

ALEPH 1.1.2

A Monte Carlo Burn-Up Code



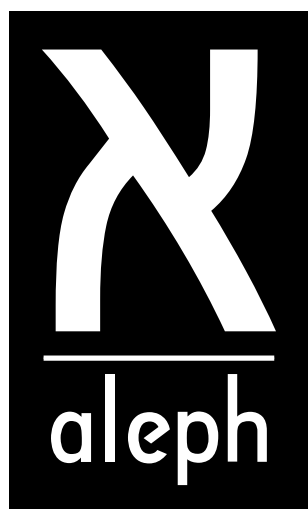
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January, 2006

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Foreword

Development of ALEPH started roughly two years ago, with Wim uttering the words “Bernard, je pourrais écrire un petit program qui peut faire ça”. At the time, we were formulating our approach to Monte Carlo burn-up to solve the burn-up problems that both of us were facing. Little did we know that - 20000 lines of C++ code later - ALEPH would exceed all of our expectations.

Initially, the code was just a simple post processor to MCNP(X) to calculate an ORIGEN library using cross section linearized by PREPRO 2002. The code didn’t even have a name back then. Very quickly, we added the possibility to run ORIGEN from within this program so that it could calculate the resulting MCNP(X) material composition. While this version - which we had called ALEPH-SPECTRUM - was a big step forward, it still required a lot of copy/paste work to perform a full burn-up calculation.

Encouraged by our initial success, we set out to fully automate the entire process (that is: run MCNP(X), read the resulting spectra, calculate the libraries, run ORIGEN, ...). By the end of June 2004, the real first version of ALEPH was completed. It was this version that was used in the VALMOX project and for the the burn-up calculations in the MYRRHA DRAFT-2 pre-design file.

Around that time, we also decided to replace PREPRO 2002 by NJOY so that ALEPH and MCNP(X) would use exactly the same nuclear data. This resulted in the creation of ALEPH-DLG (Data Library Generator) to prepare the cross section data for ALEPH and MCNP(X) by automating the entire NJOY process.

By December 2004, we decided to add features to allow for core reshuffling, multiple temperatures, ... Because these features dictated drastic changes in the original source code, we decided to rewrite the entire code. Along the way, we also added the possibility to change the geometrical specification of the MCNP(X) model to allow for variable geometry (to simulate for instance moving control rods, ...). This reports deals with this fourth incarnation of ALEPH, the first official release of ALEPH (version 1.1.2).

Before we conclude, we would like to express my gratitude to a number of people. First of all John Hendrickx (LANL) for some fruitful discussions both by e-mail and in person on the internal workings of MCNPX, Luc Borms for encouraging me to try C++ and for his technical help, Gert Van den Eynde for his help concerning numerical techniques, Ben Vanhaeren for his help concerning compilers and the Linux operating system, Thierry Aoust, Edouard Malambu, Nadia Messaoudi, Vitali Sobolev and André Beeckmans de West-Meerbeeck for their interest in ALEPH from the very beginning. Thanks also to Dirk Maes and everybody else for enduring my incessive ranting about this subject and Martine Vos for making the ALEPH logo.

Wim Haeck and Bernard Verboomen
Mol, January 2006

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Chapter 1

Introduction to ALEPH

1.1 The Monte Carlo method and burn-up applications

In the last 40 years, Monte Carlo particle transport has been applied to a multitude of problems such as shielding and medical applications, to various types of nuclear reactors, . . . The success of the Monte Carlo method is mainly based on its broad application area, on its ability to handle nuclear data not only in its most basic but also most complex form (namely continuous energy cross sections, complex interaction laws, detailed energy-angle correlations, multi-particle physics, . . .), on its capability of modeling geometries from simple 1D to complex 3D, . . . There is also a current trend in Monte Carlo applications toward high detail 3D calculations (for instance voxel-based medical applications), something for which deterministic codes are neither suited nor performant as to computational time and precision.

Apart from all these fields where Monte Carlo particle transport has been applied successfully, there is at least one area where Monte Carlo has had limited success, namely burn-up and activation calculations where the time parameter is added to the problem. The concept of Monte Carlo burn-up consists of coupling a Monte Carlo code to a burn-up module to improve the accuracy of depletion and activation calculations. For every time step the Monte Carlo code will provide reaction rates to the burn-up module which will return new material compositions to the Monte Carlo code. So if static Monte Carlo particle transport is slow, then Monte Carlo particle transport with burn-up will be even slower as calculations have to be performed for every time step in the problem.

The computational issues to perform accurate Monte Carlo calculations are however continuously reduced due to improvements made in the basic Monte Carlo algorithms, due to the development of variance reduction techniques and due to developments in computer architecture (more powerful processors, the so-called brute force approach through parallel processors and networked systems, . . .). This evolution of computer architecture is going to continue in the future. Moore's law on computer processor development clearly states that the speed of processors doubles every year. So within 10 years we will see computers that are 1000 times faster compared to our high end computers of today, although it is possible that constraints such as processor cooling will limit the validity of this law in the future (new technologies might however resolve this issue).

In recent years, these developments have created a renewed interest in Monte Carlo burn-up. As a matter of fact, work is now under way at LANL to finally include a transmutation module as a standard option into MCNPX [1, 2, 3], one of the standard Monte Carlo codes available today with a development history of over 30 years. An overview of different MC burn-up codes

can be found in table 1.1 [4]-[10].

Table 1.1: Overview of Monte Carlo burn-up codes in existence.

Code Name	MC Code	Burn-Up Code	Year	Institution
MOCUP [4]	MCNP4A	ORIGEN 2.1	1995	INEL
MC-REBUS [5]	MCNP	REBUS	1998	ANL
OCTOPUS	MCNP	FISPACT	1998	NRG
MONTEBURNS [6]	MCNP4B	ORIGEN2	1999	LANL
EVOLCODE [7]	MCNP4B	ORIGEN 2.1	1999	CIEMAT
MCB [8]	MCNP4C	Custom	1999	KTH
MCWO [9]	MCNP	ORIGEN2	2000	INEEL
MVP-BURN	MVP	Custom	2000	JAERI
BURNCAL	MCNP4B	Custom	2002	SNL
MCODE [10]	MCNP4C	ORIGEN 2.1	2002	MIT
ALEPH	MCNP/MCNPX	ORIGEN 2.2	2004	SCK•CEN
MCNPX [1]	MCNPX	CINDER	2005	LANL

1.2 Improving Monte Carlo burn-up

By examining and reflecting upon the basic Monte Carlo transport algorithms, on the tally track length estimator (which is used to calculate the reaction rates) and on the basic functions of a Monte Carlo burn-up code we have identified some points of possible improvement in Monte Carlo burn-up calculations.

First of all, Monte Carlo burn-up codes are quite time consuming (and thus rather inefficient) due to the sheer number of reaction rates that have to be calculated. Because of this, most users decide to limit the number of actinides and fission products to be considered in the transmutation chains. Sometimes users also consider very few burn-up steps over long periods of irradiation or provide a small number of burn-up zones in which reaction rates are to be calculated. This can have profound consequences on the accuracy of the calculation. By adopting a new approach to reaction rate calculation (where we perform the calculation outside the Monte Carlo code) one can reduce the calculation time significantly while ensuring maximum accuracy.

The nuclear data itself should also get some attention. Apart from the reaction rates, there is still the need for accurate branching ratio and direct fission yield data. By using nuclear data evaluations in the ENDF-format [11] we have access to all this information (along with the cross sections themselves) at once. This also allows for great flexibility because we can start using new data whenever it becomes available. An automatic coupling with NJOY [12] or a similar code will also facilitate library generation.

Another weak point (either true or conceived) of Monte Carlo burn-up codes is their complexity. These codes often use a script or link approach so that the user would have to understand and manage a large number of input and output files while the conversion of data from one form into another would introduce approximate results due to successive round off [2]. This can be solved by providing an easy to use interface that actually “hides” the burn-up code (which is something the new transmutation option in MCNPX will achieve).

These insights and developments have resulted in the creation of ALEPH, a Monte Carlo burn-up interface code that is capable of using any version of MCNP [13] or MCNPX [1] with ORIGEN 2.2 [14] for the evolution calculation and NJOY 99.112 [12] for the nuclear data. ALEPH is currently under development at SCK•CEN as part of a PhD work in collaboration with Ghent University in the framework of the MYRRHA project [15]. The main idea behind ALEPH was to create a general purpose Monte Carlo burn-up code that is efficient, flexible and easy to use.

Another point that could be seen as a minor problem of burn-up codes in general (this includes deterministic codes) and that ALEPH will try to address is that the user has to specify himself when the reaction rates need to be recalculated. Because of this, a user has the inclination to recalculate the reaction rates more often than actually would be required (a standard criterion is after every GWd/ton of accumulated burn-up). A time step optimisation routine would therefore be interesting. It would give the user an initial estimate of the time steps required during the irradiation history. Such a time optimisation routine is currently being developed for ALEPH, again using a hybrid technique to reduce calculation time. From table 1.2 we can again conclude that there are no other MC burn-up codes that provide such an optimisation. It is however possible that MCB might have such a thing but it is not entirely clear.

