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Fuel Cycle Depletion Capability for the U.S. NRC Neutronics Code PARCS

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ABSTRACT

As part of the U.S. Department of Energy's Nuclear Energy Research Initiative (NERI), several advanced reactor designs are being investigated at Purdue University. This includes both evolutionary "Generation III+" designs such as the Simplified Boiling Water Reactor (SBWR) as well as revolutionary "Generation IV" designs such as the High Conversion BWR (HCBWR). The safety analysis of these systems requires both systems thermal-hydraulics and core neutronics codes. During the last several years, the U.S. NRC spatial kinetics code PARCS has been coupled to the system thermal-hydraulics codes RELAP5 and TRAC-M using an innovative general interface design. In order to perform fuel cycle analysis of advanced reactor designs, it has been necessary to add a depletion capability to the spatial kinetics code PARCS. The depletion capability was implemented using the same basic general interface design used to couple PARCS to TRAC-M and RELAP5. An external depletion module, DEPLETOR, was developed that communicates with PARCS and the general interface code using PVM. This design has the advantage of minimizing changes to the PARCS code and simplifying code maintenance. An additional module, GENPXS, was also developed to process the output files from lattice physics codes and to generate the tabulated cross section file PMAXS for DEPLETOR. The code depletion system was verified using several test problems, to include simple multi-assembly models and a practical model of the Simplified Boiling Water Reactor (SBWR) coupled to the thermal-hydraulics code RELAP5.

1. INTRODUCTION

The design and analysis of existing and advanced reactor systems requires the solution of the coupled temperature/fluid and neutron/nuclide field equations. Several code systems have been developed that successfully perform the coupled field solution such as SIMULATE-3 (Smith, 1992) and FORMOSA (Karve, 2000). These code packages utilize advanced nodal methods for the core neutronics solution and are coupled to core thermal-hydraulics codes that are capable of accurately predicting the temperature/fluid solution for both Pressurized and Boiling Water Reactors. Both of these code packages also provide efficient interfaces to lattice physics codes for the burnup dependent few group cross sections.

During the past several years the PARCS (Purdue Advanced Reactor Core Simulator) code has been developed by the U.S. NRC for best estimate core neutronics analysis and was coupled to the U.S. NRC system thermal-hydraulic codes RELAP5 and TRAC-M (Barber, 1998) (Miller, 1999a). As shown in Figure 1 below, this coupling was performed using an innovative General Interface design which allowed the codes to remain autonomous and exchange field solutions using the PVM message passing software. This design had the advantage of minimizing changes to any of the codes and also of simplifying code maintenance. Validation of the coupled code system was performed for PWR transients such as the OECD TMI Main Steam Line Break (MSLB) benchmark transient (Ivanov, 1999), (Miller, 1999b) and for BWR transients such as the OECD Peach Bottom Turbine Trip transient (Solis, 2000).

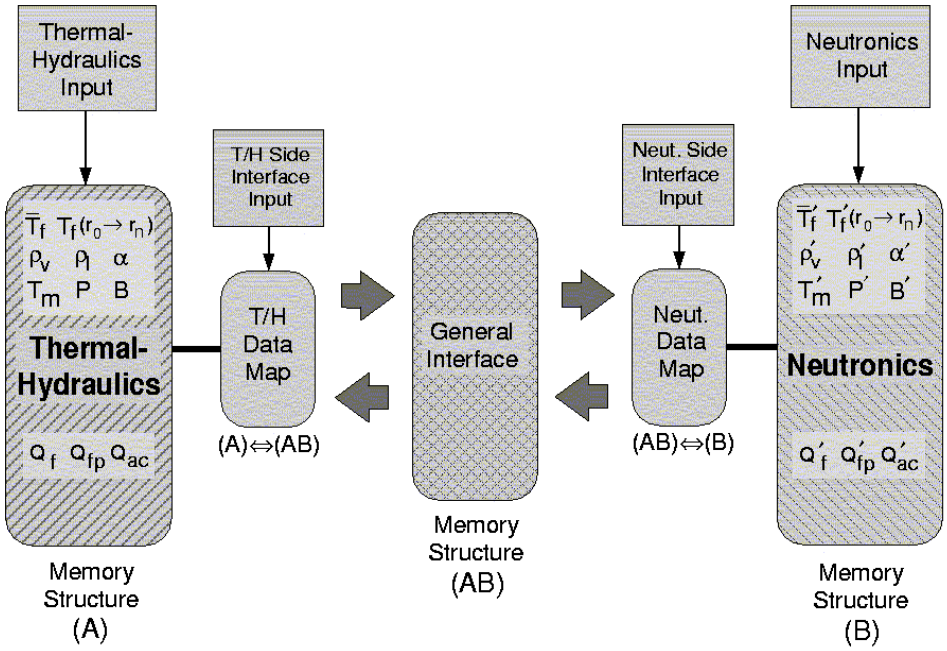


Fig. 1 Code Coupling of PARCS to Thermal-Hydraulics Codes

As part of the U.S. Department of Energy's (DOE) Nuclear Energy Research Initiative (NERI), several advanced reactor designs are currently being investigated at

