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A REACTOR PRESSURE VESSEL DOSIMETRY CALCULATION USING ATTILA, AN UNSTRUCTURED TETRAHEDRAL MESH DISCRETE-ORDINATES CODE

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ABSTRACT

Recently, a new state-of-the-art discrete-ordinates code, ATTILA, was developed. ATTILA provides the capabilities to solve geometrically complex 3-D transport problems by using an unstructured tetrahedral mesh. In this paper we describe the application of ATTILA to a 3-D reactor pressure vessel dosimetry problem. We provide numerical results from ATTILA and the Monte Carlo code, MCNP. The results demonstrate the effectiveness and efficiency of ATTILA for such calculations.

I. INTRODUCTION

The assessment of pressure vessel metal embrittlement in nuclear reactors, caused by neutron irradiation, requires accurate calculations of the fast neutron flux. Such fast neutron flux calculations require the use of Monte Carlo codes or discrete-ordinate codes. Traditional methods for use in calculating the neutron fast flux have relied on the 3-D spatial-synthesis methodology[1-3]. Here two dimensional R-θ and R-Z and one-dimensional R (infinite cylindrical) calculations are combined to approximate the 3-D solution. Such methodology makes assumptions on the spatial seperability of the neutron flux and results in additional analysis uncertainty. Three-dimensional calculations offer the possibility of more accuracy and efficiency.

Monte Carlo calculations[4] have been used for reactor pressure vessel calculations, but require extensive and perhaps, prohibitive, computing time for routine calculations. Historically, traditional 3-D discrete ordinate codes, which use rectangular meshes, require too many mesh cells to efficiently model such problems. Urban[5], et al, have recently applied the THREEDANT[6] code to such problems. This required the use of the FRAC-IN-THE-BOX code[7] to specify the geometry description and resolve it onto a X-Y-Z rectangular spatial mesh by means of volume averaging the transport data in multimaterial spatial cells. Such multimaterial spatial cells arise from the use of rectangular meshes.

We have recently applied the new state-of-the-art discrete-ordinates code, ATTILA[8], to a representative reactor pressure vessel dosimetry problem[9]. ATTILA solves the multigroup discrete-ordinates equations on an unstructured tetrahedral mesh using linear discontinuous finite element (LD) spatial differencing. The unstructured mesh allows for the accurate, explicit modeling of complex 3-D geometries, such as those arising from reactor pressure vessel dosimetry problems. The LD spatial differencing provides more accurate results with coarse meshes than the standard weighted diamond-difference scheme employed in traditional discrete-ordinates codes. We compare our results with those obtained from the 3-D Monte Carlo code, MCNP[10].

The remainder of this paper proceeds as follows: in Section II, we describe the problem to be solved, in Section III we describe the ATTILA model of the problem, in Section IV we describe the MCNP model of the problem, in Section V we provide numerical results, and in Section VI, we draw some conclusions.

II. REACTOR PRESSURE VESSEL PROBLEM DESCRIPTION

The pressure vessel dosimetry problem solved is shown in Figure 1. A more detailed description of the model is given in reference 9, which is part of these proceedings. This problem is identical to that in reference 9 except that it is symmetric about the z axis (same materials above and below the cavity regions). The symmetry has enabled determination of MCNP results more efficiently.