As can be seen in table 1.2, ALEPH is one of the first MC burn-up codes to use a more efficient approach to reaction rate calculation. It is also one of the first MC burn-up codes that is capable of using MCNPX with all of its functionality. For ADS systems such as MYRRHA, the use of MCNPX is of crucial importance due to the necessity of high energy physics (for the high energy reactions in the spallation target) and because the coupled neutron-proton transport in the system can then be treated in a single code without making any approximation [16]. Some of the MC burn-up codes mentioned in table 1.1 are being or have been used to calculate burn-up in ADS systems (notably MCB [17] and EVOLCODE [18]). In these cases, the external proton source has to be calculated with a separate code, for instance LAHET [19] (before MCNPX was created) or even MCNPX itself. Depending upon the size of the spallation target, the primary external neutron source will also change due to burn-up of the assemblies around the spallation target. To take into account the change in this primary source, the source would also have to be recalculated every burn-up step. This would be done by default if MCNPX is used in the burn-up code.

1.3 Inner workings of ALEPH

1.3.1 Calculation flow and features of ALEPH

ALEPH is in essence an interface code between NJOY 99.90 [12], ORIGEN 2.2 [14] and any version of MCNP [13] or MCNPX [1] as can be seen in figure 1.1. 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 Monte Carlo code would be quite easy because of this modular design (we would only have to replace the object responsible for the MCNP(X)-ALEPH interface by a similar object for the new Monte Carlo code). And the same applies to ORIGEN as well. A great effort has also been made to optimize ALEPH for speed (the transition to fully object oriented code was essential for this).

Table 1.2: Monte Carlo burn-up codes implementation details.

Code Name	Language	Reaction Rates Inside MC Code	Time Step Optimisation
MOCUP	C	Yes	No
MC-REBUS		Yes	No
OCTOPUS			
MONTEBURNS	Fortran - Perl	Yes	No
EVOLCODE			
MCB	Fortran	Yes	?
MCWO	UNIX Script	Yes	No
MVP-BURN		Yes	No
BURNCAL	Fortran	Yes	No
MCODE	C	Yes	No
ALEPH	C++	Yes/No ^a	Yes ^b
MCNPX	Fortran	Yes ^c	No

^a ALEPH calculates the reaction rates outside the Monte Carlo code but the possibility to calculate them within the MC code will be added in the future for comparison purposes.

^b This will be implemented in a future version.

^c MCNPX uses a mixed method. Principal reaction (such as (n,γ) , $(n,2n)$, $(n,3n)$, (n,p) , (n,α) and fission) are calculated by MCNPX using multiplier bins. A 63 group flux is used to take into account the other reactions using 63 group cross section.

An argument against Monte Carlo burn-up codes that is often used is their complexity because most codes use a script or link approach to the problem. As a result, the user would have to understand and manage a large number of input and output files while the conversion of data from one form into another would introduce approximate results due to successive round off. ALEPH strives to solve this problem (either true or conceived) as well. ALEPH is indeed an interface code but it actually wraps itself around the codes involved and automates the entire process. The ORIGEN input files for instance are created by ALEPH itself without any intervention of the user so that the use of ORIGEN is actually “hidden” from the user. By providing an easy to understand user interface, we also take away the burden from the user. For the user, it is as if he is running a simple MCNP(X) problem - with some extra options.

A typical ALEPH calculation starts by the processing of the input file (the black arrow at the top of figure 1.1). The input itself consists of the ALEPH code options, along with an initial MCNP(X) input file. These ALEPH code options are the irradiation history, the group structure to be used, the materials and libraries to be used, the ORIGEN and MCNP(X) executable names, volumes, densities, ... Other essential information like the initial material composition, temperatures, ... are read from the initial MCNP(X) input file itself.

When the input file has been processed, ALEPH will build a new MCNP(X) input file based upon the input options of the user and start an MCNP(X) calculation. The neutron spectra for the different burn-up zones considered are then passed on for building the new ORIGEN libraries and ORIGEN input files (one for every zone with burnable materials). The MCNP(X) output file is also processed to determine if MCNP(X) hasn't encountered any problems. In the case of criticality calculations, ALEPH also reads the value of the effective multiplication factor which will be used as an initial estimate for the following calculation. In that case, the fission

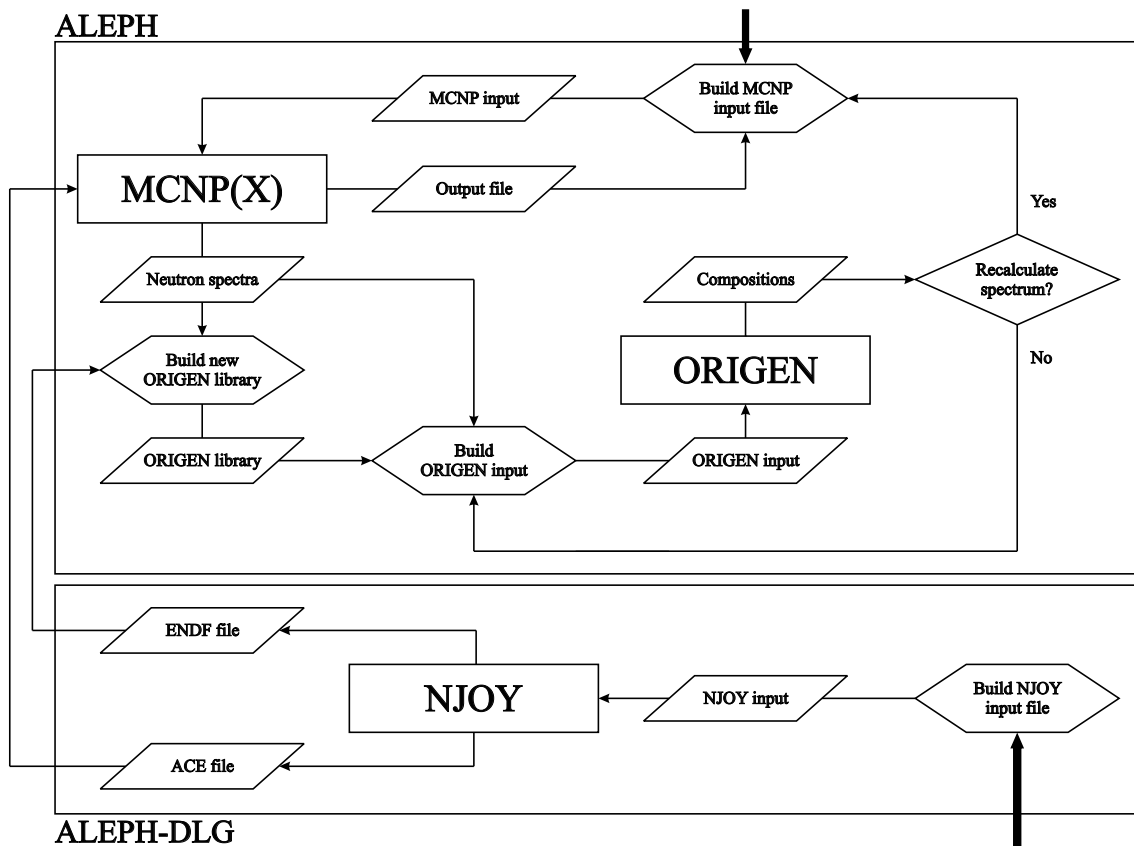


Figure 1.1: Calculation flow inside ALEPH and ALEPH-DLG.

source calculated in the previous calculation will also be used in the following calculation.

ALEPH is capable of using all irradiation features of ORIGEN. It provides for constant power irradiation, constant flux irradiation and simple decay. ALEPH will use a relative power distribution to determine the absolute levels of flux or power in every zone. After the ORIGEN calculation, ALEPH reads the results and cleans up all the temporary files from ORIGEN. The number of significant digits used by ORIGEN was increased from 3 to 5 to address the perceived round off problem mentioned above, although tests showed little to no influence on the final result. The new compositions are then stored and passed on either to build a new MCNP(X) input file (for a new burn-up step) or new ORIGEN input files (to obtain compositions at intermediate points within the burn-up step).

We have also added the possibility to change materials and geometry in the model during the irradiation. ALEPH distinguishes between 2 different types of materials: variable materials and burnable materials. Variable materials are materials that can be changed by the user but that can not be burned. A user can therefore change the density and/or temperature of such a material (to for instance simulate heating effects of water) or even replace the material by another one (to take into account changes in the boron concentration in the coolant of a PWR, ...). Geometry changes (by using surface transformations) are also possible, for instance for the simulation of control rod movement, ...

Burnable materials are (obviously) being burned. As was the case with variable materials, a user can change the temperature of such a material or even replace it with another burnable material (which doesn't necessarily have to be one that is being burned, this is to simulate core reshuffling and reloading). For obvious reasons, a burnable material's density cannot be

changed by the user. Burnable materials that are being taken out of the model will, by default, undergo decay.

At the beginning of every new burn-up step, the compositions of the materials that are being burned are updated along with the other material and geometry changes requested by the user. 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. This entire process continues until the end of the calculation.

1.3.2 Nuclear data for burn-up applications

The Monte Carlo code and the burn-up code have different demands on nuclear data. The Monte Carlo code requires specific data (being microscopic cross sections, angular distributions, energy spectra, ...) for every nuclide used in the transport simulation. ORIGEN on the other hand needs microscopic cross sections for (n, γ), (n,2n), (n,3n), (n, α), (n,p) and fission reactions - and this for every nuclide in the transmutation chains. To correctly calculate the distribution of fission products, ORIGEN also requires 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). The (n,3n), (n, α), (n,p) and fission reaction rates can be used immediately but for the (n, γ) and (n,2n) reaction we also need branching ratios towards the ground state and the first metastable state. And finally, we also require accurate decay data for every nuclide considered.