Purdue University. This includes both Generation III+ designs such as the Simplified Boiling Water Reactor (SBWR) and Generation IV designs such as the High Conversion BWR (HCBWR). In order to perform fuel cycle analysis of these advanced reactor designs, it was necessary to add a depletion capability to the spatial kinetics code PARCS. The depletion capability was implemented using the same basic general interface design used to couple PARCS to TRAC-M and RELAP5. An external depletion module, DEPLETOR, was developed that communicates with PARCS using PVM and the general interface code. This design has the advantage of minimizing changes to the PARCS code and simplifying code maintenance. This design is innovative from the standpoint of fuel cycle design and reactor safety analysis because each code solves a different set of equations and performs a separate function. The PARCS code is used only to perform eigenvalue calculations, all depletion functions are performed in DEPLETOR, and all temperature/fluid field solutions are performed in RELAP5 or TRAC-M. So if it became necessary to obtain a higher order flux solution during depletion, PARCS could simply be replaced by an appropriate transport code. An additional module, GENPXS, was also developed to process the output files from lattice physics codes and to generate the tabulated cross section file PMAXS for DEPLETOR.

The following paper will first describe the design of the PARCS based code depletion system. Results will then be presented of verifying the depletion package first with multi-assembly test models and then with a practical neutronics model of the Simplified Boiling Water Reactor (SBWR) coupled to a RELAP5 thermal-hydraulics model which provides the two-phase flow distribution throughout the burnup cycle.

2. A MODULAR FUEL CYCLE ANALYSIS CODE SYSTEM

A modular code system was designed in order to minimize changes to the PARCS code and to simplify code maintenance. However, it was also introduced to provide the maximum flexibility to employ different neutronics or TH codes during fuel cycle depletion or safety analysis. The depletion capability was implemented with an external depletion module, DEPLETOR. The PARCS code is used only to perform an eigenvalue calculation and all depletion functions are performed in DEPLETOR. The same general interface design shown in Figure 1 that was used to couple thermal-hydraulics to neutronics was used to couple PARCS to DEPLETOR.

The basic functions of the DEPLETOR code are:

- Read in the macroscopic cross sections and other assembly data from PMAXS
- Calculate assembly wise macroscopic cross sections as a function of burnup
- Transfer the assembly wise macroscopic cross sections to PARCS
- Obtain the node wise fluxes from PARCS
- Calculate assembly burnup increment at each step based on the assembly fluxes
- Tabulate and store cross section history effects

All information transfer between PARCS and DEPLETOR is performed using the standard message passing interface software PVM (Geist, 1994).. It was necessary to insert only four “entry points” in the PARCS code. An additional module, GENPXS, was

also developed to process the output files from lattice physics codes and to generate the tabulated cross section file PMAXS for DEPLETOR. The following section will describe the methodology and structure of the DEPLETOR/PARCS code system and the last section will present results of benchmarks that verify and validate the code performance.

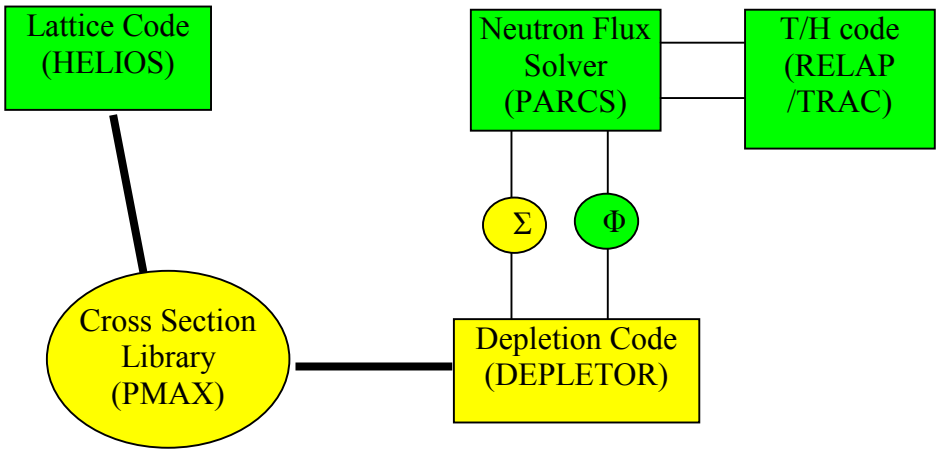


Fig. 2 Fuel Cycle Depletion Methods for PARCS

2.1 Cross Section Model

The macroscopic Cross Section (XS) representation used in PARCS is fairly standard and represented mathematically as follows:

$$\Sigma(ppm,Tf,Tm,D)=\Sigma^{r}+\frac{\partial\Sigma}{\partial ppm}\Delta ppm+\frac{\partial\Sigma}{\partial\sqrt{Tf}}\Delta\sqrt{Tf}+\frac{\partial\Sigma}{\partial Tm}\Delta Tm+\frac{\partial\Sigma}{\partial D}\Delta D+\frac{1}{2}\frac{\partial^{2}\Sigma}{\partial D^{2}}(\Delta D)^{2} \quad (1)$$

