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Benchmark Analysis of the DeCART MOC Code with the VENUS-2 Critical Experiment

Z.Zhong[1] T.J.Downar[1] H.G.Joo[2] J.Y.Cho[2]

1- *Purdue University, IN 47907-1290 USA*
2- *Korea Atomic Energy Research Institute, Yusung, Daejeon 305-353 Korea*

Computational benchmarks based on well-defined problems with a complete set of input and a unique solution are often used as a means of verifying the reliability of numerical solutions. VENUS is a widely used MOX benchmark problem for the validation of numerical methods and nuclear data set. In this paper, the results of benchmarking the DeCART (Deterministic Core Analysis based on Ray Tracing) integral transport code is reported using the OECD/NEA VENUS-2 MOX benchmark problem. Both 2-D and 3-D DeCART calculations were performed and comparisons are reported with measured data, as well as with the results of other benchmark participants. In general the DeCART results agree well with both the experimental data as well as those of other participants.

KEYWORDS: benchmark, VENUS, DeCART

1. Introduction

As part of a U.S.-ROK collaborative INERI project, a comprehensive high-fidelity reactor-core modeling capability is being developed for detailed analysis of current and advanced reactor designs. The neutronics calculation involved in this project is performed using DeCART (Deterministic Core Analysis based on Ray Tracing), a three-dimensional (3-D) whole-core discrete integral transport code. DeCART solves the heterogeneous reactor problem in which the actual detailed geometrical configuration of all pin cell components such as fuel, moderator, and cladding is explicitly retained. For the analysis here, DeCART cross sections were obtained from the 45 group cross section library in HELIOS ver 1.7 [3].

The integral transport solution in DeCART is performed using the method of characteristics (MOC) which employs discrete modular ray tracing. Because the direct application of MOC to 3-D core configurations would require a considerable amount of memory and computing time, an approximate 3-D solution method was developed for DeCART based on combining 2-D/1-D solutions. This approximate method employs planar 2-D MOC solutions and a 1-D solution which are coupled using a transverse leakage approximation within the framework of a 3-D coarse mesh finite difference (CMFD) formulation. The method is described in detail in reference [7].

Results for benchmarking DeCART with numerical benchmarks have been previously reported [4]. The purpose of the work here was to benchmark DeCART using the VENUS-2 a critical experiment [5]. The following section will first describe the VENUS-2 experiment, and then compare the results of DeCART against the measured data, as well as against the results of other codes.

2. Model Problem Description

VENUS-2 is an international benchmark with both two- and three-dimensional exercises. The objective of the benchmark was to validate and compare the nuclear data sets and production codes used for MOX-fuelled system calculations. The VENUS facility is a zero power critical reactor located at SCK CEN in Belgium. The core consists of twelve 15×15 assemblies with the typical pitch of 17×17 assembly, 1.26 cm. The four central assemblies consist of the 3.3 w/o UO_2 fuel pins, with 10 Pyrex pins each. The 8 assemblies on the periphery of the core consist of UO_2 and MOX fuel: 7 internal rows contain 4.0 w/o UO_2 fuel pins, 8 external rows contain MOX fuel with 2.0/2.7 w/o high-grade plutonium. The core is 50 cm in height. The configuration of the VENSU-2 core is shown in Fig.1.

The 2-D VENUS-2 experimental data consists of pin power distribution measurements in 121 of the 325 fuel rods in 1/8th of the core: 41 with 3.3 w/o UO2, 35 with 4.0 w/o and 45 with 2.0/2.7 w/o MOX. The remainder of the pin powers were interpolated from the measured values. The 3-D VENUS-2 experimental data provides radial pin power measurement and axial fission power of six selected pins [1]. A complete description of the facility is given in the benchmark specifications, which includes all geometry and material composition data required to create a detailed computational model of the VENUS-2 core.