The microscopic cross sections used in the Monte Carlo simulation must be the same as the ones used for the reaction rate calculation, as is the case for traditional Monte Carlo burn-up calculations. This is why we have chosen to read the linearized microscopic cross sections used by ALEPH to calculate the multi-group cross section from ENDF files generated by NJOY. These ENDF files are the ones used by the ACER module of NJOY to prepare the MCNP(X) nuclear data files (also known as ACE files).

To automatically generate these ENDF files and the corresponding ACE files for Monte Carlo transport calculations, we are developing a utility called ALEPH-DLG (Data Library Generator) [20] that wraps itself around NJOY. This approach will allow us to quickly change our data when newer (and better) evaluations become available, making ALEPH very flexible in its use of nuclear data.

ALEPH comes with its own data libraries for both ALEPH and MCNP(X) (ALEPH-LIB). This library consists of 5 major evaluations (JEF 2.2, JEFF 3.0, JEFF 3.1, JENDL 3.3 and ENDF/B-VI.8) at 6 temperatures (300, 600, 900, 1200, 1500 and 1800 K). The atomic densities used by MCNP(X) are also updated (for over 3000 nuclides) by using the Atomic Mass Evaluation 2003 included into NUBASE [21] from the Atomic Mass Data Center. This has been done to ensure data consistency between ALEPH and MCNP(X) (both codes now use the same values for atomic masses).

For now, we have limited ourselves to microscopic cross section data. All of the other data required by ORIGEN (being the branching ratios, the direct fission yield, ...) can also be found in the different nuclear data evaluations that use the ENDF format. By using this data from the ENDF files, we would have no need of other third party data or models. We are currently implementing this into ALEPH and ALEPH-DLG. By only using data from a single source (being an ENDF file), we can ensure full nuclear data consistency within the entire code system.

Chapter 2

ALEPH input options

2.1 The ALEPH input file

The ALEPH input file consists of two distinct parts. This chapter deals with the different input options for ALEPH, being the first part of the input file. We have chosen to use a keyword approach similar to that used in ORIGEN. Some keywords are even copied from ORIGEN (such as the `IRP`, `IRF` and `DEC` keywords). As we pointed out before, we strived to make ALEPH as simple to use as possible and this reflects in these input options. The number of keywords that are actually required is kept as small as possible (see table 2.1). This part of the input file is ended with the `END` keyword (see section 2.2) after which the MCNP(X) input file will follow. The details concerning this MCNP(X) input file are discussed in the following chapter (chapter 3). Before starting, we would like to make the following remarks concerning the input and the notations used in this manual:

- File and directory specification can be done using the rules under unix. Specifying directories is done with the “/” character (and not the backslash character as is done under windows). To specify a path from the root directory, the directory must begin with a “/” character. For a subdirectory from the current working directory this not required. It is also advisable to use directory names without white space.
- Anything appearing between `< . . >` is optional input. This means that the user has either to choose between different options, or that this is not required if certain conditions are met (for instance the previous use of a certain keyword).
- Although all the keywords in this manual are in capital letters, ALEPH will also accept keywords in small letters. As such, keywords like `NSP` or `nsp` are accepted but `Nsp` will not be accepted.

2.2 End ALEPH input - END keyword

The `END` keyword is used to terminate the ALEPH input options and to indicate that the MCNP(X) input file will follow. The MCNP(X) input starts either with `MESSAGE` (to supply input directives that are not used in the command line) or a problem title (with or without the `TITLE` keyword). If this keyword is not used, ALEPH will continue to read the MCNP(X) input file as if it was regular ALEPH input, causing the code to terminate with errors.

Table 2.1: Overview of the ALEPH input keywords.

Keyword	Required	Keyword Use	Section
ABS	yes	The fractional absorption criterion to be used	2.6.1
BURN	yes ^a	The Burnable materials used in the problem	2.7.1
C	no	Comment line	2.9.2
CHBM		Change a burnable material	2.8.6
CHCM		Change the material of a cell (variable material only)	2.8.6
CHMD		Density change of a variable material	2.8.5
CHMT		Temperature change of a burnable or variable material	2.8.4
CHTR		Change the TR-card on a surface	2.8.7
DAT	yes	The data path and the name of the xsdir file	2.4.1
DEC		A decay sub step	2.8.3
EGS	yes	The group structure to be used	2.3.1
END	yes	Ends the ALEPH input options	2.2
GWS	no ^b	The weight spectrum to be used for all isotopes	2.3.2
HIS	yes	The irradiation history	2.8
IRF		An irradiation sub step of constant flux	2.8.2
IRP		An irradiation sub step of constant power	2.8.1
LIB	yes	The ORIGEN libraries and library numbers	2.5.2
MAT	yes	The isotopes that have to be used	2.4.3
MCNP	yes	The MCNP(X) executable and the calculation type	2.6.3
ORI	yes	The ORIGEN 2.2 executable	2.5.1
OUT	no	ALEPH output options	2.9.3
STP		An irradiation step	2.8
TAL	yes	The tally number	2.6.2
TIT	no	A title for the new ORIGEN libraries	2.9.1
TMP	yes ^c	The temperatures used in this ALEPH run	2.4.2
VAR	no	The variable materials used in the problem	2.7.3
VOL	yes	The volumes of the materials are being burned	2.7.2
\$	no	Comment after a keyword	2.9.2

^a This keyword must always precede the HIS keyword if IRP option -1 is used.

^b If this keyword is not used, the weight spectrum must be specified for every isotope in the MAT keyword. If it is present, it must always precede the MAT keyword.

^c Because the temperatures are linked to the MAT keyword, it must always precede the MAT keyword.

2.3 Multi-group cross sections and spectra

2.3.1 Group structure - EGS keyword

The group structure to be used by MCNP(X) is specified using the EGS keyword:

```
EGS NG[1] EG[1] < NG[2] EG[2] .. NG[NGR] EG[NGR] >
```

where NG[i] is the number of groups to be used between EG[i-1] and EG[i] (specified in MeV). The energy corresponding to EG[0] has been set to 1e-11 MeV (which is in most cases the lower energy boundary of cross sections). Values for NG[1] and EG[1] are required. To

specify complex group structures, an unlimited number of values for NG[i] and EG[i] are allowed but the user should be aware of the fact that rounding problems can arise when using a group structure which is too fine. The group structure itself is calculated using the constant lethargy approach (the energy interval between EG[i-1] and EG[i] is subdivided into NG[i] groups of constant lethargy). The energy group values E_k between EG[i-1] and EG[i] are therefore given by:

$$E_k = EG[i-1] \exp\left(-\frac{k}{NG[i]} \ln\left(\frac{EG[i]}{EG[i-1]}\right)\right) \quad (2.3.1)$$

where $k = 1$ to $NG[i] - 1$.

2.3.2 Weight option - GWS keyword

In the multi-group ALEPH approach, reaction rates σ are calculated as follows:

$$\sigma = \frac{\sum_g \sigma_g \phi_g}{\sum_g \phi_g} \quad (2.3.2)$$

in which σ_g and ϕ_g are the cross section and spectrum of group g with boundaries E_{g-1} and E_g . The group cross section σ_g itself is calculated analytically by ALEPH using the following formula:

$$\sigma_g = \frac{\int_{E_{g-1}}^{E_g} \sigma(E) \varphi(E) dE}{\int_{E_{g-1}}^{E_g} \varphi(E) dE} \quad (2.3.3)$$

with $\sigma(E)$ the energy dependent microscopic cross section and $\varphi(E)$ the spectrum used to weigh the cross section.

ALEPH forseees in two possible weight spectra. The first being the constant weight spectrum (the weight is constant over the entire energy range) and the second one being the non self shielded PWR spectrum (consisting of a Maxwellian spectrum, a slowing down spectrum and a fission spectrum) [22]:

$$\varphi(E) = \begin{cases} \frac{E \exp\left(-\frac{E}{kT}\right)}{E_{max,th}^2 \exp\left(-\frac{E_{max,th}}{kT}\right)} & E \leq E_{max,th} \\ \frac{1}{E} & E_{max,th} \leq E \leq E_{max,epi} \\ \frac{\sqrt{E} \exp\left(-\frac{3E}{2E_{fis}}\right)}{E_{max,th}^{3/2} \exp\left(-\frac{3E_{max,epi}}{2E_{fis}}\right)} & E_{max,epi} \leq E \end{cases} \quad (2.3.4)$$

where $E_{max,th}$ is the upper energy boundary of the thermal region, kT is the thermal energy, $E_{max,epi}$ is the upper energy boundary of the epithermal region where E_{fis} is the mean energy of a fission neutron.

The GWS keyword is used to specify this weight spectrum. The syntax of this keyword is simply:

GWS < weightoption >

where `< weightoption >` is one of the following possibilities:

- For the constant weight spectrum:

-1

- For the non self shielded PWR spectrum:

-2 ETH T EEPI EFIS

where `ETH` is the upper energy boundary of the thermal region, `T` is the nuclear temperature, `EEPI` is the upper energy boundary of the epithermal region and where `EFIS` is the mean energy of a fission neutron. All the energies must be specified in MeV and the temperature must be specified in K.

The `GWS` keyword is used to select this weight spectrum globally. This means that all group cross sections will be calculated using the same weight spectrum. If the user wants to mix different weight spectra, then he may not use this keyword. Instead he will need to specify the weight spectrum for every isotope in the `MAT` keyword (see section 2.4.3). Also: if this keyword is used, it must be used before the `MAT` keyword.