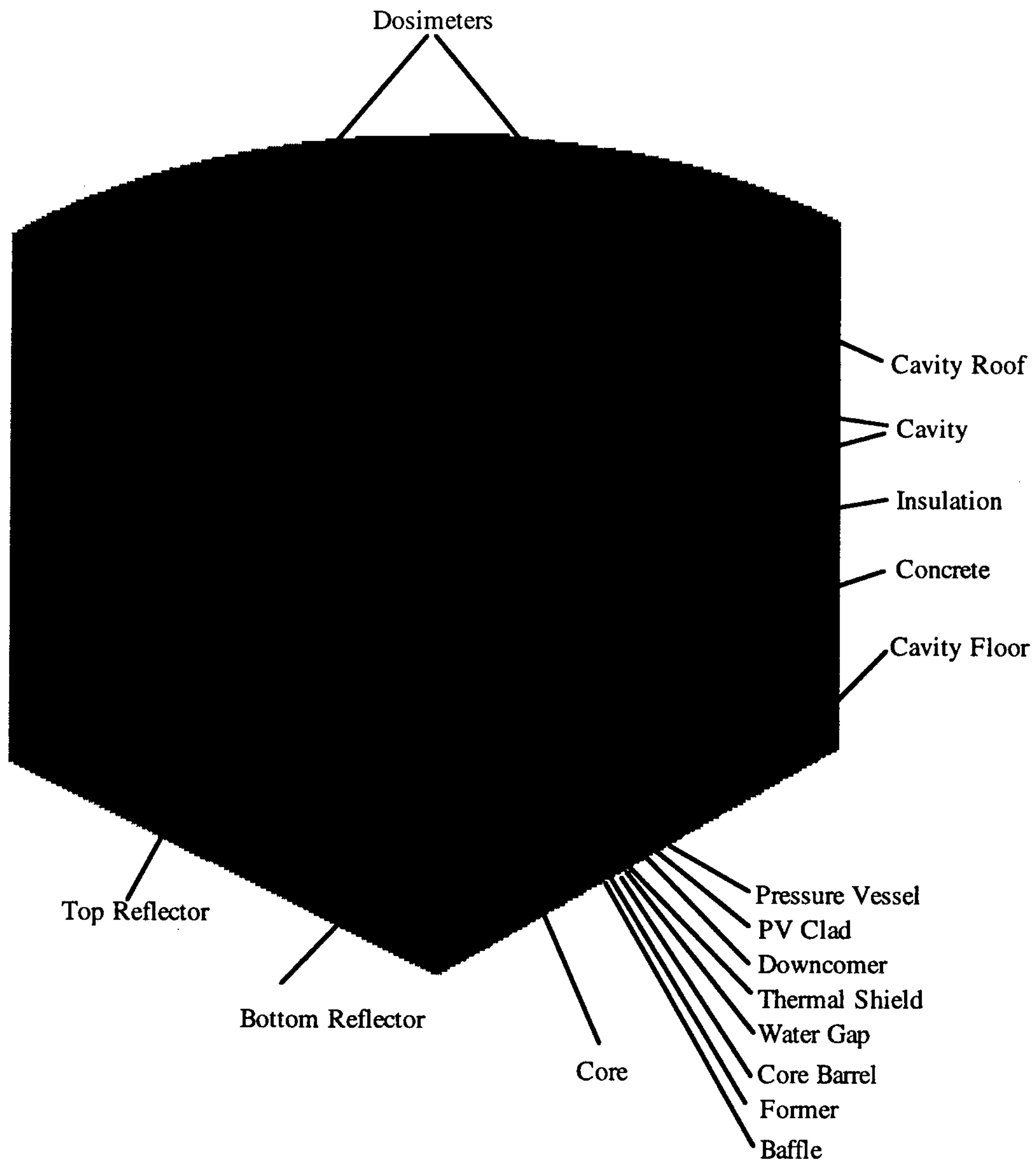

Figure 1: Reactor Pressure Vessel Problem

The main simplifications of this problem, relative to actual reactors, is the use of a homogeneous core with a constant fixed source. More advanced cores can be added to the model, but is not necessary for this analysis. Note that this problem represents one-fourth of the core, with reflective boundary conditions along the x and y axes and vacuum boundaries along all others. Because of the symmetry at 45 degrees, this can also be represented by one-eighth core with appropriate boundary conditions. We use one-fourth of the core because of the limitation of the 3-D discrete-ordinate quadrature sets in X-Y--Z geometry which only allow for 90 degree rotational symmetry.

The materials for the regions shown in Figure 1 are given as follows:

1. Core: homogeneous reactor fuel mixture.
2. Baffle Plates: stainless steel.
3. Former: water and steel mixture.
4. Core Barrel: stainless steel.
5. Thermal Shield: stainless steel.
6. Downcomer: water.
7. PV Clad: stainless steel.
8. Pressure Vessel: low carbon steel.
9. Cavity: air.
10. Insulation. low density steel.
11. Cavity Roof/Floor: low carbon steel.
12. Top/Bottom Reflector: water and steel mixture.
13. Dosimeters: low carbon steel cylinder filled with aluminum

The source for this problem is a homogenous fixed source with an energy integrated strength of 10^{13}. The energy spectrum for the source is provided in reference 9. The main objective is to find the fast neutron flux for six detector points at energies (MeV): Group 1 (17.33>E>14.19); Group 2 (2.466>E>2.365); Group 3 (0.608>E>0.498) and for all energies greater than 1 MeV and 0.1 MeV. The six detector locations are as follow:

1. In PV Clad at (x,y,z) = (0,216.93,0)
2. In PV Clad at (x,y,z) = (187.87,108.47, 0)
3. In PV Clad at (x,y,z) = (187.87,108.47,100)
4. In Pressure Vessel [3/4 T] at (x,y,z) = (201.96, 116.6,0)
5. In Cavity Dosimeter at (x,y,z) = (303.97,175.5,20)
6. In Cavity Dosimeter at (x,y,z) = (303.97,175.5,50)

III. ATTILA MODEL

The tetrahedral mesh used by ATTILA for the reactor pressure vessel problem is shown in Figure 2. The mesh consists of 90,045 tetrahedra and was generated with the mesh generation code, X3D, developed at Los Alamos National Laboratory. Since this particular problem is axially symmetric, one could create a mesh with roughly half the tetrahedra. We have chosen to use the full mesh since we are simultaneously running a similar problem using this mesh, which is not axially symmetric (the cavity floor material is concrete instead of low carbon steel).