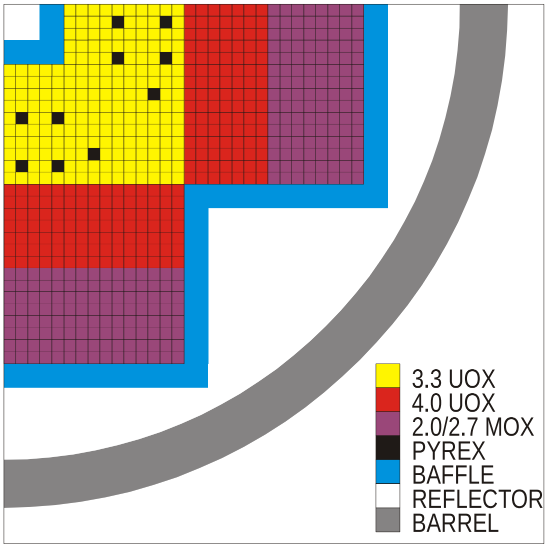


Fig. 1 VENUS-2 Configuration (1/4 Core)

3 . Benchmark Results

The 2-D version of the VENUS-2 benchmark consists of both pin cell and core calculations. Results will be reported first for the performance of DeCART using pin cell and assembly calculations.

3.1 Pin Cell Calculations

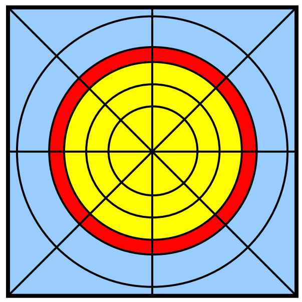


Fig. 2 DeCART Pin-Cell Discretization

The discretization of the DeCART pin-cell model is shown in Fig.2. Eight equally spaced azimuthal regions is introduced to divide the pin-cell. In the fuel pellet there are three equal-area rings, the air gap is neglected and homogenized with the cladding into one ring, and the moderator is also divided into two rings so that the flux shape can be considered in this region. In this pin cell model, there are totally 48 flat source regions. In the DeCART pin cell calculation, 8 azimuthal and 4 polar angles were used to discretize the angular flux, and the spacing between rays was 0.02cm.

Table 1 shows the pin cell k_{inf} results of DeCART compared with other benchmark participants. As indicated, there is reasonably good agreement between DeCART and HELIOS, which used the same 45g library as DeCART . However there exists a relatively large k_{inf} difference between DeCART and NEWT, especially for the MOX pin cell calculation (about 800 pcm). This relative large k_{inf} discrepancy could attributed primarily to cross section library differences. This was verified by performing a second DeCART calculation using the 44 group NEWT cross section library in DECART. [DeCART can bypass the process of reading data from the 45g HELIOS library as well as the associated resonance calculation, and instead use a set of user specified cross section.] As indicated in the Table, DeCART k_{inf} are very close to that of NEWT when the same 44 group library is used.