2.4 Nuclear data

2.4.1 Data library - DAT keyword

ALEPH requires microscopic cross sections which can be linearly interpolated for every isotope that the user wants to change in the `ORIGEN` input file. These cross sections have to be supplied in the ENDF 6 format [11]. We have chosen the ENDF format (and not some other home made format) because it is universally accepted and because there exist numerous cross section processing codes that are capable of linearizing cross sections in the ENDF format. Examples of such data processing codes are `PREPRO 2002` [23] and `NJOY` (the ALEPH-DLG utility to generate `MCNPX` and ALEPH cross section files uses `NJOY 99.112`). Furthermore, it is not required to use the complete ENDF file. Only the reactions given in table 2.2 have to be present in file 3 (the cross section file) of the ENDF file. If one of those entries is missing, ALEPH will assume that the cross section is zero.

Table 2.2: Cross sections required by `ORIGEN 2.2` and their ENDF reaction numbers (MT number).

MT	Reaction	Material Types
16 or 875-891	(n,2n)	all materials
17	(n,3n)	actinides
18 or 19-21, 38	(n,fission)	actinides
102	(n, γ)	all materials
103 or 600-649	(n,p)	activation and fission products
107 or 800-849	(n, α)	activation and fission products

The `DAT` keyword has to be used to specify the path where ALEPH can find the ENDF files that are specified in the ALEPH cross section directory file. This path is the common path to the cross section files, separate subdirectories can still be specified using the cross section directory file. The structure of the cross section directory file is given in section 4.1. The syntax of this keyword is as follows:

```
DAT datapath alephxmdir
```

2.4.2 Temperature - TMP keyword

ALEPH allows the use of multiple temperatures, both for variable materials and burnable materials. The `TMP` keyword has to be used to specify all the temperatures $T[i]$ (the unit used is K) that the user will require. The order of the temperatures is also the order in which libraries are specified in the `MAT` keyword. The syntax for this keyword is:

```
TMP T[1] < T[2] .. T[NT] >
```

with `NT` the number of temperatures to be used. At least one temperature value must be specified, this will be the default temperature.

2.4.3 Specifying nuclides - MAT keyword

One of the most important keywords in the input file is the `MAT` keyword used to specify the isotopes for which reaction rates have to be recalculated and which isotopes MCNP(X) can use for transport purposes. Depending on the previous input of keywords, the syntax for the `MAT` keyword is:

```
MAT
..
ZAMID[j] LIB[1] < LIB[2] .. LIB[NT] > < weightoption >
..
```

where `ZAMID[j]` (similar to the `ZAID` identification used by MCNP(X)) is the ORIGEN identification number of the isotope `j` (using the element number `Z`, the atomic mass number `A` and the metastable state `M` which is either 0 or 1):

$$\text{ZAMID} = 10000 Z + 10 A + M = 10 \text{ZAID} + M \quad (2.4.1)$$

`LIB[i]` is the MCNP(X) and ALEPH library number (between 1 and 99) corresponding with temperature $T[i]$ specified in the `TMP` keyword. In other words, the number of library numbers given here must be the same as the number of temperatures (`NT`) specified using the `TMP` keyword and the order in which the libraries are specified must also be the same as the order of temperatures in the `TMP` keyword. The library number `LIB[i]` can be specified as a simple integer (for instance 15) or with a suffix `c` (the MCNP(X) library notation, for instance 15c). The library numbers themselves can be positive, negative or zero. A positive library number indicates a library that will be used for reaction rates calculation and for transport calculations. Negative library numbers are used when the library is only to be used for reaction rates calculation. This way, cross section files that are not suitable for transport calculations (for instance the EAF-99 neutron activation files) can still be used to calculate reaction rates. Using zero as library number will cause the nuclide to be skipped in reaction rates calculations and transport

calculations for this temperature. This can be used when a certain temperature is only required by a variable material (and not a burnable material).

< weightoption > is optional input and has only to be included if the weight option keyword GWS is not used. This option can be used to specify different spectral weight options for certain nuclides. The input of this option itself is the same as the input for the GWS keyword. The user should note that using this when the GWS keyword is present will lead to an error message. On the other hand, placing the GWS keyword after MAT will also lead to errors.

It is advised to make this isotope list as complete as possible. Because ALEPH must ensure that MCNP(X) runs without any problem, only materials with positive library numbers that are in this list will be used in MCNP(X) runs. If somehow a nuclide is created that is not in this list, it will be omitted and a warning will be printed. Also, only isotopes and no natural elements may be used for the moment. Adding a natural element to this list is possible but it will never be used.

2.5 Calculating ORIGEN libraries

2.5.1 Running ORIGEN - ORI keyword

The ORI keyword is used to specify the ORIGEN 2.2 executable `origenexe`:

```
ORI origenexe
```

This is required because there exist different versions of ORIGEN (one for thermal reactors and one for fast reactors).

2.5.2 Libraries - LIB keyword

ORIGEN 2.2 needs three types of libraries to run: the cross section libraries (ALEPH uses an original library and will adapt it where necessary), the decay library and the photon libraries. The LIB keyword is used to specify these libraries:

```
LIB xsfile APL ACL FPL photonfile decayfile
```

where `xsfile`, `photonfile` and `decayfile` are the names and path of the files in question. The integers APL, ACL and FPL are used to specify the identification numbers of the activation product, actinide and fission product libraries in the original ORIGEN library that the user wants to change. If the user has specified an isotope in the MAT keyword that is not present in this library, it will not be added. Nuclides present in the original file will not be touched if they do not appear in the MAT keyword. The new libraries will receive new identification numbers to distinguish them from the original library: 701 for activation products, 702 for actinides and 703 for fission products.

2.6 Running MCNP(X)

2.6.1 MCNP material composition - ABS keyword

For the purpose of transport calculations ALEPH will truncate the material composition calculated by ORIGEN using a fractional absorption criterion. ALEPH will calculate the total

absorption of every nuclide (being the sum of all reactions given in table 2.2) and use it to determine to what amount this isotope contributes to the total absorption. The nuclides are sorted in decreasing absorption importance and they will be added to the list as long as the cumulative fractional absorption is not equal to or greater than the fractional absorption criterion specified by the user. After that, only nuclides that were originally present are still added. As such, the initial nuclides are used by default. The user needs to use the `ABS` keyword to specify this fractional absorption criterion `FRAC`:

```
ABS FRAC
```

Because it is a fractional criterion, `FRAC` must be a number between 0 and 1. If this number is 0, the original nuclides with their new composition will be used. Using 1 is not advised because it will add all nuclides (some of which will probably not have a library associated with them). Acceptable values are for instance 99 % and 99.9 %. The density used by `MCNP(X)` will be the density of this truncated nuclide list in order to conserve the absolute number of atoms.

2.6.2 MCNP tally specification - `TAL` keyword

The `TAL` keyword has to be used to specify the tally number `TNR` (this must be a type 4 tally) used to calculate the spectra for the purpose of an `ORIGEN` library calculation:

```
TAL TNR
```

2.6.3 MCNP execution - `MCNP` keyword

The `MCNP` keyword is used to specify the `MCNP(X)` executable `mcnpexe` to be used within the program, followed by the parallel option `< parallel >`:

```
MCNP mcnpexe < parallel >
```

where `< parallel >` is one of the following:

- for serial runs (single processor calculation):

```
-1
```

- for parallel runs (multi processor calculation):

```
-2 NSL
```

where `NSL` is the number of parallel processors. It is up to the user to ensure that enough processors are reserved and that `mcnpexe` points to an executable capable of parallel processing.

For every burn-up step with library calculation `ALEPH` will create an `MCNP(X)` input file and `MCNP(X)` will create output files and tally files. The names for these files consists of the step number (starting with 0 for the initial library calculation) with an extension (“`.i`” for an input file, “`.o`” for an output file and “`.m`” for a tally file). The so called runtape files (with the standard name `runtape`) are deleted by `ALEPH` to reduce disk space because these files can take up quite a lot of space. The user should ensure that enough disk space is available to store all these files (a single pin calculation of 50 steps takes already 500 MB of disk space).

`ALEPH` will always check for the existence of tally files before running `MCNP(X)`. If a tally file exists, `ALEPH` will skip the `MCNP(X)` run for that step. This was added to allow for continue runs (to add more steps after a calculation was already finished or to restart a calculation with a slightly different irradiation history for which previously calculated spectra can be used).

2.7 Specifying variable and burnable materials

2.7.1 Burnable materials - BURN keyword

The `BURN` keyword has to be used to specify the number `NB` of materials that are burned at any given time (which is the same as the number of spectra to be calculated and the number of cells or collection of cells that are found in the tally specification in the `MCNP(X)` input file) and to provide the material numbers of every burnable material used. `ALEPH` allows for material reshuffling so the total amount of materials used in the problem may be greater than `NB`. The syntax for this keyword is:

```
BURN NB BURNMAT[1] .. BURNMAT[NB] < BURNMAT[NB+1] .. BURNMAT[NB+k]>
```

where `BURNMAT[i]` is a `MCNP(X)` material number. The materials with `i` between 1 and `NS` are the materials that are to be burned at the start of the calculation. The order in which these material numbers are given must be the same as the cell order on the tally used to calculate the spectra. Additional material numbers for burnable materials that will be used later on in the calculation (for instance through reshuffling) are given after the first `NB` library numbers.