Where Σ^{r} : Macroscopic XS at reference state
ppm: soluble boron concentration (ppm)
Tf: fuel temperature (K)
Tm: moderator temperature (K)
D: moderator density (g/cc)
$\frac{\partial\Sigma}{\partial x}$: derivative of XS at reference state with respect to x, x=ppm, Tf,Tm,andD
$\frac{\partial^{2}\Sigma}{\partial D^{2}}$: second derivative of XS at reference state with respect to D

In this formulation, PARCS requires node-wise XS and derivatives at a specified burnup state point. The data provided in the PMAXS cross section files are the tabular

XS at specified base states, which are usually different from the node burnup states specified in PARCS. Therefore, it is necessary to employ some type of interpolation method with the PMAXS data to calculate the XS at the appropriate burnup state.

The burnup distribution is calculated using the fluxes provided by PARCS as follows:

$$\Delta B_i = \Delta B_c \frac{P_i}{G_i} / \frac{P_c}{G_c} \tag{2}$$

where: i : ith depletion region, one region is one Z-direction node of a assembly,
ΔB_i : burnup increase of ith region,
ΔB_c : Core average burnup increment in one step, specified in DEPLETOR input,
G_i : the heavy metal loading in ith region,
G_c : total heavy metal loading in the core($=\sum G_i$),
P_i : power in ith region,
P_c : Total power in core ($=\sum P_i$).

G_i, P_i can be calculated as following:

$$G_i = \rho_i \sum_{j \in i} V_j \tag{3}$$

$$P_i = \sum_{j \in i} V_j \left[\sum_{ig} \left(\Phi_{ig,j} \times \kappa\Sigma_{f\,ig,j} \right) \right] \tag{4}$$

where: j: jth neutronic node in PARCS,
ig: igth energy group,
V_j: volume of jth node, given by PARCS,
ρ_i : heavy metal density in ith region, provided in PMAXS,
$\Phi, \kappa\Sigma_f$: Fluxes and fission energy XS, given by PARCS.

Linear interpolation is used between 2 burnup points as:

$$\Sigma(B_i) = \Sigma(B_n) \frac{B_{n+1} - B_i}{B_{n+1} - B_n} + \Sigma(B_{n+1}) \frac{B_i - B_n}{B_{n+1} - B_n} \tag{5}$$

where: Σ represents the node XS and derivatives at the reference state

B_n, B_{n+1} are assembly burnups of two XS sets in PMAX.

The base state in PMAX can be different from the reference state specified in the PARCS input deck. The XS at each reference state is calculated with the following formula:

$$\Sigma^r = \Sigma_0 + \Delta\Sigma_{ppm} + \Delta\Sigma_{Tf} + \Delta\Sigma_{Tm} + \Delta\Sigma_D \tag{6}$$

where : Σ_0 : XS at base state

$\Delta\Sigma_{ppm}, \Delta\Sigma_{Tf}, \Delta\Sigma_{Tm}, \Delta\Sigma_D$: the XS difference between reference states specified in PARCS input deck and the base state due to the difference in *ppm*, *Tf*, *Tm*, and *D* respectively.

In DEPLETOR, each independent variable (e.g. *ppm*, *Tf*, *Tm*, or *D*), is treated separately. Here, x is used to represent each independent variable. The formulation then becomes:

$$\Sigma(x) = \Sigma_0 + \Delta\Sigma_x + \frac{\partial\Sigma}{\partial x}\Delta x + \frac{1}{2}\frac{\partial^2\Sigma}{\partial x^2}(\Delta x)^2 \tag{7}$$

(Note: The second order derivative is only evaluated for x=*D*)

For the case with no branch:

$$\Delta\Sigma_x = \frac{\partial\Sigma}{\partial x} = \frac{1}{2}\frac{\partial^2\Sigma}{\partial x^2} = 0 \tag{8}$$

For the case with one branch:

$$\Delta\Sigma_x = (x_r - x_0)d_1, \quad \frac{\partial\Sigma}{\partial x} = d_1, \quad \frac{1}{2}\frac{\partial^2\Sigma}{\partial x^2} = 0 \tag{9}$$

