The Monte Carlo Method: Versatility Unbounded in a Dynamic Computing World
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ALEPH: AN EFFICIENT APPROACH TO MONTE CARLO BURN UP

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ABSTRACT

The application of the Monte Carlo method to the field of burn up calculations leads to powerful and accurate tools which are however quite demanding on calculation time because the reaction rates required for burn up calculations are always calculated within an MC code. Trying to solve this problem, we have formulated a more efficient approach to Monte Carlo burn up where we calculate the reaction rates outside the MC code. To demonstrate this, we have implemented it in ALEPH, a Monte Carlo burn up code using MCNP or MCNPX, ORIGEN 2.2 and NJOY 99.90. A decrease of a factor 30 in calculation time has been observed while the results obtained are in excellent agreement with the NEA/OECD Burn-up Credit Criticality Benchmark. It has also been shown that a statistical error of 0.5 % on the total flux in a cell is sufficient to obtain reliable results on the isotope composition.

Key Words: MC Burn Up, Fuel Cycle

1 INTRODUCTION

The application of the Monte Carlo method to the field of burn up calculations leads to powerful tools with a broad area of applications: from simple 1D to complex 3D geometries, either normal critical systems, sub-critical systems with an external fixed source, ... The use of Monte Carlo also allows for multi-particle physics, complex interaction laws and detailed energy-angle descriptions which can be of crucial importance in applications such as Accelerator Driven Systems (ADS), ... These tools are however quite demanding on calculation time because the reaction rates required for burn up calculations are always calculated within an MC code, examples are MONTEBURNS [1], MOCUP [2], MCB [3], ...

The primary purpose of the Monte Carlo code in an MC burn up code is to calculate the spectrum weighted reaction rates σ for every nuclide and reaction considered in the transmutation chain:

$$\sigma = \frac{\int \sigma(E)\,\phi(E)\,dE}{\int \phi(E)\,dE} \tag{1}$$

in which $\sigma(E)$ is the energy dependent microscopic cross section of the nuclide in question and $\phi(E)$ is the neutron energy spectrum in the cells with the material that we wish to burn. A code such as MCNP [4] or MCNPX [5] estimates these quantities as a sum over all histories and interactions going through the cell in which we want to know the reaction rate [4, 6]:

$$\int dV \int \sigma(E)\,\phi(E)\,dE = \frac{1}{N}\sum_h \sum_i l_{i,h} w_{i,h} \sigma(E_{i,h}) \tag{2}$$

$$\int dV \int \phi(E)\,dE = \frac{1}{N}\sum_h \sum_i l_{i,h} w_{i,h} \tag{3}$$

where $E_{i,h}$ is the energy of a particle within the cell where we want to calculate the reaction rate with a corresponding track length $l_{i,h}$ and weight $w_{i,h}$. In MCNP(X), these quantities are accumulated during the simulation of all the particles. As such, the following operations have to be performed for every history, every interaction and for every reaction rate that we want:

- calculate the cross section value $\sigma(E_{i,h})$ (that is, look for the right interval and perform a linear interpolation)
- calculate the product $l_{i,h} w_{i,h} \sigma(E_{i,h})$ and add it to the previous result

If the number of interactions and histories is large, looking up the cross section value every time will become a very time consuming operation. If we calculate for instance the (n,γ) reaction rate of ^{238}U we already see an increase of 8 % in calculation time. Adding more reaction rates only makes it worse: when calculating about 1000 reaction rates (which are required for burn up calculations) we can observe an increase in calculation time of a factor 30.

A solution for this problem would be to calculate the required reaction rates after the MC calculation finished - allowing us to reduce the number of operations required and thus reduce the total calculation time. For this purpose we have developed two different strategies.