The temperature of a burnable material can be changed using the `CHT` keyword (see section 2.8.4) during an irradiation step specified with the `HIS` keyword (see section 2.8) and a burnable material can be changed to another by using the `CHBM` keyword (see section 2.8.6).

You may use any number of materials (both to be burned and to be used later on), there are no limitations except maybe for the memory available on the system used to run the program (in our present time, that shouldn't be much of a problem).

2.7.2 Volumes - VOL keyword

`ALEPH` requires the volumes of the cells containing the burnable materials to recalculate the total fluxes, power distributions, ... Because these cells can consist of multiple parts and because they can be repeated in lattices, it is not possible to rely upon `MCNP(X)` to normalize the flux tallies. The user has to use the `VOL` keyword to specify the total modeled volume of the cells containing burnable materials:

```
VOL V[1] .. V[NB]
```

where `NB` is the total number of materials that are burned as any given time (see the `BURN` keyword, section 2.7.1). The order in which these volumes are given must be the same as the order of materials on the `BURN` keyword.

2.7.3 Variable materials - VAR keyword

The `VAR` keyword is used to specify the variable materials in the problem. Variable materials can help in better modeling the irradiation conditions in certain problems because they allow the change of parameters such as composition, temperature, ... This is for instance useful for simulating the boron concentration in water for a `PWR`. If the user has no need to change materials, this keyword can be omitted. The use of this keyword is similar to that of the `BURN` keyword:

```
VAR VARMAT[1] .. VARMAT[NV]
```

where `VARMAT [i]` is a MCNP(X) material number and `NV` is the total number of variable materials to be used. The order in which these materials are specified is not important.

The temperature of a variable material can be changed using the `CHT` keyword (see section 2.8.4) during an irradiation step specified with the `HIS` keyword (see section 2.8). The density of a variable material is changed by the `CHMD` keyword (see section 2.8.5) and the content of a cell is replaced by another variable material by using the `CHCM` keyword (see section 2.8.6).

2.8 Specifying burn-up History - HIS keyword

The burn-up history has to be specified with the `HIS` keyword. This keyword must be followed by at least one burn-up step. A burn-up step is simply a point in the irradiation history where a user can ask to output the material compositions or where the library needs to be recalculated. Such a burn-up step is specified using a block starting with the keyword `STP` and an integer `ICAL` to specify if the library has to be recalculated for this point (`ICAL = 1` to recalculate and `ICAL = 0` to use the previously calculated libraries). The `STP` block ends when another `STP` or when any other keyword is encountered:

```
HIS
  STP ICAL
  ..
  STP ICAL
  ..
```

Within every `STP` block, there are three different types of burn-up keywords (the usual `ORIGEN` options `IRP`, `IRF` and `DEC`), four material control keywords (`CHT`, `CHD`, `CHCM` and `CHBM`) and one geometry control keyword (`CHTR`).

2.8.1 Power irradiation - IRP keyword

The `IRP` keyword is used to specify a sub step of constant power irradiation, along with the irradiation time:

```
IRP < IRP option > TU TIME
```

where `< IRP option >` is the power normalisation option, `TU` the time unit to be used (see table 2.3) and `TIME` the total time elapsed at the end of this sub step since the beginning of the step (referenced from the beginning of the `STP` block in which this keyword appears).

The power renormalisation option `< IRP option >` is used to determine the power for every burnable material so that every material is burned relatively to the other materials in the system (according to the power distribution). The power in a system (and in the different materials that compose the system) is determined by the power distribution, which is in turn determined by the flux distribution. The power produced in a material j (consisting of N_j different nuclides i characterised by a proton number Z_i , mass number A_i with density ρ_i and fission cross section $\sigma_{f,i}$) is proportional to what we call the specific normalisation power $P_{0,j}$. This power $P_{0,j}$ represent the relative power distribution in all materials. In essence, $P_{0,j}$ is the total power produced through direct fission and delayed energy (expressed in MW):

$$P_{0,j} = e 10^{-24} \sum_{i=1}^{N_j} Q_{f,i} \frac{\rho_i V_j N_a}{A_i} (\sigma_{f,i} \phi_{0,j}) \quad (2.8.1)$$

Table 2.3: Time units in the irradiation history.

TU	Time Unit
1	seconds
2	minutes
3	hours
4	days
5	years
7	10 ³ years
8	10 ⁶ years
9	10 ⁹ years

in which e is the elementary electron charge, N_a is the number of Avogadro, $\sigma_{f,i}$ is the one group fission cross section for nuclide i (this is taken from the modified ORIGEN libraries for the material in question), $\phi_{0,j}$ is a measure of the total flux in the material j (in fact, MCNP(X) will provide us with $\phi_{0,j}V_j$ per source particle for every material that we are burning) and where $Q_{f,i}$ is the total fission Q -value (both the prompt and delayed) of the nuclide i expressed in MeV by the following formula (this is the same formula as the one used inside ORIGEN) [14]:

$$Q_{f,i} = 1.29927 \cdot 10^{-3} (Z_i^2 A_i^{0.5}) + 33.12 \quad (2.8.2)$$

ALEPH will use the specific normalisation power $P_{0,j}$ corresponding to the last spectrum calculated. In other words, the power is calculated by using the composition of the material when its spectrum was recalculated. So if the user has specified points without a spectral recalculation, the specific normalisation power $P_{0,j}$ will not be updated with the new composition. This is currently under investigation.

It should be noted that - for now - the specific normalisation power $P_{0,j}$ will be zero for a material that doesn't contain actinides. It is therefore impossible to calculate the evolution of such materials by using constant power irradiation. Constant flux irradiation is the only possibility to do this. This will be fixed in a future version of ALEPH.

There are four possibilities for this power normalisation option:

- The power for every material i is specified. This option must be followed by a number of power values $P[i]$ equal to the number NS of materials to be burned:

```
-1 P[1] .. P[NS]
```

In this case no further normalisation of the power will occur. This option should be avoided because it doesn't take into account the relative power distribution in the system.

- The total power P_{TOT} for all materials is given:

```
-2 PTOT
```

The power of every material j is now determined by using the relative power level $P_{0,j}$ of the material to that of all materials together:

$$P_j = P_{TOT} \frac{P_{0,j}}{\sum_{l=1}^N P_{0,l}} \quad (2.8.3)$$

- The power P of a specific material IK is given:

-3 $IK P$

The relative power level of every other material j to material IK is now used to determine the power values of those materials:

$$P_j = P \frac{P_{0,j}}{P_{0,IK}} \quad (2.8.4)$$

- The total power P_{TOT} of a collection of materials with index $I[i]$ ($i = 1 \dots NC$) is given:

-4 $NC I[1] \dots I[NC] P_{TOT}$

This option is somewhat similar to the second and third option. For materials in the collection, the relative power level of the material to that of all materials in the collection is used (see equation 2.8.3). For materials that aren't in the collection the relative power of that material to the power of any material from the collection is used (see equation 2.8.4).

All of the power values used in these options have to be specified in MW. When a single material is being burned, all of the options described above are equivalent.

2.8.2 Flux irradiation - IRF keyword

As was the case with the `IRP` keyword, the `IRF` keyword is used for a substep of constant flux irradiation. The syntax is similar to that of the `IRP` keyword:

`IRF < IRF option > TU TIME`

There are two possibilities for the `IRF` renormalisation option `< IRF option >`:

- The absolute source strength S is specified:

-1 S

Because MCNP(X) provides us with flux values per source particle multiplied with the volume of the material, the flux for every material j is calculated as:

$$\phi_j = S \frac{\sum_{l=1}^{N_g} \phi_{0,j,l}}{V_j} \quad (2.8.5)$$

where $\phi_{0,j,l}$ is the flux per source particle of group l for material j (as calculated by MCNP(X)) and where V_j is the total volume of material j present.

- The flux PHI of a specific material IK is given:

-2 $IK \text{PHI}$

The flux ϕ_j of the other materials j is then calculated as:

$$\phi_j = \text{PHI} \frac{V_{IK} \sum_{l=1}^{N_g} \phi_{0,j,l}}{V_j \sum_{l=1}^{N_g} \phi_{0,IK,l}} \quad (2.8.6)$$

2.8.3 Decay - DEC keyword

Using the `DEC` keyword, we can specify a sub step of natural decay. The only input required is the time unit `TU` and the end time `TIME` of the sub step referenced from the start of the step:

```
DEC TU TIME
```

2.8.4 Change temperature - CHMT keyword

The `CHMT` keyword is used to assign a different temperature with value `TEMP` to the material with `MAT` as MCNP(X) material number:

```
CHMT MAT TEMP
```

This keyword can be applied to both variable and burnable materials. This could for instance be useful to change the temperature of a burnable material during a step where it will produce a lot more or less power compared to the previous step. The temperature `TEMP` must also have been declared using the `TMP` keyword. If the temperature has not been specified or if the `TMP` keyword is used after the `HIS` keyword, ALEPH will issue an error.

This keyword can appear anywhere within an `STP` block, but only if the libraries are recalculated. The changes will be performed at the beginning of the step. If this keyword is used in an `STP` block where the spectrum is not recalculated (`ICAL = 0` for the block), ALEPH will issue an error. This also applies to the `CHMD`, `CHCM`, `CHBM` and `CHTR` keywords.

2.8.5 Change density - CHMD keyword

The `CHMD` keyword is used to change the density of a variable material `MAT` to `DENSITY`:

```
CHMD MAT DENSITY
```

This can only be applied to variable materials. If a burnable material is chosen, an error will be issued. As was the case with the `CHMT` keyword, this can only be used in an `STP` block where the spectrum is recalculated.