Where : x_r : the reference state

x_0 : the base state

x_1 : the first branch state

d_1 : the average derivative between x_0 and x_1

And for the case with two branches:

$$\Delta\Sigma_x = (x_r - x_0)\frac{d_1 \times (x_2 - x_r) - d_2 \times (x_1 - x_r)}{x_2 - x_1}$$

$$\frac{\partial\Sigma}{\partial x} = \frac{d_1 \times (x_2 + x_0 - 2x_r) - d_2 \times (x_1 + x_0 - 2x_r)}{x_2 - x_1} \qquad (10)$$

$$\frac{1}{2}\frac{\partial^2\Sigma}{\partial x^2} = \frac{d_2 - d_1}{x_2 - x_1}$$

Where : x_2 : the second branch state

d_2 : the average derivative between x_0 and x_2

2.2 Code Structure

The general algorithm for coupling DEPLETOR and PARCS is shown in Figure 3.

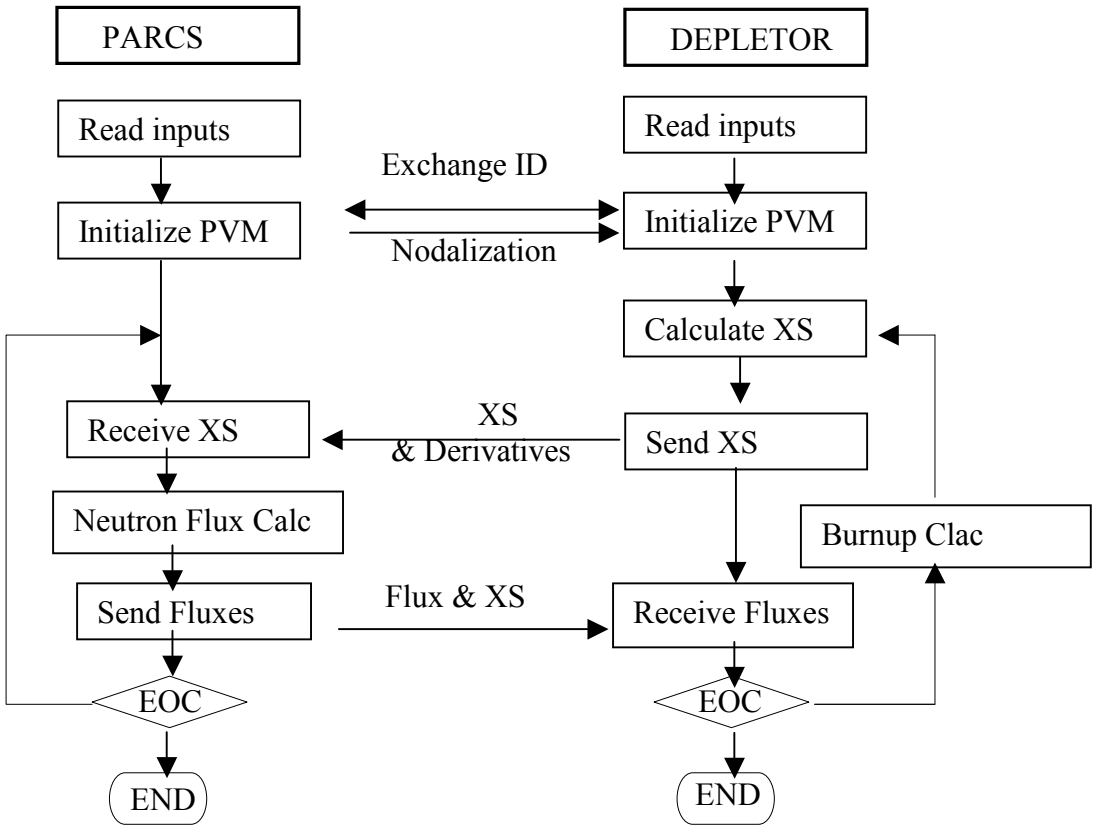


Fig. 3 Schematic of the Depletion Procedure for the DEPLETOR/PARCS Codes

DEPLETOR generates the cross-sections and their derivatives at each burnup state and transfers them to PARCS. PARCS then solves the diffusion equations with the given macroscopic cross sections and their derivatives and transfers the resulting flux distribution to DEPLETOR.

2.3 Code Benchmarking

In order to validate the capability of PARCS for depletion and to verify the PMAXS format, several benchmark problems were analyzed. In the following section only three of these benchmarks will be presented. In the first two problems, results will be compared to HELIOS and to the KAERI Depletion code MASTER. The **MASTER** (Multi-purpose Analyzer for Steady state and Transient Effects of Reactors) is a reactor core design code developed by KAERI (Lee, 1998), (Cho, 1999), (Kim,1996) for analyzing light water reactors. The MASTER code has the capability to deplete with the cross sections of HELIOS and has been well validated with several benchmark and actual reactor core simulations. Because the depletion code of PARCS also uses the cross sections from HELIOS, it provided a convenient reference for benchmarking purposes. The last test problem will be a model of the GE Simplified Boiling Water Reactor (SBWR). This problem demonstrates the versatility of the depletion code system and results will be compared to the GE calculations reported in the SSAR (GE, 1992).