The first one uses a multi-group approach to the problem and has already been implemented in ALEPH [7]. ALEPH is our own Monte Carlo burn up code capable of using any version of MCNP or MCNPX for spectral calculations, a slightly modified version of ORIGEN 2.2 [8] for evolution calculations and data read from the ENDF-VI format by using NJOY 99.90 [9]. In this multi-group ALEPH approach, we calculate the reaction rate σ as:

$$\sigma = \frac{\sum_g \sigma_g \phi_g}{\sum_g \phi_g} \tag{4}$$

in which σ_g and ϕ_g are the cross section and spectrum of group g with boundaries E_{g-1} and E_g. Only the multi-group spectrum has now to be calculated by the Monte Carlo code. The group structure has been chosen so that the reaction rates calculated by equation (4) are within one standard deviation of the values calculated by MCNPX using formulas (2) and (3). The resulting group structure is quite large (of the order of 10^4 groups) and can be assumed to be practically continuous. During the Monte Carlo simulation, the code has only to determine in which energy bin to accumulate the flux. The extra calculation time that this operation takes is so small that it is

barely visible, even for our large group structure. During a test with a structure of around 10^5 groups (10 times more than we actually need) we observed an increase in calculation time of about 2 %.

The group cross section σ_g itself is calculated analytically by ALEPH using the following formula:

$$\sigma_g = \frac{\int_{E_{g-1}}^{E_g} \sigma(E)\,\varphi(E)\,dE}{\int_{E_{g-1}}^{E_g} \varphi(E)\,dE} \tag{5}$$

with $\sigma(E)$ the energy dependent cross section and $\varphi(E)$ the spectrum used to weigh the cross section (which can be a constant spectrum or a spectrum composed of a Maxwellian spectrum, a slowing down spectrum and a fission spectrum).

The total time required to calculate the reaction rates using formula (4) and (5) is constant regardless of the number particles simulated and is of the order of seconds to minutes depending upon the system on which the code runs. On a dual Xeon 3 GHz system for instance, it takes 15 seconds to calculate all multi-group cross sections and reaction rates for 296 nuclides of the JEF 2.2 library. This is negligible compared to the calculation time of a single MCNP or MCNPX run - unless very few particles are simulated. By using this multi-group ALEPH approach we have effectively reduced the calculation time by a factor 30.

The second strategy to solve this time problem is to gather the required data (being the energy $E_{i,h}$, the track length $l_{i,h}$ and weight $w_{i,h}$) and write them to a separate file. After the MC code finishes the simulation, the data should be sorted in increasing values of energy so that we can go over these values energy by energy while going through the linearised cross sections interval by interval. This way, we have to go through the entire cross section only once to calculate a single reaction rate. We will implement this strategy in the near future, but it will require some changes to the MCNP and MCNPX source code to extract the necessary data.

2 INNER STRUCTURE OF ALEPH

ALEPH is in essence an interface code between NJOY 99.90, ORIGEN 2.2 and any version of MCNP or MCNPX (we currently use MCNPX 2.5.e) as can be seen in figure 1. Except for some minor modifications to ORIGEN 2.2 to improve output accuracy (the number of significant digits were increased from 3 to 5) and to increase the memory allocation no changes have been made whatsoever to the source code of the programs involved. ALEPH itself has been written in C++ using a highly modular design to allow for great flexibility. Replacing for instance MCNP or MCNPX by another MC code would be quite easy because of this modular design (we would only have to replace the object responsible for the MCNP-ALEPH interface by a similar object for the new MC code).

The input required by ALEPH is the irradiation history, along with an initial MCNP(X) input file and other code options. Information such as initial material composition, temperatures, volumes, ... are read from the initial MCNP(X) input file. Before every MCNP(X) run ALEPH generates a new input file based upon the input options of the user. First of all, the material