2.8.6 Change material - CHCM and CHBM keywords

Changing materials in a cell is done through the `CHCM` and `CHBM` keywords, depending upon the type of material (variable or burnable). For a variable material for instance, you change the material of a single cell with the `CHCM` keyword:

```
CHCM CELL NEWMAT
```

where `CELL` is the cell in which the new variable material with number `NEWMAT` will be used. The temperature of the new material will be set to that of the old material, unless the new material is already in use. Because every material can only be associated with a single temperature, the temperature that is already in use will be assigned to the cell. It is up to the user to make sure that variable materials are not assigned to cells with different temperatures.

For burnable materials, it is only allowed to exchange an old burnable material `OLDMAT` with a new burnable material `NEWMAT` with the `CHBM` keyword:

```
CHBM OLDMAT NEWMAT
```


It is not possible to change specific cells because that would involve changing the tally used to calculate the spectra. This might be added in a future version but for now it is not possible. If one of both materials is not being burned, the material that is being taken out will undergo decay for the rest of the calculation (or until it is used again in a CHBM keyword). The temperature of the new material will be set to that of the old one. If both materials are being burned, the materials will simply swap positions. Their respective temperatures will be swapped as well. Again, these keyword can only be used in an STP block where the spectrum is being recalculated.

2.8.7 Change TR-card - CHTR keyword

The previous change keywords were used to change things on the material level. The CHTR keyword can be used to perform changes on the geometry level. It allows a user to change the tr-card number of a surface entry SURF to another tr-card number NEWTR:

```
CHTR SURF NEWTR
```

The user should test if the surface transformation works properly before using this option. As was the case with the previous change keywords, this keyword can only be used in an STP block where the spectrum is being recalculated.

2.9 Optional keywords

2.9.1 ORIGEN library title - TIT keywords

The TIT keyword can be used to specify a title for the calculation. It will be used as the title of the ORIGEN libraries:

```
TIT title
```

2.9.2 Inputfile comment - C and \$ keywords

To put comments in the input file, two different keywords have been foreseen : C and \$. The C keyword can be used to comment out entire lines while the \$ keyword is used to comment out parts of lines. The \$ keyword can be used everywhere when the regular input is present. This means that comment after every isotope in the MAT keyword like:

```
MAT
  922350 03c 15c      $ U235 from JEF 2.2
  942380 03c 15c      $ U238 from JEFF 3.0
```

or comment in the HIS keyword like this:

```
HIS
  STP 1              $ point 1, calculate spectrum
  IRP -2 0.25 4 30 $ constant power irradiation for 30 days
  STP 0
  IRP -2 0.25 4 30 $ constant power irradiation for 30 days
```

is permitted. Using the C keyword in those keywords is however not permitted.

2.9.3 Output - OUT keyword

The OUT keyword is used to set certain output options of ALEPH. For now, there are four options: full output (OUTFULL), library changes (LIBCHANGES), full library output (LIBFULL) and ORIGEN output (ORIGENOUTPUT):

```
OUT  OUTFULL  LIBCHANGES  LIBFULL  ORIGENOUTPUT
```

If `OUTFULL = 1`, everything that is written to the screen will be written to the output file (see section 6.3.1). When performing large amounts of steps with library recalculation, this can lead to large output files. For `LIBCHANGES = 1`, the changes made to the original ORIGEN file will be reported (see 6.3.2). If `LIBFULL = 1`, ALEPH will print the libraries generated to separate files. This last option can be used when preparing updated libraries for normal ORIGEN calculations. Again, in the case of large calculations with many materials and steps this may lead to a large amount of files. If `ORIGENOUTPUT = 1`, ALEPH will print the ORIGEN output files to separate files with the following naming convention:

This keyword is not required. By default, all output options are assumed to be 0.

Chapter 3

MCNP(X) input

3.1 The MCNP(X) input file

This chapter deals with the second part of the ALEPH input file: the MCNP(X) input file. For the ALEPH interface to work, ALEPH must be capable of easily going through the input file. For this, some basic rules have to be established (the ALEPH MCNP(X) parser is not as complete as the one used by MCNP(X) itself). But apart from those rules, anything goes.

When ALEPH reads the MCNP(X) input instructions, it will read in all cells, surfaces and material compositions and take whatever information it needs. Apart from these points, ALEPH will also look for the tally specified with the `TAL` keyword to see if it is present. ALEPH will also determine if the calculation is a criticality calculation or a fixed source calculation. In the case of a criticality calculation, ALEPH will look for a source file (called `srctp`, the default MCNP source file name). If that file is present, the source specification (using the `ksrc` or `sdef` keywords) will be commented out to force MCNP(X) to use the source file generated by a previous run. ALEPH will also read the value of the effective multiplication factor k_e from a previous run to use it as a k_e estimate for the next run. This is done by default.

3.2 Cell specification

For the specification of a cell, constructions using the “like ... but ...” scheme are not permitted. This means that the cell number must be followed by the material number, and that the third number must be the density (provided that the material number was not 0). The density itself may be specified in g/cm^3 or in atoms $\text{barn}^{-1} \text{cm}^{-1}$ as per normal MCNP(X). The input of these 3 cell parameters (or 2 when it concerns a void cell) may not be interrupted by comments (either `c` or `$`). The line continuation card `&` is also not allowed because ALEPH uses the first 5 blank characters on a line to identify entries on multiple lines. Due to this, it is also not allowed to cut an entry in two by using the `c`-comment. If the user still wants to comment out entire lines in an entry, he should use the `$`-style comment. Whenever the entry ends, `c`-style comments are allowed.

ALEPH also requires the temperature of the cell. For this purpose, every cell containing a variable or burnable material must have the option `tmp=` within its declaration. If this temperature specification is missing, the default temperature will be used (the first entry on the `TMP` keyword, see section 2.4.2).

3.3 Surface specification

MCNP(X) distinguishes between three types of surfaces: a normal surface (designated by a simple integer), a reflective boundary surface (designated by a simple integer preceded by an *) and a white boundary surface (designated by a simple integer preceded by an +). ALEPH will read this surface number, along with the surface transform number that follows the surface number (if a surface transform is present of course).

All the previous rules for cell specification still apply: the surface number and the surface transformation number (if any is given) may not be interrupted by comment, the surface entry may not be interrupted by c-style comment and the line continuation card & is not allowed (the first 5 blank characters on a line indicate a continuation of the previous line).

3.4 Material specification

The initial material compositions of burnable materials and the composition of the variable materials to be used in the ALEPH run are read from the material specification of MCNP(X). A variable or burnable material is specified according to the following rules. First, the first line of the material specification of a material `<matnr>` may not contain any isotope and it must be ended by a \$-style comment containing the density `< density >` (as it was given in the cell entries if the material is in use or the density foreseen by the user when it will be used):

```
m<matnr>                                $ < density >
```

The different isotopes that compose the material have to be specified on the following lines using this syntax:

```
ZAID<.LIB> FRAC    $ < origen type > < metastable >
```

where ZAID is the MCNP(X) material ID (see equation 2.4.1) and FRAC is either the weight fraction (in MCNP(X) this must be a negative number) or the atom fraction (this is a positive number) of this isotope in the material. The library number LIB is optional. Library numbers that are specified here will be skipped as only the numbers given in the MAT keyword will be used.

To perform ORIGEN calculations, some additional information on the isotope are still required (the ORIGEN material type `< origen type >` and the metastable state `< metastable >`). All this is specified after the weight fraction within a \$ comment. ORIGEN distinguishes between 3 different types of materials: activation products, actinides and fission products. If the isotope is an activation product (for instance ^{16}O), then `< origen type > = -1`. For actinides (for instance ^{235}U) this is `< origen type > = -2` and for fission products it is `< origen type > = -3`. ORIGEN also distinguishes between isotopes in the ground state and in a metastable state (something which is not provided in MCNP(X)). If the isotope is in the ground state, then `< metastable > = 0` while it will be `< metastable > = 1` for metastable nuclides.

ALEPH can read both types of material specification possible in MCNP(X): weight fractions and atomic fractions. The same counts for the densities specified on the cell entries: it may be specified in g/cm^3 or in atoms $\text{barn}^{-1} \text{cm}^{-1}$ as per normal MCNP(X). And it is also allowed for the input to be mixed (density in g/cm^3 and composition in atomic fractions and vice versa). By default, ALEPH will recalculate variable and burnable materials to densities given in atoms $\text{barn}^{-1} \text{cm}^{-1}$ and compositions given in atom fractions, as MCNP(X) does internally.

To recalculate compositions and densities from one formalism to another, ALEPH requires precise values of the atomic mass of every nuclide. And this is where the isotopes files comes in (see section 4.2).

Chapter 4

ALEPH auxiliary files

4.1 The cross section directory file

The cross section directory file `alephxsdir` that has to be specified in the `DAT` keyword is a simple text file that is used to specify the file names of the ENDF files for use with ALEPH. With the `MAT` keyword, the user specifies the library numbers for every isotope to be used in the calculation. For every non-zero library number `lib` (both positive and negative) in an entry of an isotope with a `ZAMID` identification on the `MAT` keyword, the following line must be in the cross section directory file:

```
ZAMID lib endf_file_name
```

where `endf_file_name` is the name (along with subdirectories if required) of the ENDF file containing the required information. Please note that the common data path specified with the `DAT` keyword should not be included here.