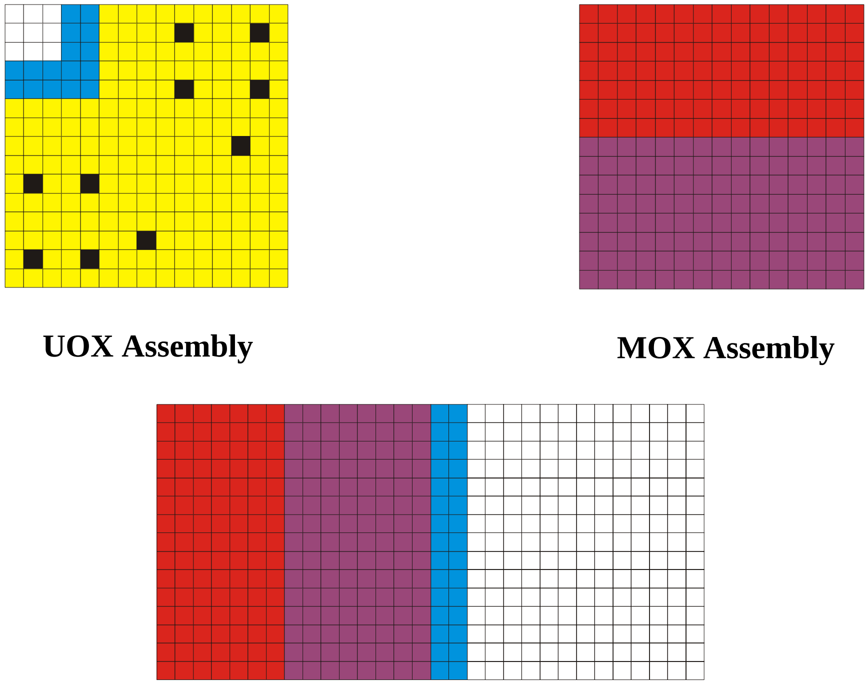
Table 1. Results for VENUS-2 Pin Cells

Code	UO_2 3.3%		UO_2 4.0%		MOX	
	k_{inf}	%Dev.*	k_{inf}	%Dev.	k_{inf}	%Dev.
HELIOS 1.7 (190g)	1.40850	0.18	1.34331	0.45	1.26339	0.53
HELIOS 1.7 (45g)	1.40691	0.07	1.34189	0.35	1.26332	0.52
NEWT (44g)	1.40424	-0.12	1.33259	-0.35	1.25435	-0.19
DeCART (44g NEWT)	1.40261	-0.24	1.33194	-0.39	1.25356	-0.25
DeCART (45g HELIOS)	1.40322	-0.19	1.34147	0.31	1.26207	0.42
MCNP-4B	1.40670	0.06	1.33775	0.04	1.25769	0.08
Average**	1.40593		1.33726		1.25673	

Average for Deterministic Method : 1.40400 1.33527 1.25546
Average for Monte Carlo Method : 1.40786 1.33925 1.25800

3.2 Assembly Calculations

Three different models were used to assess the performance of DeCART for fuel assembly calculations. The configuration of these assemblies is shown in Fig.3. In each of these calculations, 8 azimuthal and 4 polar angles were used to discretize the angular flux, and the spacing between adjacent rays was 0.02cm.



UOX Assembly **MOX Assembly**

MOX-Reflector Assembly

Figure.3 VENUS-2 Assembly Models

The UOX assembly consists of a central water hole, center baffle, 210 3.3 w/o UO_2 fuel pins and 10 pyrex pins; the MOX assembly consists of 105 4.0 w/o UO_2 pins and 120 2.0/2.7 w/o MOX pins; the MOX-Reflector assembly model adds an outer baffle and outer reflector region onto the MOX assembly. The k_{inf} of these three assemblies calculations is shown in Table 2.

Table 2. Results for Assembly Calculation of VENUS-2

Code	UOX-Assembly	MOX- Assembly	MOX-Reflector
HELIOS-45g	1.17502	1.29843	1.15420
MCNP 4B	1.17570	1. 29459	1.14882
DeCART (45g HELIOS)	1.17497	1.29752	1.14886
DeCART (44g NEWT)	1.17206	1.28959	1.14092
NEWT 44g	1.17316	1.12896	1.14419

From the results listed in Table 2, it can be seen that when using the same 45g library, there exists more than 500 pcm k_{inf} difference between DeCART and HELIOS for the MOX-Reflector assembly model. However when using the 44g cross section from NEWT, the k_{inf} difference between DeCART and NEWT is only about 200 pcm. Part of this 200 pcm difference in k_{inf} can be attributed to differences in treatment of the scattering cross section. NEWT uses P1 scattering, whereas DeCART uses isotropic scattering with a transport correction.

3.3 Core Calculation

The configuration of the VENUS-2 whole core model of DeCART is shown in Fig.4[7], some simplifications were made in the model. The core barrel is approximated using a series of pin size square mesh, and all other external structure material was neglected and replaced by the reflector. Eight azimuthal and 4 polar angles were used to discretize the angular flux, and the spacing between 2 adjacent rays was 0.02cm.