We use the SAILOR 47 energy group cross section library[11]. Only neutron fluxes at energies less than 0.1 MeV are of concern; therefore, the calculations are terminated after the 26-th group. We use the triangular, Tchebyschev-Legendre quadrature sets and P_3 scattering. Petrovic[12], et al, have shown that the SAILOR multigroup cross sections with P_3 scattering and S_8 triangular quadrature are adequate for 2-D pressure vessel calculations with weighted diamond-difference spatial differencing.

To obtain the six detector results, the tetrahedron is identified which the detector point lies within. The linear discontinuous flux representation for the tetrahedron is then used to calculate the flux at the detector location. Some of these tetrahedra are relatively large and this procedure could conceivably introduce some uncertainties in the solution. The extent of these uncertainties is problem dependent. A more rigorous alternative could be to create very small tetrahedra around the detector points when the mesh is generated, which could mitigate such uncertainties. We have not followed this approach for this calculation, primarily due to time limitations; however, from the results given later in the paper, this does not appear to introduce much error.

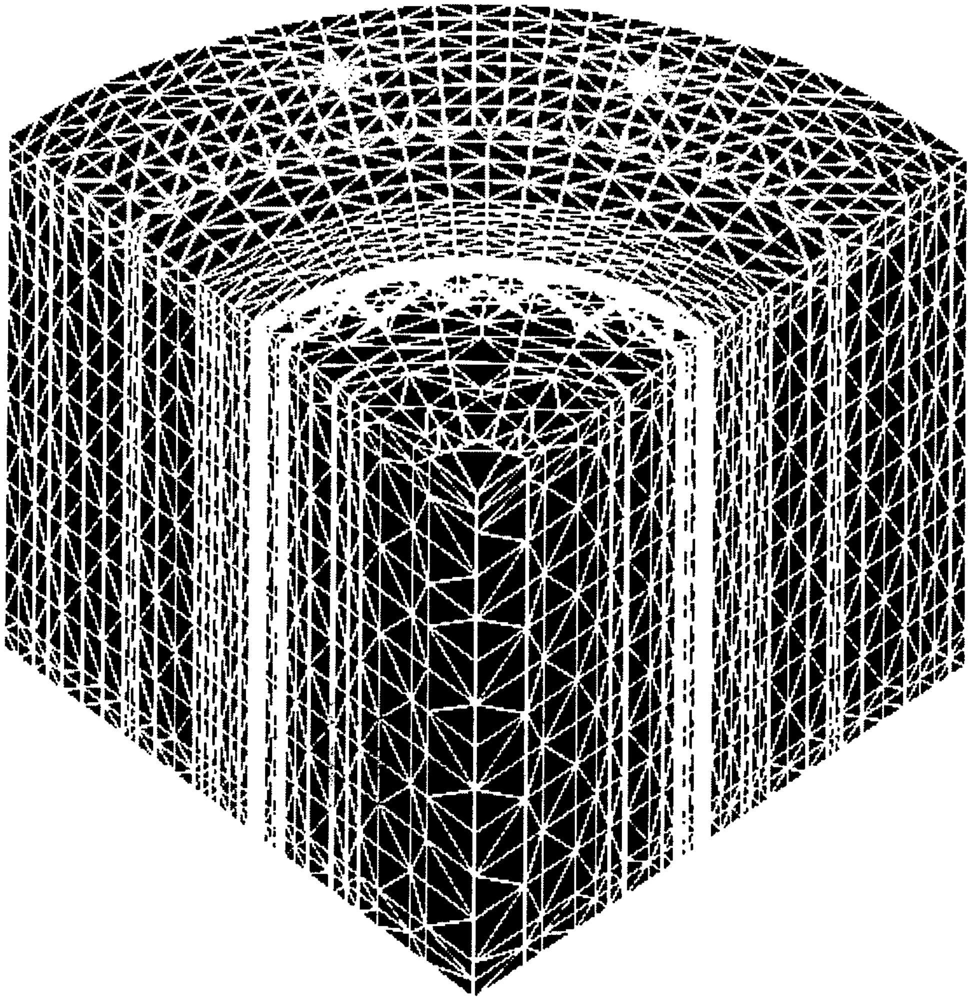

Figure 2: ATTILA Model of Reactor Pressure Vessel Problem

IV. MCNP MODEL

The MCNP model is essentially Figure 1, using one-eighth of the upper half of the problem with appropriate symmetry boundary conditions. We use the SAILOR multigroup cross section library. Some variance reduction techniques have been used, including source biasing, geometric splitting, and larger than nominal volumes for detector flux tallies.

V. NUMERICAL RESULTS

The fast neutron fluxes, at the specified energies, for the six detector locations are provided in Table 1 for the multigroup MCNP calculation and the ATTILA calculations using S_8-S_{12}. The respective average fast neutron fluxes, at the specified energies, within the PV clad, pressure vessel and cavity dosimeter are provided in Table 2. The ratio of the ATTILA S_{12} and the MCNP results are also provided in each table. All ATTILA calculations were run on a Sun Ultra 2 workstation. The calculations required approximately 18 hours for the S_8 calculation and approximately 36 hours for the S_{12} calculation. Note that we could have run this particular problem using only the upper half with a reflecting boundary on the bottom. This would have reduced the mesh size by one-half and the running time would have been approximately 9 hours for the S_8