3. APPLICATIONS

3.1 Multi-assembly Test Problems

The first application was to a simple multi-assembly model to verify functionality of the depletion code by comparisons to the HELIOS lattice physics code. The problem consists of four fuel assemblies with a zero net current boundary condition as shown below.

The calculation conditions for the problem were as follows:

- Core power = 22.7681 MWth
- Boundary condition = reflective (net current zero) boundary condition
- Core geometry = 2D
- Xenon/Samarium state = Equilibrium
- Moderator temperature = 290.04 C
- Fuel temperature = 480.04 C
- Moderator density = 0.74568 g/cc
- Soluble boron concentration = 1 ppm

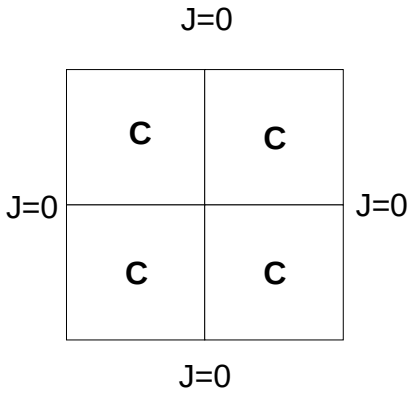


Fig. 4 Multi-Assembly Test Problem

The purpose of this problem is to verify the performance of the depletion routines of DEPLETOR and their interface to PARCS, as well as the PMAXS cross section interface to the HELIOS code. The difference in the predicted k-infinite of PARCS/DEPLETOR and HELIOS is shown in Figure 5 below.

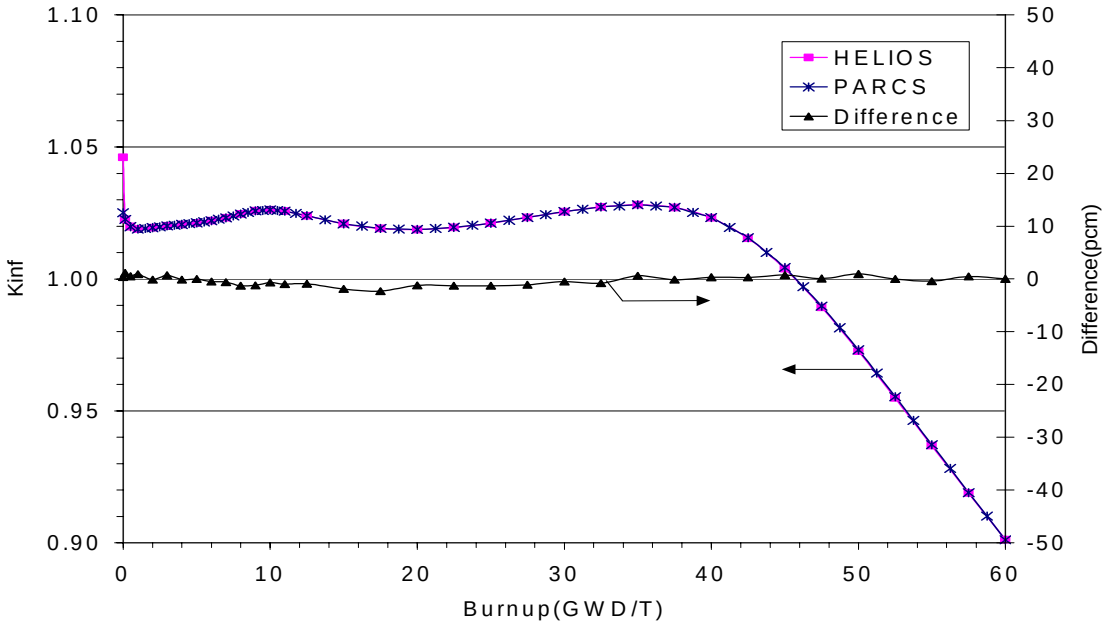


Fig. 5 Difference in the Burnup Predictions of HELIOS and PARCS/DEPLETOR

A second problem was analyzed with a three-dimensional model of a simplified PWR as shown in Figure 6 below. The results were compared to the KAERI MASTER depletion code (Lee, 1998). It should be noted that the MASTER code performs

microscopic depletion whereas PARCS currently employs only macroscopic depletion. The results are shown in Figure 7 below.

