Validation of the ALARA Activation Code

P.P.H. Wilson, H. Tsige-Tamirat,
H.Y. Khater, D.L. Henderson

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UNIVERSITY OF WISCONSIN

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Paul P.H. Wilson
Fusion Technology Inst.
U. of Wisconsin-Madison
1500 Engineering Drive
Madison, WI 53706
paul.wilson@inr.fzk.de

H. Tsige-Tamirat
FZK, INR
Postfach 3640
76021 Karlsruhe
Germany
tsige@inr.fzk.de

Hesham Y. Khater
Fusion Technology Inst.
U. of Wisconsin-Madison
1500 Engineering Drive
Madison, WI 53706
khater@engr.wisc.edu

Douglass L. Henderson
Fusion Technology Inst.
U. of Wisconsin-Madison
1500 Engineering Drive
Madison, WI 53706
henderson@engr.wisc.edu

ABSTRACT

ALARA [Analytic and Laplacian Adaptive Radioactivity Analysis] v1.0,[1,2] a new activation code released in January 1998 and developed specifically for the analysis of radioactivity in fusion energy systems, has been validated by comparison to other commonly used activation codes, FISPACT-97[3] and DKR-Pulsar 2.0[4] using the International Atomic Energy Agency [IAEA] Fusion Evaluated Nuclear Data Library [FENDL] Calculational Activation Benchmark.[5] The solutions to the benchmark problem for both steady-state and pulsed operation have been calculated with all three programs on the same IBM RS/6000 workstation. In addition to comparing the total activity in each of the 44 non-void zones and the isotopic contributions to the activity at a specific spatial point, the required computing time has been compared. For the steady state problem, agreement between ALARA and FISPACT-97 for the total activity was within 2.5% in all zones at all cooling times, and within 0.5% in most zones. For both the steady state and pulsed problem, agreement between ALARA and DKR-Pulsar 2.0 was within 1% in all zones and at all cooling times where tritium inventories were not significant. The agreement between ALARA and FISPACT-97 for the individual isotopic inventories in the stainless steel first wall backplate were within 1% for all dominant isotopes at all cooling times, while the DKR-Pulsar 2.0 results showed some significant discrepancies. The processing time for ALARA is 2/3 of that for DKR-Pulsar 2.0 and less than 1/5 of that for FISPACT-97. This validation exercise proves that ALARA is an accurate and fast computational tool for the calculation of induced activity in fusion power systems.

I. INTRODUCTION

Following a detailed analysis of the physical approximations and mathematical methods used to calculate induced activation,[6] ALARA [Analytic and Laplacian Adaptive Radioactivity Analysis] v1.0[1,2] has been developed to implement the conclusions of this analysis with modern computer programming techniques. In particular, various choices and decisions were made in the software design process to improve the accuracy of the physical and mathematical models while ensuring that the program would run quickly and be easy to use.[1,6]

For all new computer programs, an important step in the development process is the validation of the program against other computational tools. In the field of fusion activation calculations, there are many such tools. The newest version of DKR,[7] DKR-Pulsar 2.0[4] [hereafter referred to simply as DKR], is often used in the United States for the simultaneous calculation of induced activation at many spatial points. DKR's analytical solution methods have been extended in DKR to model exactly pulsed fusion power systems using matrix methods.[8] The standard fusion activation program in Europe is FISPACT-97 which calculates the induced activation and gas production at a single spatial point using a time-step based ordinary differential equation solver. Both FISPACT-97 and DKR have been shown in the past to agree well with analytical solutions to multi-step activation pathways.[9] ALARA offers improvement over DKR because it is able to accurately model loops in the decay trees and calculate the gas production. In comparison to FISPACT-97, ALARA has many of the advantages of DKR, including the ability to exactly model pulsed irradiation histories and simultaneously calculate the solution at many spatial points. In comparison to both codes, ALARA uses modern programming practices and data handling to increase the flexibility of operation and reduce memory requirements.