calculation and 18 hours for the S_{12} calculation. The MCNP calculations were also run on a Sun Ultra 2 workstation. Three separate MCNP calculations were made: one for all energies above 0.1 MeV; one for all energies in Group 11 and higher; and one for Group 1 alone. This energy cutoff expedited the solution time required to get reasonable variances. This is justified by the fact that only downscatter appears in this problem. The MCNP runs required approximately 230 hours, 150 hours, and 17 hours, respectively.

Table 1: Neutron Scalar Fluxes at Detector Points

Detector Number	Energy Group	MCNP Multigroup	ATTILA S_8	ATTILA S_{10}	ATTILA S_{12}	ATTILA S_{12} / MCNP
1 (PV Clad)	1	8.81+6 (.024)[a]	8.60+6	8.64+6	8.65+6	0.98
	11	1.23+9 (.029)	1.22+9	1.23+9	1.23+9	1.00
	21	3.37+9 (.039)	3.23+9	3.24+9	3.25+9	0.96
	>1.0 MeV	2.20+10 (.024)	2.11+10	2.12+10	2.12+10	0.96
	> 0.1 MeV	4.59+10 (.016)	4.39+10	4.40+10	4.41+10	0.96
2 (PV Clad)	1	7.59+6 (.020)	7.17+6	7.36+6	7.43+6	0.98
	11	1.13+9 (.022)	1.17+9	1.17e+9	1.17+9	1.04
	21	3.31+9 (.030)	3.27+9	3.28+9	3.28+9	0.99
	> 1.0 MeV	2.05+10 (.016)	2.01+10	2.02+10	2.02+10	0.99
	> 0.1 MeV	4.30+10 (.012)	4.30+10	4.32+10	4.32+10	1.00
3 PV Clad	1	7.63+6 (.013)	6.85+6	7.17+6	7.30+6	0.96
	11	1.15+9 (.015)	1.11+9	1.13+9	1.13+9	0.98
	21	3.22+9 (.021)	3.05+9	3.07+9	3.06+9	0.96
	> 1.0 MeV	2.01+10 (.012)	1.90+10	1.94+10	1.94+10	0.96
	> 0.1 MeV	4.27+10 (.009)	4.03+10	4.08+10	4.08+10	0.96
4 (Pressure Vessel 3/4 T)	1	6.09+5 (.017)	5.53+5	5.74+5	5.76+5	0.95
	11	8.60+7 (.018)	8.43+7	8.51+7	8.53+7	0.99
	21	1.78+9 (.011)	1.80+9	1.80+9	1.80+9	1.01
	> 1.0 MeV	2.40+9 (.012)	2.41+9	2.43+9	2.43+9	1.01
	> 0.1 MeV	1.70+10 (.006)	1.71+10	1.71+10	1.71+10	1.01
5 (Cavity Dosimeter)	1	1.23+5 (.018)	9.88+4	1.19+5	1.17+5	0.95
	11	1.57+7 (.036)	1.47+7	1.53+7	1.56+7	0.99
	21	4.56+8 (.016)	4.33+8	4.51+8	4.61+8	1.01
	> 1.0 MeV	5.14+8 (.016)	4.81+8	5.01+8	5.12+8	1.00
	> 0.1 MeV	5.41+9 (.005)	5.16+9	5.32+9	5.41+9	1.00
6 (Cavity Dosimeter)	1	1.21+5 (.018)	9.65+4	1.19+5	1.16+5	0.96
	11	1.55+7 (.035)	1.45+7	1.51+7	1.53+7	0.99
	21	4.58+9 (.016)	4.30+8	4.44+8	4.53+8	0.99
	> 1.0 MeV	5.14+8 (.016)	4.74+8	4.93+8	5.00+8	0.97
	> 0.1 MeV	5.31+9 (.006)	5.11+9	5.25+9	5.32+9	1.00