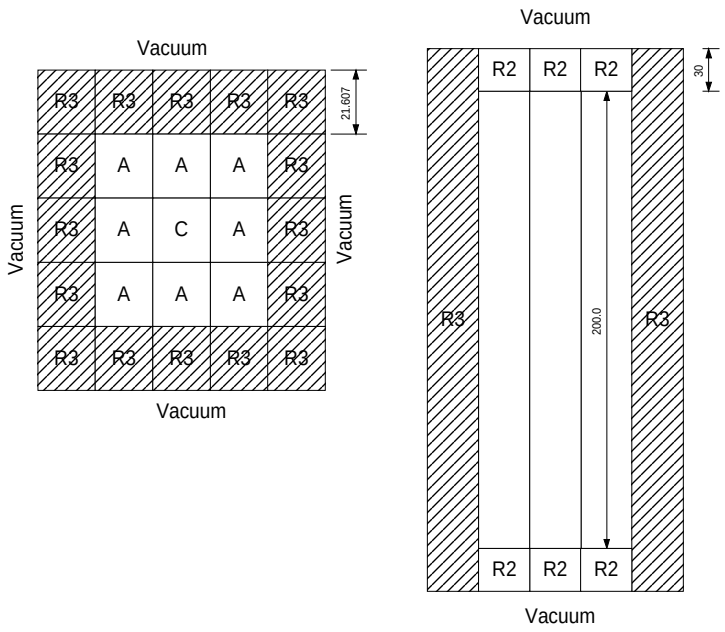


Fig. 6. Three-Dimensional Model of a Simplified PWR Test Problem

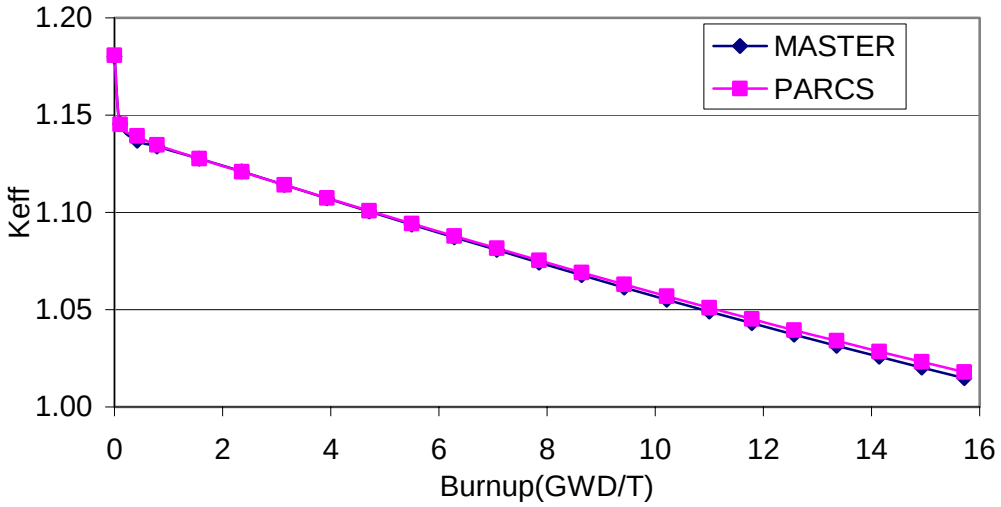
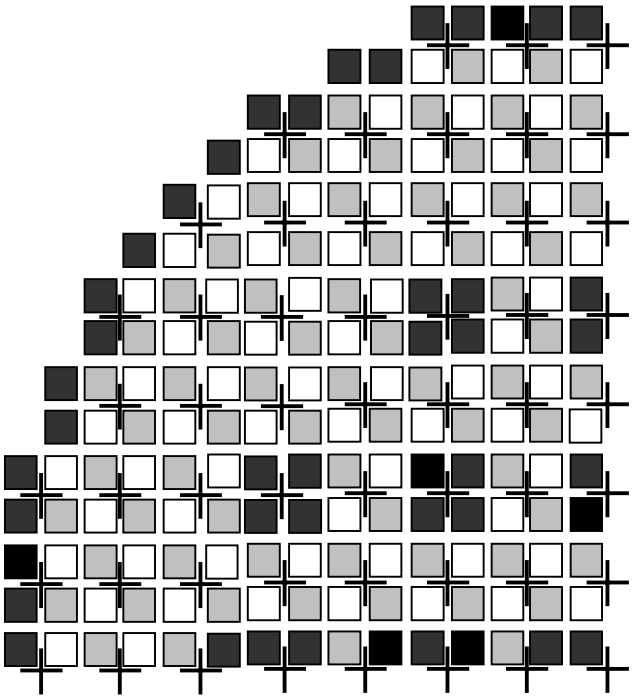


Fig. 7 Difference in the Burnup Prediction of MASTER and PARCS/DEPLETOR

As indicated in the Figure, the agreement in the predicted keff is fairly good, especially at the beginning of the burnup cycle. Towards the end of the burnup cycle the difference is larger (about 0.3% k) which can be attributed partly to macroscopic versus microscopic depletion effects. In the future, a microscopic depletion capability will be added to DEPLETOR.