II. BENCHMARK SPECIFICATIONS

The IAEA FENDL Calculational Activation Benchmark[5] problem is based on the reference steel/water shielding blanket design in the ITER outline design, including all materials from the inboard magnet to the outboard vacuum vessel. The neutron fluxes are provided by the benchmark in the VITAMIN-J 175 group energy structure for each of the

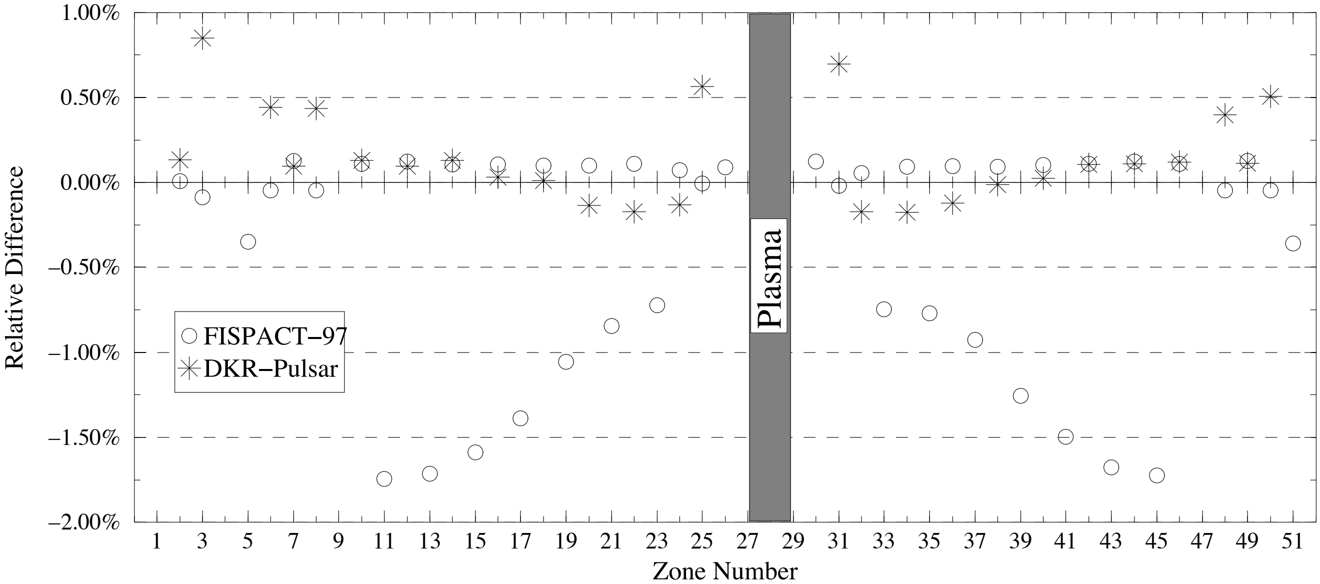

Figure 1: Relative difference between ALARA and other codes for steady state problem at a cooling time of 1 hour.

468 fine mesh intervals. Zones 27 through 29 (see Figures 1 through 4) represent the plasma. These fluxes were calculated using the ONEDANT[10] deterministic neutron transport code with a 14.1 MeV isotropic neutron source normalized to inboard and outboard neutron wall loadings of 1 and 1.5 MW/m^2, respectively. In all cases the FENDL-2/A activation library was used.

The first activation calculations were performed with a steady state operation time of 3 years and cooling times of 1 hour, 1 day, 1 week, 30 days, 1 year and 100 years. A pulsed activation calculation was performed by ALARA and DKR using 94500 pulses of 1000 s with a dwell time of 1200 s between pulses. Based on the time (14 minutes) required to solve the first 100 pulses at a single spatial point, FISPACT-97 was determined to be unsuited to such pulsed operation calculations. Assuming that the total operation time scales linearly with the number of pulses, the full problem would require more than 220 days for each of the 317 spatial points – a total computation time of over 190 years!

III. STEADY-STATE PROBLEM

In ALARA, this calculation built 111 reaction trees with a total of 45075 nodes and a longest chain of length 14, producing 770 different isotopes in the steel-containing intervals, of which 550 were radioactive.