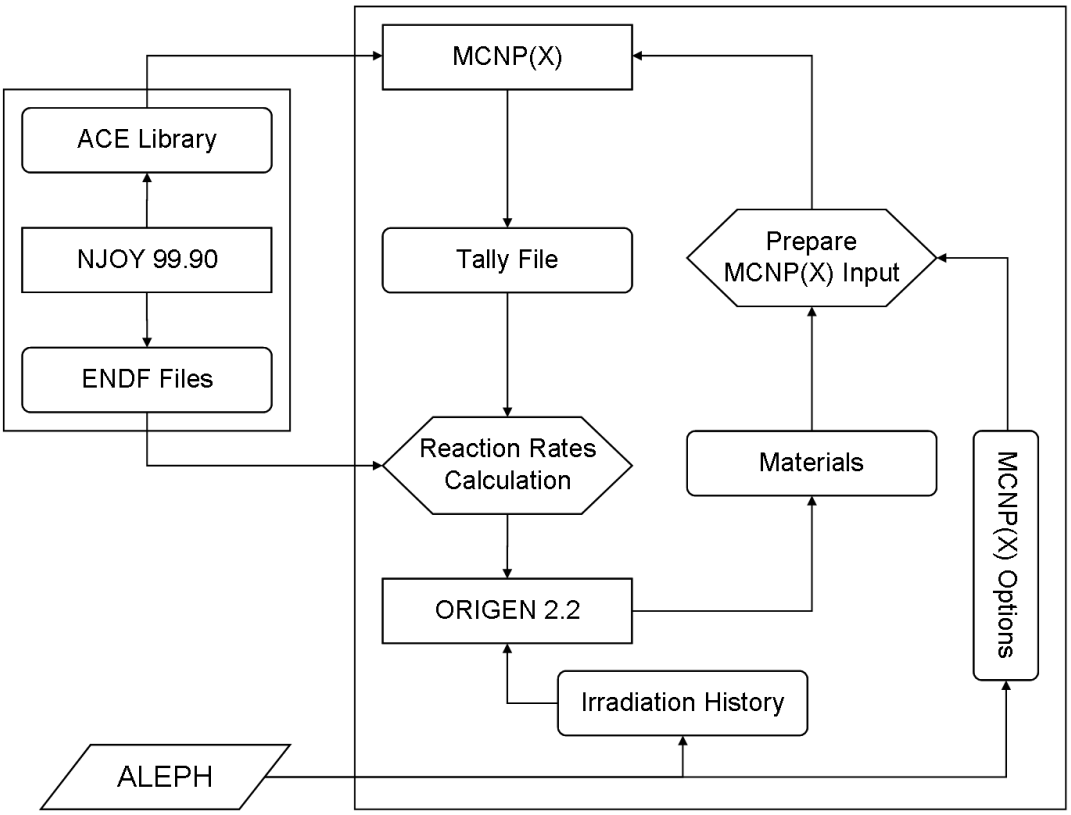

Figure 1: Calculation flow in ALEPH

composition of the materials that are being burned are updated. For the purpose of transport calculations we truncate the material composition calculated by ORIGEN using a fractional absorption criterion specified by the user. Only those nuclides responsible for e.g. 99 or 99.9 % of all absorptions are included - nuclides that were originally present are added by default and do not necessarily contribute to this fractional absorption criterion. If requested by the user, ALEPH will also change the position of burnable materials and replace materials (to represent reshuffling). ALEPH can also change the temperature of any material (both materials that are being burned or materials that are left unchanged) and density and/or composition of a material that is not being burned.

After every MCNP(X) run, the multi-group spectra are read from the tally file. ALEPH will now generate the reaction rates required by ORIGEN. ORIGEN makes a distinction between three fundamental types of materials: activation products, actinides (including their daughter nuclei) and fission products. The required input of reaction rates and other data depends upon the type of material. Activation products require cross sections for (n,γ) (both to the ground state and the first metastable state), (n,2n) (both to the ground state and the first metastable state), (n,α) and (n,p) reactions. In the case of actinides, the (n,α) and (n,p) reactions have been replaced by fission and the (n,3n) reaction. Fission products have the same cross sections as activation products but some of the fission products have direct fission yield data, associated with 8 primary actinides

(^{232}Th, ^{233}U, ^{235}U, ^{238}U, ^{239}Pu, ^{241}Pu, ^{245}Cm and ^{252}Cf). ALEPH will use an original ORIGEN cross section library and only change the values for isotopes for which data is available.