3.2 Simplified Boiling Water Reactor (SBWR)

A more practical benchmark problem was performed which is related to the DOE NERI project at Purdue on the Simplified Boiling Water Reactor (SBWR). This problem has the additional advantage of testing the coupling of PRACS/DEPLETOR to the thermal-hydraulics code RELAP5. A PARCS neutronics model was developed (Figure 8) and coupled to a RELAP5 model of the SBWR shown in Figure 9. Cross sections were generated using the HELIOS lattice physics code and the core was depleted using PARCS/DEPLETOR. An equilibrium cycle was developed and comparisons were made to the depletion predictions of the GE Safety Analysis Report of the SBWR (GE, 1992).



Fresh fuel, 69 bundles

1st Cycle Fuel, 69 bundles

2nd Cycle Fuel, 45 bundles

Fig. 8 Quarter Core Loading Pattern for the 600 MWe SBWR

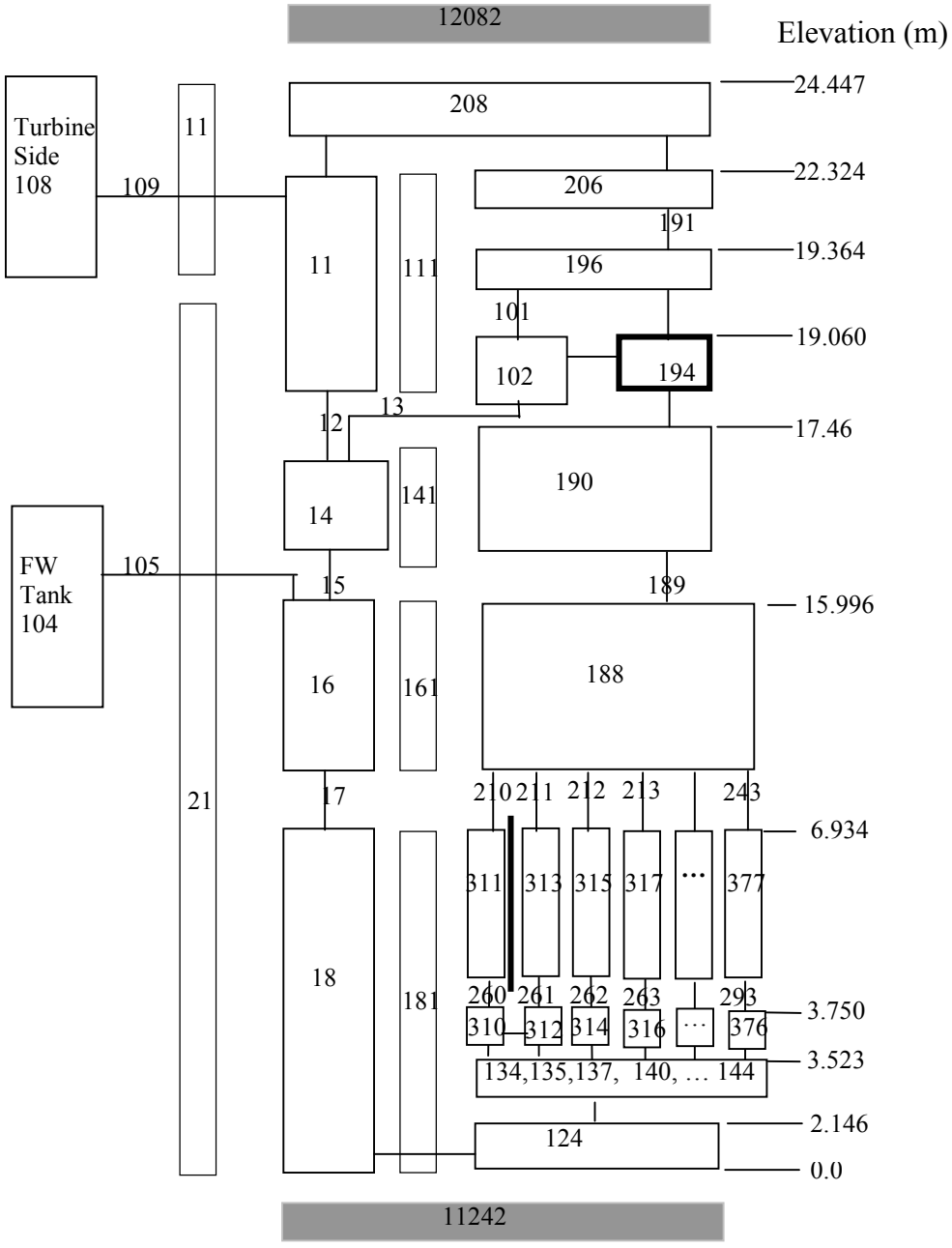


Fig. 9 The RELAP5 Model for the 600 Mwe SBWR

The results of depleting the SBWR with PARCS/DEPLETOR/RELAP5 are shown in Table 1 below. Core criticality is maintained at each burnup step by searching for the critical rod configuration with PARCS. The control rod notches inserted (C.R. Notches in Table 1) are indicative of the excess reactivity in the core and when the rods are fully removed (C.R. = 0) the core has achieved its reactivity limited end of cycle. The prediction of a 14.3GWd/T cycle length coincides with the prediction by GE (GE, 1992).

Table 1 Results of SBWR Depletion with PARCS/DEPLETOR/RELAP5

B(GWd/T)	C.R. notches	Max Peak	Radial Peak	Axial Peak	Ave. Burnup
0.000	571	2.105	1.398	1.491	14.049
1.1	556	1.994	1.456	1.355	15.149
2.2	551	2.051	1.433	1.352	16.249
3.3	527	2.178	1.383	1.370	17.349
4.4	527	2.385	1.353	1.436	18.449
5.5	527	2.764	1.336	1.534	19.549
6.6	480	3.055	1.336	1.619	20.649
7.7	501	3.053	1.391	1.681	21.749
8.8	501	2.599	1.371	1.579	22.849
9.9	473	2.158	1.376	1.396	23.949
11.0	456	2.019	1.394	1.353	25.049
12.1	379	1.982	1.392	1.408	26.149
13.2	302	1.999	1.394	1.388	27.249
14.3	0	1.948	1.399	1.323	28.349

It is also worthwhile to analyze the execution time profile for depletion with PARCS/DEPLETOR/RELAP5. The amount of time spent in each of the modules is summarized in Table 2. As indicated, the largest amount of time is spent in PARCS, however this can be deceiving since an excessive number of neutronics calculations are required as RELAP5 converges to a steady-state using a "null transient" at each burnup step. This has motivated the investigation of alternate hydrodynamics models for depletion analysis.

Table 2 Execution Time Profile for a Single Burnup Step (CPU seconds)