The results have been compared by calculating the relative difference between ALARA and the other codes:

$$\text{Relative Difference} = \frac{\text{ALARA}}{\text{X}} - 1,$$

where X is either FISPACT-97 or DKR.

Figures 1 and 2 show the relative difference between the results of the steady state problem from ALARA and FISPACT-97 and between ALARA and DKR at a cooling time of 1 hour and 1 century, respectively. Since the methods implemented in this version of DKR were not designed to compute the accumulation of light ions (^{1}H, ^{2}H, ^{3}H, ^{3}He, and ^{4}He) emitted by nuclear reactions, its total activity for all zones with dominant tritium inventories is much too small. Since these differences were up to a few orders of magnitude, the relative difference between ALARA and DKR in these zones has not been shown in Figure 1 in order to compare the differences in the other zones.

At a cooling time of 1 hour, the ALARA results are within 1.8% of the FISPACT-97 results throughout the entire geometry, with most zones having a difference of less than 0.4%. The largest differences occur in the 14 water-filled zones of the blanket, increasing in directions away from the plasma in the zones with lower and softer fluxes. The absolute activity in these regions is as low as 2.1×10^9 Bq/m^3 (zone #11) and dominated by very low levels of tritium (5.4 tritium atoms per 10^{12} source atoms) and ^{14}C (2.8 atoms per 10^9 source atoms). This demonstrates a difference in the precision of the two calculations and the way that this precision is defined. In this case, the ALARA calculation had a precision defined directly as 1 atom per 10^{10} source atoms whereas FISPACT-97 calculated inventories as low as 10^5 atoms corresponding to 1 atom per 10^{18} source atoms in water. At a cooling time of 1 century, the differences between ALARA and FISPACT-97 are as high as 2.5%, with the largest differences still occurring in the water-filled zones where, after more than 8 tritium half-lives, the dominant isotope is now ^{14}C. The differences in the other zones remain below 0.4%.

In those zones with insignificant tritium inventories, the differences between ALARA and DKR are less than 0.2%