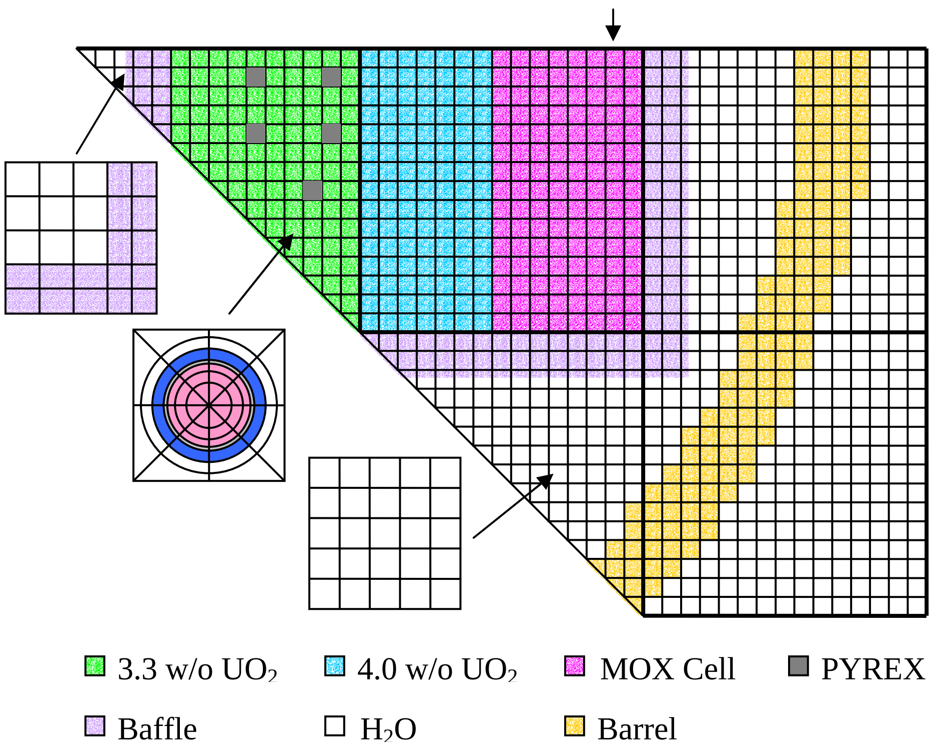


Fig. 4 DeCART Modeling for VEMUS-2 MOX Critical Core Problem

In the axial direction, the model is divided into 7 nodes. The bottom and top reflector nodes are 10 cm each, and 5 axial nodes are used to discretize the active part of the core, with the height of the axial nodes of 5.5, 13.0, 13.0, 13.0 and 5.5 cm.

The 2-D and 3-D k_{eff} are shown in Table 3. The 2-D DeCART k_{eff} is very close to that of MCNP and the k_{eff} predicted by DeCART for the 3-D calculation is close to 1.0, which is the critical condition. Although DeCART uses the same 45g library as HELIOS, there is a significant 700 pcm k_{eff} difference for the 2-D calculation

Table 3. Results for VENUS-2 Core Calculation

Code	2-D	3-D
Helios-45g	1.08901	
DeCART-45g	1.08209	0.99724
MCNP 4B	1.08277	1. 00201

The calculated pin power distribution is shown in Tables 4 and 6. Because the core is diagonal symmetric (see Fig.4), it is only necessary to show the pin power distribution of 2 assemblies. The pin power distribution in the central UOX assembly and right MOX assembly are shown here. The calculated pin power was compared with the experimental data and the ratios of the calculated value to the experimental value are shown in Table 5 and Table 7 [5]. From Tables 5 and 7, it is apparent that the largest error between calculated and experimental pin power is only about 8%, which occurs at the MOX assembly.