[a] Values in parenthesis are fractional errors and represent 1σ.

The ATTILA results compare very well with the MCNP results with less than 10 % difference for the six detector points at the specified energies. The groupwise fluxes for the six detector points have standard deviations in the range of 2 to 9 %. The regionwise fluxes also compare very well with the MCNP results. The PV Clad and the Pressure Vessel fluxes are all within 4% of the MCNP results which had standard deviations of less than 0.5 %. The Cavity Dosimeter fluxes are within 10% of the MCNP results which had standard deviations between 0.2 and 2.0%. Some of the differences here could be attributed to the angular quadrature order; the results for group 1 have changed by 20 % between the S_{10} and S_{12} calculations and by 4% for all energies > 0.1 MeV. We note that no effort has been made to spatially refine the ATTILA mesh; however, it appears that this mesh is sufficient for this problem. Also no effort was made to create a small tetrahedron around each detector point to localize conceivable uncertainties in the detector fluxes. Although the SAILOR cross sections with P_3 scattering appear to be adequate, the S_8 quadrature appears to be insufficient. We see that S_{10}-S_{12} quadratures are required to resolve the solution at the cavity dosimeter.

Table 2: Average Neutron Scalar Fluxes in PV Clad, Pressure Vessel and Cavity Dosimeter

Region	Energy	MCNP Multigroup Sailor	ATTILA S_8	ATTILA S_{10}	ATTILA S_{12}	ATTILA S_{12}/ MCNP
PV Clad	1	6.95+6 (.002)	7.05+6	7.05+6	7.06+6	1.00
	11	1.10+9 (.002)	1.13+9	1.13+9	1.13+9	1.03
	21	2.97+9 (.002)	2.97+9	2.97+9	2.97+10	1.00
	>1.0 MeV	1.87+10 (.002)	1.93+10	1.93+10	1.93+10	1.03
	> 0.1 MeV	3.98+10 (.002)	4.00+10	4.01+10	4.01+10	1.01
Pressure Vessel	1	1.87+6 (.002)	1.90+6	1.90+6	1.91+6	1.01
	11	3.10+8 (.002)	3.17+8	3.18+8	3.18+8	1.03
	21	2.39+9 (.002)	2.41+9	2.41+9	2.41+9	1.01
	> 1.0 MeV	6.41+9 (.001)	6.57+9	6.58+9	6.57+9	1.02
	> 0.1 MeV	2.45+10 (.001)	2.47+10	2.47+10	2.47+10	1.01
Cavity Dosimeter	1	1.04+5 (.005)	9.41+4	7.92+4	9.47+4	0.91
	11	1.36+7 (.008)	1.16+7	1.19+7	1.26+7	0.93
	21	4.14+8 (.003)	3.62+8	3.78+8	3.96+8	0.95
	> 1.0 MeV	4.48+8 (.004)	3.82+8	3.94+8	4.14+8	0.92
	> 0.1 MeV	4.96+9 (.002)	4.37+9	4.52+9	4.69+9	0.94

VI. CONCLUSIONS

The state-of-the-art discrete-ordinates code, ATTILA, has been applied to a representative reactor pressure vessel dosimetry problem. The use of a unstructured tetrahedral mesh provides the capability to accurately model this problem with relatively few mesh cells (90,045). The results demonstrate that ATTILA generates very accurate results. ATTILA results match the MCNP results within 10%. ATTILA is very efficient for such calculations; an S_{10} calculations can be done within a 24-30 hour period on a typical desktop workstation. MCNP, modeling only 1/4 of the ATTILA model requires over 200 hours on a typical desktop workstation to obtain reasonable results. Smaller variances would require several more hours.

Future plans include making a parallel version of ATTILA which can be run on a cluster of workstations. This could ultimately lead to reactor pressure vessel calculations that would require only several minutes to a few hours, depending on the type and number of processors.

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