The reaction rates σ for the (n,α), (n,p), fission and (n,3n) reactions calculated by equation (4) can be used immediately by ORIGEN. In the case of (n,γ) and (n,2n), we still need to distinguish between the reaction rate to the ground state and the first metastable state. For this purpose, ALEPH uses a branching ratio obtained from the original ORIGEN library:

$$\lambda = \frac{\sigma^o_{mt}}{\sigma^o_{gr} + \sigma^o_{mt}} \tag{6}$$

where σ^o_{gr} is the original reaction rate to the ground state and σ^o_{mt} the one to the first metastable state. The new reaction rates σ_{gr} and σ_{mt} will then be given by:

$$\sigma_{gr} = (1 - \lambda)\,\sigma \tag{7}$$

$$\sigma_{mt} = \lambda\sigma \tag{8}$$

in which σ is the reaction rate calculated with equation (4).

The direct fission yield Y of an isotope used by ORIGEN can also be recalculated using a formula similar to equation (4):

$$Y = \frac{\sum\limits_g Y_g \sigma_{f,g} \phi_g}{\sum\limits_g \sigma_{f,g} \phi_g} \tag{9}$$

in which Y_g is the yield of the fission product and $\sigma_{f,g}$ is the fission cross section of the actinide that produces the fission product in group g. This will be done in a future version of ALEPH. For the moment, ALEPH leaves the original yield values from ORIGEN unchanged.

Another significant feature of ALEPH is that it reads microscopic cross sections directly from an ENDF file prepared by NJOY (in linear interpolated form). To automatically generate these ENDF files and the corresponding ACE files (at several different temperatures) for transport calculations, we have created a utility called ALEPH-DLG (Data Library Generator) [10]. This way, we ensure that exactly the same nuclear data is used within the entire code system. The probability tables in the unresolved resonance energy region are switched off during the MCNP(X) calculations because the multi-group approach in ALEPH cannot use these probability tables like MCNP(X) can as these change the cross section for a single particle while for a collection of particles we see an average cross section. Whenever we adopt the second strategy described above, we can use the probability tables as they are meant to be used.

The JEF 2.2 nuclear data evaluation is preferred for use by ALEPH due to its completeness compared to other evaluations (such as ENDF-B6.8) in high energy reactions such as (n,p), (n,γ), (n,2n) and (n,3n) that are required by ORIGEN.

3 BENCHMARKING ALEPH

To assess the abilities of ALEPH, we have performed the Burn Up Credit Criticality Benchmark - Phase IV-B for first recycle MOX fuel [11]. The investigation of burn up credit for