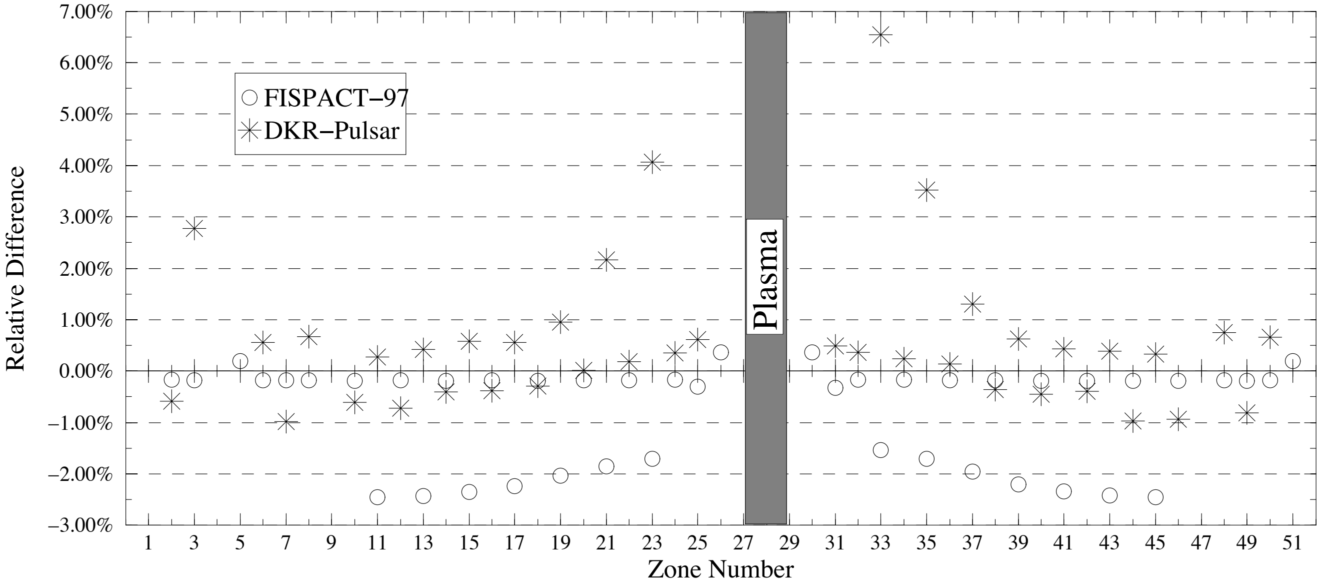

Figure 2: Relative difference between ALARA and other codes for steady state problem at a cooling time of 1 century.

throughout the geometry at a cooling time of 1 hour. After 1 century, although the relative contribution of tritium has increased in some of those same zones, the relative differences are still less than 1%. DKR's inability to account for the light ion production results in tritium inventories which are as much as 6 orders of magnitude too low in the first wall's Be coating, and up to 3 times too low in the blanket's water cooling zones. Even after more than 8 tritium half-lives (1 century), when tritium is responsible for less than 10% of the total activity, the difference between ALARA and DKR in the water can be as high as 7% (zone #33).

A single fine mesh interval was chosen in which to compare the activity of various nuclides in detail. The 1 mm thick stainless steel (SS316) inboard first wall back plate is modeled as a single interval (#242) in zone #24. The large number of initial isotopes in steel and the high flux due to its proximity to the plasma make this a good choice for comparison.

Table 1 shows the seven most dominant isotopes at a cooling time of 1 hour, which together account for over 95% of the total activity. Table 2 shows the five most dominant isotopes at a cooling time of 1 century, accounting for more than 99.7% of the total activity.

Table 1: Detailed differences in interval #242 at 1 hour.

Isotope	ALARA [10^{16}Bq/m^3]	Relative Difference [%]	
		FISPACT-97	DKR-Pulsar 2.0
^{56}Mn	114.6	-0.051	0.15
^{55}Fe	85.5	0.24	-0.10
^{51}Cr	75.7	0.019	-0.041
^{57}Co	24.4	-0.081	3.0
^{54}Mn	20.0	0.97	0.15
^{58m}Co	10.3	-0.053	0.30
^{58}Co	8.32	-0.048	-13.74

The agreement between ALARA and FISPACT-97 is seen to be within 1% in all cases. DKR, on the other hand, has relative differences of up to 16%. These discrepancies are most probably caused by the inability of DKR to model certain kinds of loops in the decay chains and the influence which this has on the decay chain creation calculations.

IV. PULSING PROBLEM

The results of ALARA and DKR for the pulsing problem are compared in Figure 3 for both 1 hour and 1 century. Once again, tritium plays an important role in the discrepancies, which are nearly identical to the discrepancies between ALARA and DKR for the steady state problem. In the glass insulator of the TF coil (zone #3), the discrepancy in the pulsing problem is twice as high as in the steady state problem at 1 hour, but the same at 1 century. This demonstrates the true physical effect of pulsing on the importance of the tritium inventory at relatively short cooling times. Basically,

Table 2: Detailed differences in interval #242 at 1 century.

Isotope	ALARA [10^{13}Bq/m^3]	Relative Difference [%]	
		FISPACT-97	DKR-Pulsar 2.0
^{63}Ni	27.8	-0.17	0.40
^{59}Ni	3.80	-0.18	-1.2
^{91}Nb	3.37	-0.21	1.3
^{14}C	0.86	-0.22	-0.19
^{93}Mo	0.69	-0.21	16