	PARCS	RELAP5	GI	Depletor
CPU secs	750	260	117	74

4. CONCLUSIONS

A fuel cycle depletion capability was implemented with the U.S. NRC spatial kinetics code PARCS using an innovative general interface design similar to that used to couple PARCS to TRAC-M and RELAP5. An external depletion module, DEPLETOR, was developed that communicates with PARCS using PVM and a general interface code. This design had the advantage of minimizing changes to the PARCS code and simplifying code maintenance. This design is also innovative from the standpoint of fuel cycle design and reactor safety analysis because each code solves a different set of equations and performs a separate function. The PARCS code is used only to perform eigenvalue calculations, all depletion functions are performed in DEPLETOR, and all temperature/fluid field solutions are performed in RELAP5 or TRAC-M. So if it became necessary to obtain a higher order flux solution during depletion, PARCS could simply be replaced by an appropriate transport code. An additional module, GENPXS, was also developed to process the output files from lattice physics codes and to generate the tabulated cross section file PMAXS for DEPLETOR. The code depletion system, to include the coupling to TRAC-M and PARCS, was verified and validated using simplified PWR models and a practical model of the Simplified Boiling Water Reactor (SBWR).

A cross section history effect capability has been added to DEPLETOR which uses a multidimensional interpolation scheme. This method is currently being validated using the Ringhalls benchmark problem [Lefvert, 1994]. Work is continuing on DEPLETOR to include the implementation and testing of PARCS/DEPLETOR with alternate thermal-hydraulics models which will help reduce the computational burden. Also, future work will include the implementation of a microscopic depletion capability.

NOMENCLATURE

B: Burnup
d: Derivative of Macroscopic XS
D: Moderator density (g/cc)
G: Heavy metal loading
P: Power
ppm: Soluble boron concentration (ppm)
Tf: Fuel temperature (K)
Tm: Moderator temperature (K)
V: Volume
x: independent variable, represents ppm, Tf, Tm, or D
Σ: Macroscopic XS
ρ: Heavy metal density
Φ: Flux
$k\Sigma_f$: Fission energy XS

Subscript or superscript:

i: *i*th depletion region, one region is one Z-direction node of a assembly,
j: *j*th neutronic node in PARCS,
ig: *ig*th energy group,
c: core
r: reference state specified by PARCS input deck
0,1,2: base state, first and second branches in PMAX.

ACKNOWLEDGEMENTS

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