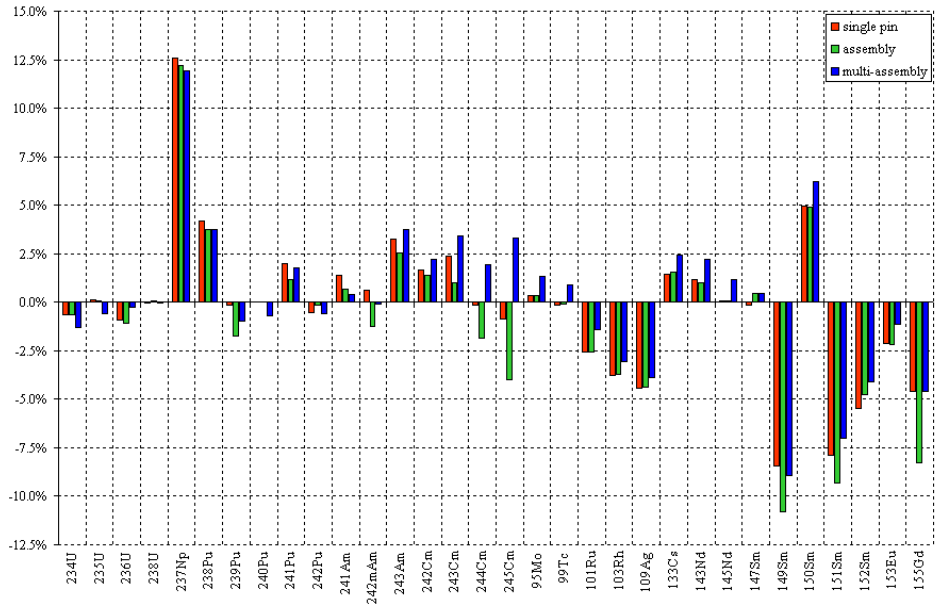

Figure 2: Relative deviation of ALEPH compared to APOLLO2 after 1320 days for the single pin, assembly and multi-assembly (supercell) model

different types of fuel is an ongoing objective of the OECD/NEA Burn Up Credit Working Group. As part of that work, the Working Group has defined a burn up credit benchmark program for MOX fuels (i.e. fuel containing a mixture of U and Pu oxides) in PWR reactors. Phase VI-B of this benchmark program concerns the calculation of irradiated MOX fuel compositions. For this benchmark, three geometrical 2D models were considered:

- A multi-assembly (or supercell) model with a MOX assembly containing 289 pins (24 guide tubes, 1 instrumentation tube, 12 low-enriched MOX pins, 68 medium-enriched MOX and 184 high-enriched MOX pins) along with three UO_2 assemblies with translational boundary conditions.
- A single MOX fuel assembly (the same as the one described above) with reflective boundary conditions.
- A single pin model which conserves the fuel-to-moderator ratio of the assembly model using an average MOX fuel composition with reflective boundary conditions.

The irradiation history consists of three cycles of 420 days full power with an End Of Cycle (EOC) burn up of 16 GWd/tHM with 30 days of downtime in between the cycles. For the calculation in ALEPH, we have subdivided every cycle into time steps of 30 days (every step thus accounts for an average burn up of about 1 GWd/tHM). For every model we have run a criticality calculation of 280 cycles (30 inactive and 250 active cycles) with 20000 neutron histories per cycle. The relative errors obtained on the total flux in the cells that were burned were (on average) 0.02 % for the single pin, 0.1 % for the assembly model and 1 % for the supercell model.

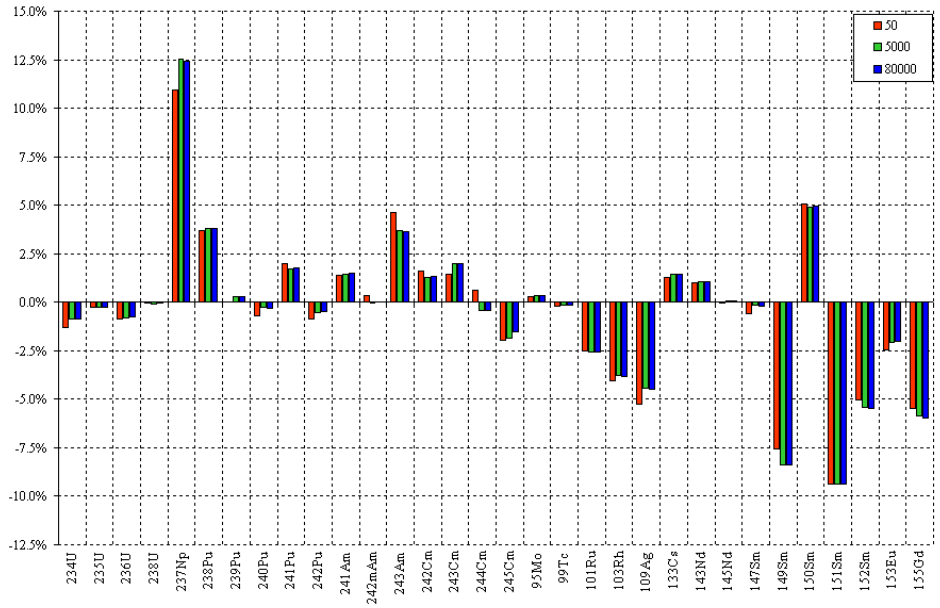

Figure 3: Relative deviation of ALEPH compared to APOLLO2 after 1320 days for the single pin model with different statistical errors on the total flux