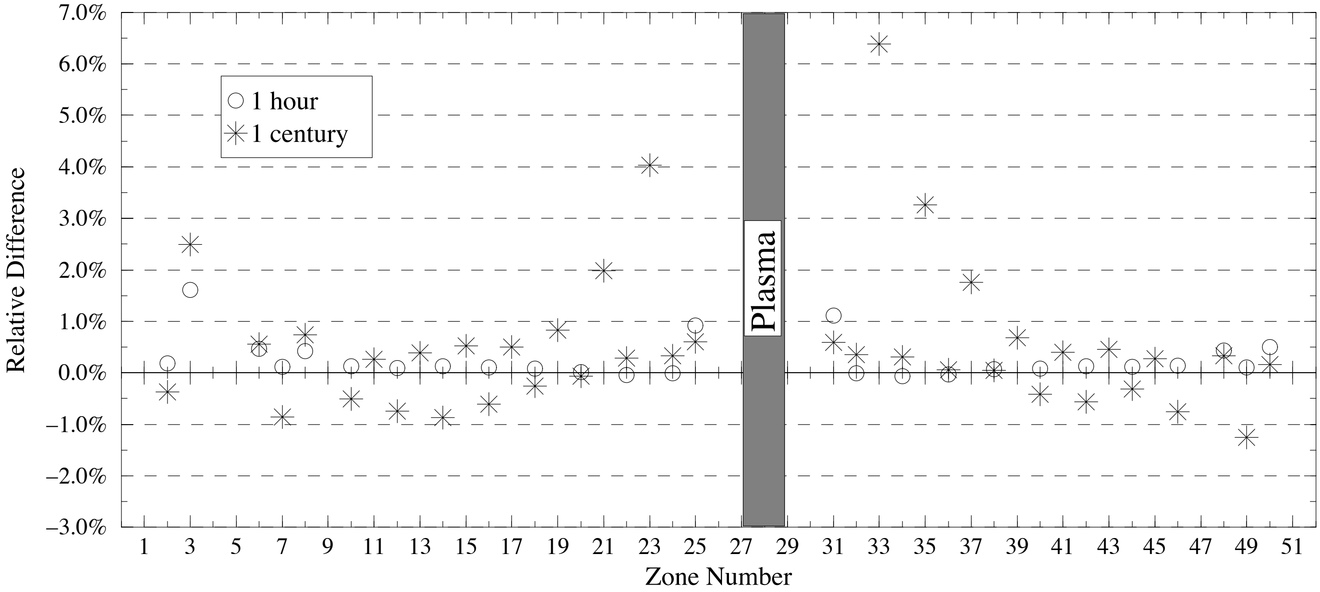

Figure 3: Relative difference between ALARA and DKR for the pulsing problem at cooling times of 1 hour and 1 century.