As was the case for the `MAT` keyword, the library number `lib` can be specified as a simple integer (for instance 15) or with a suffix `c` (the MCNP(X) library notation, for instance 15c).

4.2 The isotopes file

Although ORIGEN uses the `ZAMID` identification for input of a nuclide, it does not use this identification for the output. There, ORIGEN uses element names to identify nuclides. The isotopes file is used to link element names with the appropriate Z-number of the element.

To recalculate compositions (both from the MCNP(X) input file and the ORIGEN output files) to the standard atoms $\text{barn}^{-1} \text{cm}^{-1}$, the correct atomic mass of every possible nuclide is required. The atomic mass values used by ALEPH and by MCNP(X) itself must also be the same to ensure data consistency. MCNP(X) uses the values that are specified in the first part of the `xsdir` file, but the standard `xsdir` files only contain atomic mass data from 300 to 400 nuclides while ALEPH requires atomic mass values for at least every nuclide possible in ORIGEN. We have therefore decided to update those atomic mass values by using the Atomic Mass Evaluation 2003 included into NUBASE [21] from the Atomic Mass Data Center. These values are also specified with the isotopes file and they are also included in the `xsdir` files provided with ALEPH-LIB.

Although the user should never need to worry about the isotopes file (it is included in the libraries delivered with ALEPH), the general structure of the file is detailed here (should the

need arise). For an element with an element name EL, a proton number Z and NI different isotopes, the entry looks like this:

```
EL      Z      ZAID[0]  MASS[0]
          ZAID[1]  MASS[1]  ..  ZAID[NI]  MASS[NI]
```

where ZAID[0] and MASS[0] are the ZAID identification of the element ($Z*1000$) and the atomic mass of the element, expressed in units of neutron mass, as is the case in MCNP(X). ZAID[i] and MASS[i] (for $1 \leq i \leq NI$) are the ZAID identification and the atomic mass in units of neutron mass of isotope i.

We do not distinguish the metastable state of nuclides in this approach because a nuclide is supposed to have the same atomic mass, regardless of the metastable state.

Chapter 5

Error and Warning Messages

5.1 Reading the ALEPH input file

- Error: input file ... not found.
ALEPH tried to open the input file that was specified on the command line but couldn't find it.
- Error in line ...: path specified with DAT keyword does not exist or the isotopes file is missing

To check if the data path specified with the DAT keyword is correct, ALEPH will attempt to open the isotopes file that should be located there. If ALEPH fails to open the isotopes file, either the data path is incorrect or the isotopes file is missing. Either way, ALEPH cannot run the calculation.

- Error in line ...: the ALEPH xsdir file ... is missing
ALEPH tried to open the xsdiraleph file that was specified using the DAT keyword. Because ALEPH can't find it, the code cannot find the required cross section data required to calculate the ORIGEN libraries.
- Warning: material ... has no atomic mass in the isotopes file
atomic mass has been set to ...

When reading the xsdiraleph file, ALEPH will read the value for the atomic mass from the isotopes file for every nuclide entry in the xsdiraleph file. Although the isotopes file is as complete as possible (it contains data for over 3000 nuclides), it might be possible that the xsdiraleph file points to nuclides that are not included in the isotopes file. In that case, ALEPH will use the atomic mass number A of the nuclide as an estimate for the atomic mass.

Whenever this warning is issued, the user should check the isotopes file and add the missing data.

- Error on line ...: input of negative temperature with temperature keyword TMP

Temperature input on the TMP keyword must be non-negative and specified in eV.

- Warning: temperature above 2500 K detected in temperature keyword TMP
Temperature input on the TMP keyword must be specified in eV. To be sure that the user uses realistic temperature values, ALEPH will recalculate the temperature to K and test if the temperature is smaller than 2500 K which is a reasonable upper limit for realistic temperatures. This is just a warning message for the user to detect erroneous input.

- Error on line ...: illegal input (negative or zero) for the
... library

In the ORI keyword, the user has to specify (among others) the original ORIGEN library numbers for the activation products, actinides and fission products. These numbers must be non-negative and non-zero integers.

- Error on line ...: ORIGEN library ... found in file ...
Expected library ..., ... or ...

While reading the ORIGEN library specified on the ORI keyword, ALEPH found an ORIGEN library number different from the three numbers specified on the ORI keyword. Either a wrong ORIGEN library file was used or there is a formatting error in the file.

- Error: ORIGEN library file ... not found.

ORIGEN requires three library files to function: the cross section libraries, the decay library and the photon library. If ALEPH cannot find one of these files, the code will issue this error.

- Error on line ...: parallel option on keyword MCNP is either -1 or -2
ALEPH foresees two modes for running MCNP(X) (serial and parallel calculations) which have to be specified after the MCNP(X) executable. Option -1 has to be used for serial calculations and option -2 for parallel calculation. In this case, there probably is incorrect input in this line.

- Error on line ...: number of parallel slaves must be non-zero in
keyword MCNP

For parallel calculations, the MCNP(X) command line needs an extra argument: the number of parallel tasks. The amount of parallel slaves must be a non-negative and non-zero integer. Please note that it is up to the user to allocate the proper amount of resources to run the calculation.

- Error on line ...: illegal input (negative or larger than 1) for the
fractional absorption limit in keyword ABS

The fractional absorption criterion to be used by ALEPH is specified as an integer between 0 and 1 (the values of 0 and 1 are allowed).

- Error on line ...: illegal input (negative value) with keyword TAL
The tally number must be a positive integer.

- Error on line ...: the tally specified with the TAL keyword is not
a type 4 tally

ALEPH requires a neutron flux tally in all cells with burnable materials. This is a type 4 tally so that the tally number must end with 4 (for instance 4, 14, 24, ...). In this case, the tally number specified is not a type 4 tally.

- Error on line ...: weight option ... in the GWS keyword does not exist

ALEPH foresees in the use of two possible weight options for calculating the multi-group cross sections: either the constant spectrum (option -1) or the PWR weight spectrum (option -2). In this case, ALEPH did not find any of these options.

- Error on line ...: no input or illegal negative input for ... in keyword GWS

This error occurs when no input or illegal input (negative values) are used for any of the 4 input parameters for PWR spectrum in the GWS keyword.

- Error on line ...: keyword GWS used after the MAT keyword

ALEPH has detected the use of the GWS keyword after the MAT keyword. A global weight option can be set for the weight spectrum using the GWS keyword, but this keyword must appear before the MAT keyword. This error will most likely be accompanied by errors in the MAT keyword on the individual isotopes' weight spectra. See the input instructions for the GWS and MAT keyword for more details (see sections 2.3.2 and 2.4.3).

- Error on line ...: illegal input (negative or zero) for the number of materials burned in the keyword BURN

Because ALEPH allows for variable materials (both those that are being burned and those that are not), not all burnable materials must be burned from the beginning. In order to avoid confusion, the number of burnable materials that are being burned at any given time is the first input parameter on the BURN keyword. This must be a non-zero and non-negative integer.

- Error on line ...: illegal input in the keyword ..., the identification number of a variable material cannot be zero or negative

The BURN and VAR keywords are used to specify lists of MCNP(X) material numbers to be used in the calculation. These numbers cannot be zero or negative.

- Error on line ...: expected at least ... burnable materials but found only ... in the keyword BURN

ALEPH tested the number of burnable materials found on the BURN keyword against the number of burnable materials that are being burned at any given time. In this case, there are less materials than indicated. The user has probably forgotten to specify this number and that ALEPH has assumed that the first material number is the number of burnable materials that are being burned at any given time.

- Error on line ...: input of negative volumes with volume keyword VOL

The VOL card is used to specify the volumes of the cells containing burnable materials. It is obvious that these volumes cannot be zero or negative.

- Error on line ...: expected ... volumes but found ... volumes in the VOL keyword

The number of entries on the VOL keyword must be the same as the number of burnable materials that are being burned at any given time (the first entry on the BURN keyword).

Either the first entry on the BURN keyword is wrong or the user has not specified all volumes.

- Error on line ...: no BURN keyword specified before VOL

ALEPH has detected the use of the VOL keyword before the BURN keyword. Because the number of volume entries on the VOL keyword depends upon the input on the BURN keyword, the VOL keyword must always be used after the BURN keyword.

- Error on line ...: invalid library number for temperature T = ... eV

The library numbers specified in the MAT keyword can be negative (to indicate a library for reaction rate calculation only), positive (to indicate a transport library) or zero (for no library needed). These library numbers must be integers between (and including) -99 and 99 because the positive ones have to be valid MCNP(X) library numbers.

- Error on line ...: no TMP keyword specified before MAT

ALEPH has detected the use of the MAT keyword before the TMP keyword. Because the number of library entries on the MAT keyword equals the number of temperatures on the TMP keyword, the TMP keyword must always be used after the MAT keyword.

- Error on line ...: non existant material

Isotopes on the MAT keyword are identified using their ORIGEN identification (ZAMID). The smallest possible nuclide is hydrogen with 10010 as identification. Numbers smaller than this value are not legal identification numbers for isotopes.

- Error: no ENDF file for T = ... eV was specified in xsdiraleph
for ...

ALEPH checks the xsdiraleph file for every isotope and library number (other than zero) on the MAT keyword to see if the ENDF file exists. In this case, ALEPH found no entry in the xsdiraleph file for this isotope and temperature. The user should either fix the xsdiraleph by adding the isotope or he should remove the nuclide from the MAT keyword. Either way, ALEPH will not start the calculation.