We have chosen to compare our results with APOLLO2, the French PWR reference code. For ease of comparison we use the relative deviation of our results to the ones obtained by APOLLO2. Table I and figure 2 give these deviations for 17 actinides and 15 common fission products after the third cycle (that is after a period of 1320 days). It is obvious from this table and figure that our results are in good agreement with those obtained by APOLLO2. Our results are well within 5 % of those from APOLLO2 except for ^{237}Np, ^{149}Sm, ^{150}Sm (in the supercell case), ^{151}Sm, ^{152}Sm (for the single pin) and ^{155}Gd (for the assembly case). The benchmark results for those nuclides however showed quite large deviations from the mean value of all contributors. ^{237}Np has for instance deviations of 35.0 % for the single pin, 37.6 % for the assembly and 36.8 % for the supercell model. In the case of ^{155}Gd this is 35.9 %, 32.7 % and 31.9 %. The deviations for Sm are smaller than the previous ones, but still high enough to explain our difference with APOLLO2. ^{149}Sm shows deviations of 6.5 %, 5.4 % and 7.5 %. For ^{151}Sm these deviations are 10.1 %, 9.3 % and 11.1 %. ^{150}Sm has a deviation of 3.4% for the supercell case and ^{152}Sm has a deviation of 8.8 % for the single pin model.

Our results for the uranium and plutonium isotopes are well within 1 to 2 % of APOLLO2 except for ^{238}Pu for which we observe a 3 to 4 % difference. But again, the benchmark revealed a rather high deviation from the mean value for this isotope: 8.4 % for the single pin, 9.0 % for the assembly and 9.2 % for the supercell model.

To study the influence of the statistical error on the total flux, we have performed several calculations using the single pin model with different numbers of particles per cycle. Figure 3 and table II give the relative deviation to APOLLO2 after 1320 days for 50, 5000 and 80000 neutrons per cycle (which correspond to errors of 0.5 %, 0.04 % and 0.01 %). We observe little to no

variation in the deviations except for ^{237}Np (a difference of 1.5 %), ^{243}Am (a difference of 1 %) and the fission products ^{109}Ag and ^{149}Sm (a difference of about 0.8 %) when the statistical error on the total flux is reduced from 0.5 % to 0.01 %. It is obvious that a statistical error of 0.5 % on the total flux is more than sufficient to obtain reliable values for the isotope composition as decreasing the error below this value has little to no effect at all.

ALEPH has also been benchmarked using experimental data from the ARIANE programme [12] (for the 400 MWe PWR Beznau-1 reactor) in the framework of the European FP5 VALMOX project. ALEPH gives similar results as WIMS-8a with some significant improvements for ^{239}Pu (C/E is 0.99 for ALEPH versus 1.07 for WIMS), ^{237}Np (0.81 for ALEPH versus 0.69 for WIMS) and ^{241}Am (1.04 for ALEPH versus 1.08 for WIMS). Recalculation with JEFF 3.0 nuclear data reflects the improvements to JEF 2.2 due to changes introduced in the basic data: 1 % improvement for ^{235}U (from 1.01 to 1.00), 4 % improvement for ^{236}U (from 0.88 to 0.92), 4 % improvement for ^{237}Np (from 0.81 to 0.85), 3 % improvement for ^{242}Pu (from 0.97 to 1.00) and 5 % improvement for ^{245}Cm (from 0.92 to 0.97). These results are discussed in more detail in [13].

4 CONCLUSIONS

A more efficient multi-group approach to MC burn up has been developed, in which the required reaction rates are calculated outside the MC code. In this approach, the MC code needs only to provide a multi-group spectrum in every cell that we wish to burn. This has been implemented into ALEPH resulting in a reduction of the calculation time by a factor 30. The results of this code on the NEA/OECD Burn-up Credit Criticality (BUC) Benchmark are in good agreement with the results from APOLLO2 (below 5 % deviation) except for nuclides such as ^{237}Np and ^{155}Gd. Using the single pin model of the BUC benchmark we have also shown that a statistical error of 0.5 % is sufficient to obtain reliable isotope compositions.

