific value. Temperature parameters for the fuel, cladding, and water allow for the user to specify the values that should be used during the simulation. Reflectivity options were initially implemented to allow for 1/8th and 1/4th core simulations. Shown below in Figure 1 are fuel pins and guide tubes in a 7x7 lattice in which assemblies have been repeated to model a portion of a PWR core containing 25 assemblies.

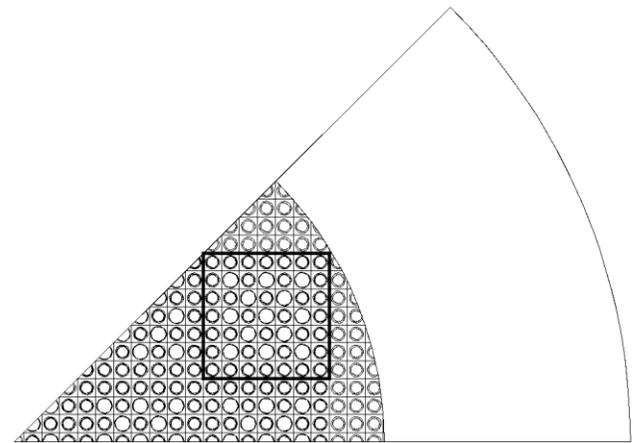


Figure 1: MCNP Plot showing 7x7 assemblies in a PWR core with 1/8th reflectivity. Because the outer most assembly has been specified as a water bundle, the emboldened assembly contains the outer most fuel pin, and was used to automatically calculate the inner core radius. The core is surrounded by 20cm of water.

After verifying the PWR models generated were correct, LWRGen was updated to include options for creating BWR cores. Channel parameters were implemented for specifying the distance from an edge fuel

pin to the box, the box's thickness, and distance to the center of a control blade. Control blades are determined by specifying the inner and outer width of the blade; the inner and outer radii of the control pins within the blade; control pin pitch within the blade; a spacing parameter determining the extent of the blade; and how many pins are within each extending section of a blade. The blades were created as quadrant sections so that they can be used in lattices and placed in the core using a blade mapping grid. Axial zoning of the moderator was also added to correctly model the variation in moderator density with height, and allows the user to specify the densities for each region. Reflectivity options were also updated for infinitely reflective assemblies to allow for greater fidelity in modeling a single fuel assembly. As seen below, Figure 2 shows the changes when generating a BWR assembly with a control blade.

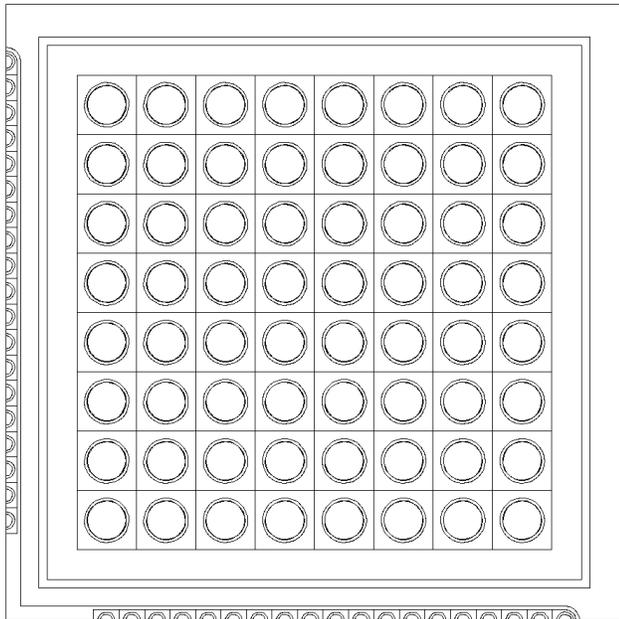


Figure 2: MCNP Plot showing a boxed 8x8 BWR assembly with a control blade in the bottom left corner. Control blades within the core are placed using blade mapping, allowing for non symmetric cores and blades to be placed on reflective boundaries.

Finally, water wings and a water channel were implemented to create an additional BWR geometry as shown in Figure 3. The water channel size is determined by a single parameter while the wings use three: distance from the channel, width of the wing, and length of the wing. One additional parameter is used for specifying the thickness of zircaloy enclosing the wings and channel. The assembly map was also updated to allow for the pins to be split into four separate grids, and an option for specifying moderator regions within the assembly without guide tubes was added. Gadolinium rods were also added for more accurate modeling of real assemblies.