Table 4 Calculated Pin Power for Central UOX Assembly

0.000	0.000	0.000	0.000	0.000	1.015	1.222	1.300	1.293	1.245	1.330	1.374	1.331	1.232	1.223
0.000	0.000	0.000	0.000	0.000	1.010	1.225	1.298	1.246	0.000	1.281	1.358	1.280	0.000	1.172
0.000	0.000	0.000	0.000	0.000	1.011	1.238	1.318	1.307	1.256	1.338	1.378	1.332	1.231	1.221
0.000	0.000	0.000	0.000	0.000	1.035	1.264	1.338	1.322	1.264	1.345	1.383	1.334	1.231	1.220
0.000	0.000	0.000	0.000	0.000	1.115	1.309	1.361	1.293	0.000	1.303	1.371	1.284	0.000	1.167
1.015	1.010	1.011	1.035	1.115	1.270	1.371	1.407	1.384	1.326	1.380	1.391	1.328	1.241	1.223
1.222	1.225	1.238	1.264	1.309	1.371	1.421	1.450	1.452	1.440	1.429	1.375	1.279	1.288	1.251
1.300	1.298	1.318	1.338	1.361	1.407	1.450	1.475	1.483	1.475	1.442	1.326	0.000	1.243	1.246
1.293	1.246	1.307	1.322	1.293	1.384	1.452	1.483	1.493	1.488	1.461	1.394	1.296	1.307	1.250
1.245	0.000	1.256	1.264	0.000	1.326	1.440	1.475	1.488	1.486	1.469	1.434	1.386	1.341	1.244
1.330	1.281	1.338	1.345	1.303	1.380	1.429	1.442	1.461	1.469	1.459	1.435	1.393	1.334	1.224
1.374	1.358	1.378	1.383	1.371	1.391	1.375	1.326	1.394	1.434	1.434	1.411	1.369	1.304	1.189
1.331	1.280	1.332	1.334	1.284	1.328	1.279	0.000	1.296	1.386	1.393	1.369	1.325	1.255	1.138
1.232	0.000	1.231	1.231	0.000	1.241	1.288	1.243	1.307	1.341	1.334	1.304	1.255	1.180	1.060
1.223	1.172	1.221	1.220	1.167	1.223	1.251	1.246	1.250	1.244	1.224	1.189	1.138	1.060	0.928

Table 5 Pin Power C/E* Ratio for Central UOX Assembly

0.000	0.000	0.000	0.000	0.000	0.940	0.979	0.978	0.969	0.963	0.952	0.984	0.986	1.007	0.990
0.000	0.000	0.000	0.000	0.000	0.959	0.980	0.965	0.971	0.000	0.970	0.971	0.998	0.000	0.991
0.000	0.000	0.000	0.000	0.000	0.985	0.982	0.992	0.958	0.948	0.964	0.988	0.981	0.999	0.980
0.000	0.000	0.000	0.000	0.000	0.962	0.995	0.965	0.956	0.967	0.979	0.997	0.977	0.995	0.976
0.000	0.000	0.000	0.000	0.000	0.986	1.009	0.990	0.968	0.000	0.979	1.007	0.978	0.000	0.984
0.940	0.959	0.985	0.962	0.986	0.974	0.995	0.986	0.955	0.965	0.986	1.009	0.988	0.985	0.989
0.979	0.980	0.982	0.995	1.009	0.995	0.974	0.978	0.964	0.968	0.983	0.983	0.994	1.007	0.989
0.978	0.965	0.992	0.965	0.990	0.986	0.978	0.977	0.979	0.974	0.976	0.959	0.000	0.978	0.977
0.969	0.971	0.958	0.956	0.968	0.955	0.964	0.979	0.981	0.980	0.979	0.971	0.968	1.002	0.978
0.963	0.000	0.948	0.967	0.000	0.965	0.968	0.974	0.980	0.976	0.975	0.979	0.997	1.009	0.982
0.952	0.970	0.964	0.979	0.979	0.986	0.983	0.976	0.979	0.975	0.972	0.982	0.988	0.979	0.984
0.984	0.971	0.988	0.997	1.007	1.009	0.983	0.959	0.971	0.979	0.982	0.974	0.987	0.966	0.983
0.986	0.998	0.981	0.977	0.978	0.988	0.994	0.000	0.968	0.997	0.988	0.987	0.979	0.994	0.990
1.007	0.000	0.999	0.995	0.000	0.985	1.007	0.978	1.002	1.009	0.979	0.966	0.994	0.952	0.992
0.990	0.991	0.980	0.976	0.984	0.989	0.989	0.977	0.978	0.982	0.984	0.983	0.990	0.992	1.002