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Table I: Relative deviation of ALEPH compared to APOLLO2 after 1320 days for the single pin, assembly and multi-assembly (supercell) model

nuclide	single pin	assembly	supercell
^{234}U	-0.6	-0.7	-1.3
^{235}U	0.1	0.1	-0.6
^{236}U	-0.9	-1.1	-0.3
^{238}U	0.1	0.0	0.0
^{237}Np	12.6	12.2	11.9
^{238}Pu	4.2	3.7	3.8
^{239}Pu	-0.2	-1.8	-1.0
^{240}Pu	0.0	0.0	-0.7
^{241}Pu	2.0	1.2	1.8
^{242}Pu	-0.5	-0.1	-0.6
^{241}Am	1.4	0.7	0.4
^{242m}Am	0.6	-1.2	-0.1
^{243}Am	3.2	2.5	3.7
^{242}Cm	1.7	1.4	2.2
^{243}Cm	2.4	1.0	3.4
^{244}Cm	-0.1	-1.8	1.9
^{245}Cm	-0.9	-4.0	3.3
^{95}Mo	0.4	0.3	1.4
^{99}Tc	-0.1	-0.1	0.9
^{101}Ru	-2.5	-2.6	-1.4
^{103}Rh	-3.8	-3.7	-3.1
^{109}Ag	-4.4	-4.4	-3.9
^{133}Cs	1.4	1.5	2.4
^{143}Nd	1.2	1.0	2.2
^{145}Nd	0.1	0.1	1.2
^{147}Sm	-0.1	0.5	0.5
^{149}Sm	-8.4	-10.8	-8.9
^{150}Sm	5.0	4.9	6.2
^{151}Sm	-7.9	-9.3	-7.0
^{152}Sm	-5.5	-4.8	-4.1
^{153}Eu	-2.1	-2.2	-1.2
^{155}Gd	-4.6	-8.3	-4.6

Table II: Relative deviation of ALEPH compared to APOLLO2 after 1320 days for the single pin model with different statistical errors on the total flux

nuclide	50	5000	80000
^{234}U	-1.3	-0.9	-0.9
^{235}U	-0.2	-0.3	-0.3
^{236}U	-0.9	-0.8	-0.8
^{238}U	-0.1	-0.1	-0.1
^{237}Np	11.0	12.5	12.4
^{238}Pu	3.7	3.8	3.8
^{239}Pu	0.0	0.3	0.3
^{240}Pu	-0.7	-0.3	-0.3
^{241}Pu	2.0	1.7	1.8
^{242}Pu	-0.8	-0.5	-0.5
^{241}Am	1.4	1.5	1.5
^{242m}Am	0.3	0.0	0.0
^{243}Am	4.6	3.7	3.6
^{242}Cm	1.6	1.3	1.3
^{243}Cm	1.4	2.0	2.0
^{244}Cm	0.6	-0.4	-0.4
^{245}Cm	-2.0	-1.8	-1.5
^{95}Mo	0.3	0.4	0.4
^{99}Tc	-0.2	-0.1	-0.1
^{101}Ru	-2.5	-2.5	-2.5
^{103}Rh	-4.0	-3.8	-3.8
^{109}Ag	-5.2	-4.5	-4.5
^{133}Cs	1.3	1.4	1.4
^{143}Nd	1.0	1.1	1.1
^{145}Nd	0.0	0.0	0.0
^{147}Sm	-0.6	-0.1	-0.2
^{149}Sm	-7.6	-8.4	-8.4
^{150}Sm	5.1	4.9	4.9
^{151}Sm	-9.4	-9.4	-9.4
^{152}Sm	-5.0	-5.4	-5.5
^{153}Eu	-2.4	-2.1	-2.0
^{155}Gd	-5.5	-5.9	-5.9