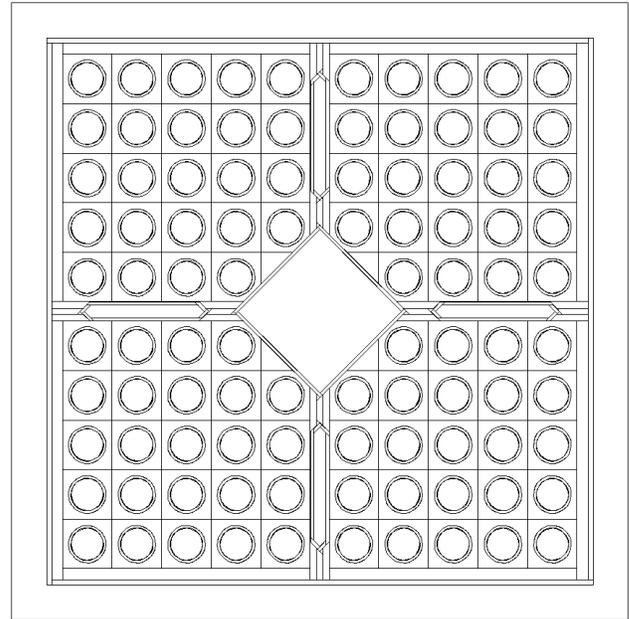


Figure 3: MCNP Plot showing boxed 4x(5x5) BWR assembly with water wings and a water channel. The four center pins were removed by specifying them as moderator, allowing for the moderator density to continue to vary with height.

LWRGen was then used to help create spent fuel library 5 (SFL5) for the NGSIs spent fuel NDA project. SFL5 contains BWR assemblies with water channels to simulate reactor irradiation on three assemblies with average fuel enrichments of 2, 2.5, and 3 percent. The assemblies have been simulated both with control blades fully inserted, and without control blades, to estimate the changes caused by these boundary conditions. The 96 fuel pins have been split into 25 axial zones, with enrichment and H₂O density/void fraction varying with height. Gadolinium has also been included in some of the fuel with radial zones increasing from one for just solely fuel to ten for axial zones that include Gd. Newer versions of MCNP and the associated linkage code *Monteburns* along with improved computing power allowed up to thousands of individually modeled materials to be burned instead of the ~50 material limit of the past. However, memory and processing constraints still limited the simulations to 2182 materials (2184 with blades inserted) in an infinitely reflected BWR assembly.

The simulations irradiated the fuel to a burnup of 48 GWd/tU in steps of 12, with 30 day cooling periods and slow start ups to account for xenon buildup. Using MCNP with CINDER90 and *Monteburns* allowed for the spent fuel libraries to be generated as a series of MCNP input files, which specify the material composition for each period in time. Cooling times of 1, 5, 20, 40, and 80 years for the assemblies were calculated with CINDER90 to determine the fuel composition after it has been

removed from the reactor and stored in a spent fuel pool or dry storage.

RESULTS

LWRGen has made it far more efficient and much easier to create models for simulating Monte Carlo neutron transport using MCNP. Because it was implemented using C++, with its Standard Template Library and Object Oriented design, it allows for additional features to be added with relative ease. New geometry models can be added in about the same amount of time that it would take to create the model by hand, and then by changing parameters in the generation input file; the model can easily be copied and varied with little effort. Rather than spending a week to type an MCNP model by hand, the generation input file can be created in less than 10 minutes, and the MCNP model generated within seconds, allowing for a year of modeling efforts to be completed in 1 or 2 days. The output functions for LWRGen follow MCNP formatting, but allow for simple additions to also create the *Monteburns* input files, or can easily be changed to create the input for another simulation for verification.

Simulating the reactor irradiation for three enrichment levels, four burnups, and with and without control blades, has created 24 additional assemblies in NGSF SFL5 in addition to those already created for PWR assemblies. The simulations used the ENDF/B-VII data set in MCNP. Using simulations of reactor irradiation, the new libraries provide additional representative assemblies of what may currently be residing in spent fuel pools or dry storage from BWRs.

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