* C/E ratio: calculated value to experimental value

Table 6 Calculated Pin Power for Central MOX Assembly

1.519	1.507	1.514	1.510	1.495	1.501	1.502	1.490	1.474	1.449	1.414	1.363	1.296	1.192	0.992
1.432	1.429	1.426	1.420	1.410	1.400	1.386	1.368	1.342	1.310	1.268	1.215	1.146	1.042	0.845
1.382	1.378	1.374	1.365	1.353	1.338	1.319	1.294	1.264	1.227	1.182	1.126	1.055	0.954	0.770
1.333	1.330	1.323	1.313	1.300	1.282	1.260	1.232	1.199	1.159	1.111	1.053	0.983	0.885	0.720
1.273	1.270	1.262	1.252	1.237	1.218	1.194	1.165	1.129	1.088	1.039	0.981	0.911	0.820	0.673
1.189	1.186	1.179	1.167	1.152	1.132	1.107	1.078	1.042	1.001	0.953	0.897	0.831	0.747	0.617
1.055	1.052	1.045	1.034	1.019	1.000	0.977	0.949	0.916	0.877	0.833	0.782	0.723	0.650	0.544
1.101	1.098	1.090	1.077	1.061	1.040	1.014	0.983	0.947	0.905	0.857	0.804	0.742	0.671	0.576
0.935	0.931	0.924	0.913	0.898	0.879	0.856	0.829	0.796	0.759	0.718	0.671	0.619	0.560	0.487
0.841	0.838	0.831	0.820	0.806	0.788	0.766	0.741	0.711	0.676	0.638	0.596	0.549	0.496	0.432
0.765	0.762	0.755	0.746	0.732	0.715	0.695	0.671	0.643	0.611	0.576	0.537	0.493	0.446	0.387
0.694	0.691	0.685	0.675	0.663	0.647	0.628	0.606	0.580	0.551	0.518	0.482	0.443	0.399	0.346
0.622	0.619	0.614	0.605	0.594	0.580	0.562	0.542	0.518	0.492	0.462	0.430	0.394	0.355	0.307
0.547	0.545	0.540	0.532	0.522	0.509	0.493	0.475	0.454	0.431	0.405	0.376	0.345	0.310	0.269
0.457	0.455	0.451	0.444	0.436	0.425	0.412	0.396	0.379	0.359	0.337	0.312	0.287	0.259	0.229

Table 7 Pin Power C/E* Ratio for Central MOX Assembly

0.973	0.969	0.972	0.978	0.973	0.977	0.984	0.981	0.979	0.980	0.978	0.975	0.976	0.986	0.974
0.975	0.976	0.981	0.978	0.975	0.974	0.973	0.965	0.968	0.962	0.956	0.957	0.957	0.983	0.960
0.992	0.991	0.996	0.994	0.995	0.986	0.979	0.979	0.983	0.977	0.969	0.968	0.977	1.004	0.979
0.995	0.996	1.000	1.001	0.997	1.000	0.997	0.997	0.999	0.994	0.992	0.985	0.994	1.003	0.991
0.996	1.000	1.000	1.002	0.997	1.004	1.017	1.016	1.014	1.012	1.006	1.006	1.005	1.012	0.999
1.010	1.014	1.016	1.023	1.023	1.078	1.024	1.021	1.018	1.009	1.000	1.016	1.029	1.039	1.016
1.020	1.018	1.017	1.012	1.003	0.999	1.006	1.006	1.006	1.008	1.012	1.008	1.010	1.016	1.014
1.040	1.031	1.027	1.027	1.029	1.026	1.037	1.033	1.022	1.024	1.038	1.038	1.030	1.043	1.026
1.036	1.027	1.016	1.020	1.018	1.023	1.016	1.022	1.008	1.023	1.042	1.032	1.020	1.038	1.048
1.046	1.051	1.042	1.038	1.032	1.042	1.041	1.036	1.032	1.033	1.030	1.024	1.014	1.030	1.021
1.073	1.063	1.054	1.057	1.058	1.063	1.069	1.069	1.068	1.057	1.069	1.056	1.043	1.044	1.029
1.082	1.074	1.065	1.070	1.080	1.081	1.085	1.084	1.085	1.089	1.087	1.079	1.070	1.051	1.023
1.078	1.073	1.075	1.075	1.086	1.091	1.096	1.097	1.093	1.095	1.078	1.091	1.077	1.053	1.017
1.058	1.060	1.066	1.064	1.050	1.067	1.094	1.063	1.077	1.072	1.079	1.062	1.042	1.049	1.009
1.056	1.039	1.020	1.038	1.032	1.036	1.056	1.037	1.034	1.046	1.062	1.042	1.031	1.032	1.022