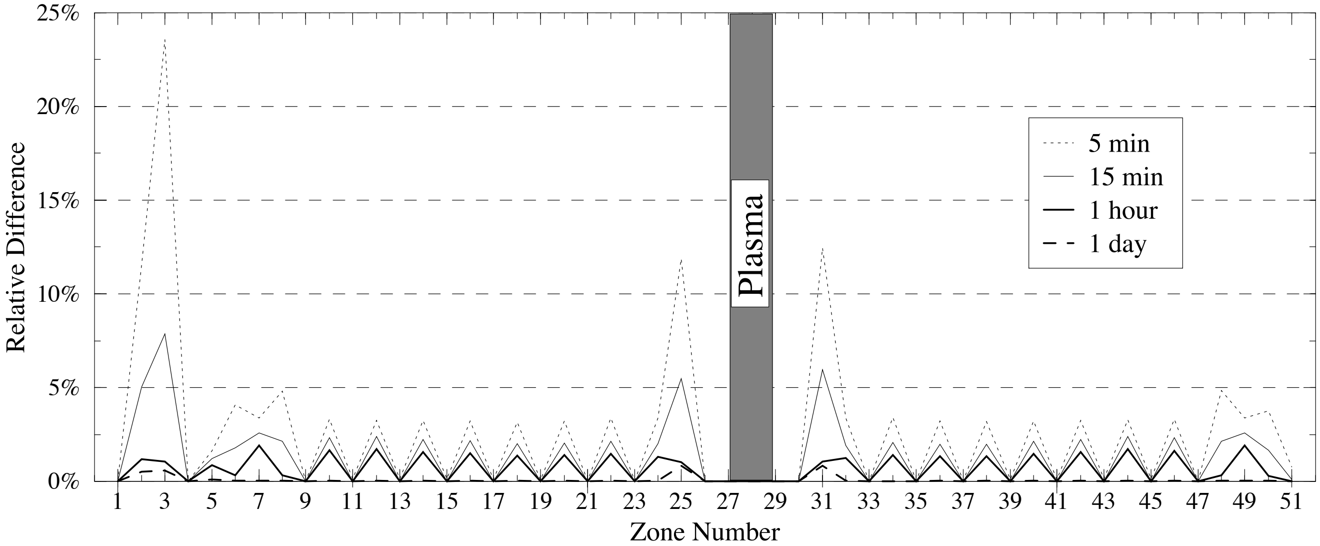

Figure 4: Relative difference between exact pulsed solution and steady state approximation at various cooling times.

the pulsed operation will tend to reduce the inventory of isotopes with half-lives which are of the same order of magnitude as the dwell time between pulses: very long-lived isotopes will decay little between pulses and slowly reach their saturation level while very short-lived isotopes will decay completely between pulses, but can reach their saturation level in a single pulse.[11] The dominant isotopes in the glass at 1 hour are ^{64}Cu and ^{24}Na, both with half-lives slightly longer than half a day. Their inventories in the pulsed problem are 50% less than in the steady state problem, while the tritium inventory is reduced by less than 10%.

One method of modeling a pulsed problem as a steady state problem is to preserve both the total fluence and the total operating time.[11–13] Using ALARA, the results of such an approximate calculation with a flux scaling factor of 1/2.2 and total operation time of 2.079×10^8 are compared to the exact solution in Figure 4, represented as

$$\text{Relative Difference} = \frac{\text{Pulsing}}{\text{Steady State}} - 1.$$

In this case, because of the nature of the pulsing history, the effect can only be seen at short cooling times. The two materials with largest discrepancies are the glass insulator (zone #3) and the first wall heat sink (Cu-Be-Ni in zones #25 and #31). In the former, the activity of ^{28}Al ($t_{1/2} = 2.25$ m), responsible for over 25% of the activity at a cooling time of

1 minute, is under-calculated by 50%. The same is true of ^{66}Cu ($t_{1/2}$ = 5.10 m) which is responsible for just under 10% of the activity in the first wall.

V. COMPUTING RESOURCES

All three codes were used on the same IBM RS/6000 Model 595 P2SC workstation. The full steady-state problem was solved by ALARA in 3425 s (57^m5^s) and by DKR in 5253 s ($1^h27^m33^s$). The same problem required 20715 s ($5^h36^m25^s$) for a previously developed shell-script system which sequentially runs FISPACT-97 for each of the intervals. The pulsed problem was solved by ALARA in 5736 s ($1^h35^m36^s$), with 44591 nodes and a longest chain of 14. DKR needed 10855 s ($3^h0^m55^s$). FISPACT-97 was unable to solve the pulsed problem.

For the steady state problem, ALARA requires a maximum of 35 MB of RAM and, other than the binary library of just over 11 MB, uses no hard drive space. DKR required as much as 107 MB of RAM and up to 250 MB of temporary hard drive space in addition to its 10 MB text library. Other than the 38 MB data libraries, FISPACT-97 uses negligible quantities of RAM and hard drive space since it solves each interval sequentially.

VI. CONCLUSIONS

The ALARA activation code has been validated for use in calculating the activation of fusion power systems. The results for a steady state activation problem have been compared to the results from two standard codes whose accuracy has been well documented:[9] FISPACT-97 and DKR. Discrepancies between the total activities calculated by ALARA and the other codes are always less than 2.5%, except where DKR is unable to calculate the tritium production from emitted light ions. The results of a pulsing problem have been compared to DKR (FISPACT-97 was unable to perform such a calculation in a reasonable time). The discrepancies in this case are once again primarily due to the lack of tritium production in DKR, and are otherwise less than 1%.

Based on this validation and its faster and less memory-intensive operation, ALARA is recommended for the solution of fusion activation problems.

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