* C/E ratio: calculated value to experimental value

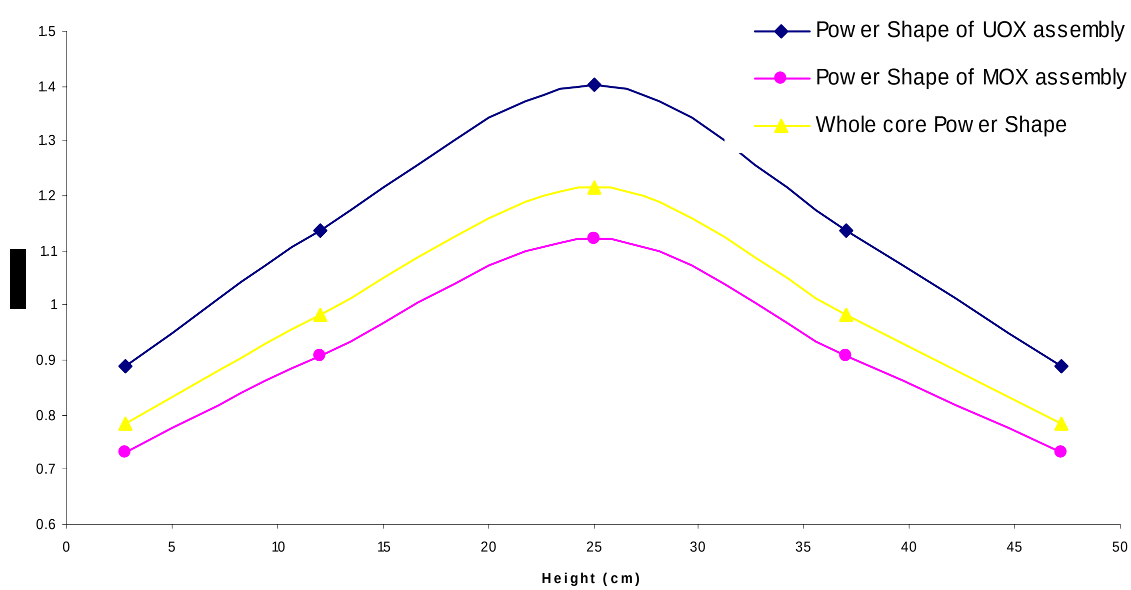


Fig.5. DeCART Axial Power Shape Prediction

4. Summary and Conclusion

The DeCART results from both the 2-D VENUS-2 benchmark appear to be in reasonably good agreement with the results of experimentally measured data, as well as with the results of other benchmark participants. Preliminary results for the 3-D benchmark are encouraging with good agreement between the eigenvalue predicted by DeCART and the measured critical condition.

Work is continuing on the refinement of the 2D/1D solution strategy in DeCART to address concerns with the numerical stability of the 2D to 1D coupling. As reported in another paper at this conference [8], when small mesh are used in the 1-D solution the transverse leakage approximation can introduce numerical instabilities. An alternate 2D/1-D coupling method based on current correction factors has been proposed that appears to be more stable and is currently being implemented in DeCART.

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