- Warning: ENDF file ... for material ... specified in xsdiraleph
does not exist
No changes will be made to the ORIGEN library for this
nuclide

ALEPH checks the alephxmdir file for every isotope and library number (other than zero) on the MAT keyword to see if the ENDF file exists. In this case, ALEPH didn't find the ENDF file pointed to by the xsdiraleph file for this isotope and temperature. This warning could indicate a badly specified data path (in the DAT keyword), a wrong entry in the xsdiraleph file or simply that the ENDF file is missing. Because this is not an error per se, ALEPH will continue as normal but no changes will be made to the ORIGEN library for this particular isotope and temperature.

- Error: irradiation history input before TMP and BURN keywords

The irradiation history requires some input from the TMP and BURN keywords; namely the temperature (for use in the CHT keyword) and the number of burnable materials that are being burned (for IRP option -1).

- Error on line ...: ... change requested without spectral recalculation

This error message indicates that a change keyword (CHD, CHT, CHCM, CHBM and CHTR) has been requested for a point where the spectrum is not being recalculated. Because these change keywords can radically change the spectra in the system, a spectrum calculation is required.

- Error on line ...: temperature has no cross sections associated to it
A temperature change to a temperature that was not specified on the TMP keyword has been requested using the CHT change keyword. Since no library numbers are specified for this temperature, ALEPH cannot perform the calculation.

- Error on line ...: density change requested for a burnable material

Because the density of a burnable material is linked to the irradiation, it is impossible to change the density of a burnable material. Only densities of variable materials can be changed.

- Error on line ...: cell material change requested to a burnable material

The CHCM keyword is used to change the material in a cell, but only cells with variable materials can be changed and no burnable materials can be used.

- Error on line ...: non-burnable material used in CHBM keyword

The CHBM keyword is used to change burnable materials. In this case, ALEPH found a material number that is not a burnable material.

- Error on line ...: unknown IRF option ...
Error on line ...: unknown IRP option ...

The constant flux irradiation (IRF) only allows two different options: input of the absolute number of source particles (-1) or the absolute flux level of a material (-2). The constant power irradiation (IRP) only allows four different options: input of the power for every burnable material (-1), the total power for all materials (-2), the power of a particular material (-3) or the total power of a subset of materials (-4).

- Error on line ...: illegal input for ... in keyword OUT

Input on the OUT keyword is with 0 and 1 only. In most cases, this simply means that not all 4 output options were specified.

- Error on line ...: unknown keyword "..."

The ALEPH input parser has detected an unknown keyword in the input file.

- Error on line ...: incorrect input detected

ALEPH tried to read an input parameter but found something else or nothing at all. In this case, ALEPH will print the line with all the input parameters that the code expects, followed by the original line that it found. Check the input option for the correct syntax to solve the problem.

- Error on line ...: unexpected input
ALEPH has detected input beyond the regular input of a keyword. Only the \$-style comment is allowed on the same line when the regular input of a keyword is finished.
- Error: no input of keyword ...
Certain keywords are required by ALEPH while others are optional (see table 2.1). In this case, ALEPH has detected that one of those keywords has not been used.

5.2 Reading the MCNP(X) input file

- Error: temperature specified for cell number ... not specified
in TMP keyword
While going through the cell entries, ALEPH has found a cell with a burnable or variable material that uses a temperature that has not been declared on the TMP keyword.
- Error: density specified for cell number ... differs from the
density specified for a previous cell
Error: temperature specified for cell number... differs from the
temperature specified for a previous cell
ALEPH has found a cell containing a variable or burnable material with a certain density or temperature different from the temperature or density for a previous cell containing the same material. Because ALEPH requires unique temperatures and densities, the code cannot start the calculation.
- Error: density of material ... (...) is
different from the density previously specified in a cell: ...
When reading through the different materials, ALEPH found a variable or burnable material where the density (specified in a \$-style comment) is different from the density found for cells containing the same material.
- Error: incomplete input for isotope ... in material ...
The input for this isotope does not conform to the input specifications (something must be missing, check section 3.4 for the correct input).
- Error: nuclide ... specified for material ...
has no libraries for temperature T = ... eV.
When reading a material composition, ALEPH didn't find a library for a certain isotope at this temperature. Either the isotope wasn't included on the MAT keyword or the library number was set to 0 for this temperature.
- Error: material type ... does not exist
use -1 for AP, -2 for AC and -3 for FP
There are only three different material types used by ORIGEN. To identify these, ALEPH uses the following three options: activation products (option -1), actinides and daughters (option -2) and fission products (option -3).

- Error: metastable option ... does not exist
Because MCNP(X) uses the ZAID identification and ORIGEN the ZAMID identification, ALEPH still requires the input of the metastable state, which is either 0 or 1.
- Error: density of material ... not found in comment
When reading through the different materials, ALEPH found a variable or burnable material where the density has not been specified in a \$-style comment. ALEPH requires this density to function.
- Error: f4 neutron tally with number ... not found
While going through the MCNP(X) input file, ALEPH will look for the f4 tally specified with the TAL keyword. In this case, ALEPH has not found the tally. The user should check if he indicated the correct tally number.
- Error: burnable material ... not found
When ALEPH is done reading the MCNP(X) input file, it will also check if all burnable material from the BURN keyword were found in the MCNP(X) input file. In this case, ALEPH has not found such a material. The user should check the materials on the BURN keyword and the materials in the MCNP(X) input file.

5.3 Running ALEPH and MCNP(X)

- Warning: no transport library specified for nuclide ...
nuclide skipped
Warning: no library specified for nuclide ...
nuclide skipped
When preparing a new MCNP(X) input file, ALEPH found an isotope that doesn't have a transport library associated to it. MCNPX would be able to continue (because MCNPX would generate cross sections using models) but MCNP would not. This is why we decided to omit such nuclides from transport calculations.
- Fatal error occurred in MCNP(X) - run terminated
A fatal error has occurred in MCNP(X). The best solution is to try the MCNP(X) input file in a pure MCNP(X) run to see what is wrong and to correct the problem. Again, it is up to the user to provide a working MCNP(X) input file for use with ALEPH.
- Bad trouble occurred in MCNP(X) - run terminated
This error is similar to the one above. The best solution is to try the MCNP(X) input file in a pure MCNP(X) run to see what is wrong and to correct the problem. Again, it is up to the user to provide a working MCNP(X) input file for use with ALEPH.
- Wrong executable for MCNP(X) or unknown trouble in
MCNP(X) - run terminated
When the operating system returned control to the ALEPH executable, the code didn't find the MCNP(X) output file. It is possible that the MCNP(X) executable is wrong or that there was another unexpected problem with MCNP(X).

- Error: this is not a linearized ENDF file.
Fault detected in file 3, mt = ...

When calculating the multi-group cross sections, ALEPH has found an ENDF file with a cross section that it requires that has not been linearized or that has multiple interpolation zones. This can happen when an unprocessed ENDF file is used or when there is something wrong with the index of the ENDF file (in file 1, mt451). In this last case, the index can be corrected by using the DICTIN code from the PREPRO package [23].

- Error: no ENDF file found.

ALEPH tried to open the ENDF file but couldn't find it. Normally, this error should not occur because this is checked before running ALEPH but it is still possible that something else happened.

- Warning: material ... has no atomic mass in the isotopes file
atomic mass has been set to ...

When reading the ORIGEN output, an isotope was found that does not appear in the isotopes file. The isotopes file does contain data for over 3000 nuclides but this does not mean that it is complete. This error message might also indicate a problem with the isotopes file itself (the element name field might be incorrect).

- Error: no ORIGEN output files found - check executable

ALEPH failed to open the ORIGEN output file. Either there is something wrong with the executable (compiler related problems,...) or the name and path of the executable were wrong.

Chapter 6

ALEPH test problem and output

6.1 The NEA-BUC single pin problem

The NEA-OECD BUC IV-B benchmark [24] has been proposed by the expert group on burn-up Credit (BUC) of the Working Party on Nuclear Criticality Safety (NEA - WPNCS). The investigation of burn-up credit for different types of fuel is an ongoing objective of the NEA-OECD Burn-Up Credit (BUC) expert group. For this specific benchmark, three geometrical 2D models were considered:

- A single pin in a moderator cell, with reflective boundary conditions. This model is representative for an infinite medium and provides information about reactivity and fuel inventory as a function of burn-up. The pitch of the cell must be modified to take into account the assembly global moderation ratio that the pin cell simulates.
- An assembly model with reflective boundary conditions. This model provides more information than the pin cell model, since the pin power distribution and pin material inventory can be computed. The assembly calculation is a standard calculation step in a complete design core calculation.
- A supercell model that aims to calculate a fuel assembly while taking into account its environment. It is especially recommended when dealing with MOX fuel, as this type of fuel is loaded in cores filled with a larger number of UO₂ fuel assemblies: the MOX fuel assembly behavior depends on the neutron spectrum established in the neighboring assemblies. In particular, power peaking at the MOX fuel assembly border needs to be carefully assessed.

Two types of MOX fuels were considered in the benchmark specifications: MOX made with reactor-grade plutonium (RG-MOX) and MOX made with weapon-grade plutonium (WG-MOX). The depletion was assumed to be at constant power and the irradiation history consists of three cycles of 420 days with 30 days of downtime in between the cycles. The third cycle is then followed by a cooling time of 5 years. At the end of the irradiation, the spent fuel must have reached a final burn-up of 48 GWd/tHM.

As a test problem, we consider the pin cell problem. For the calculation in ALEPH, we have subdivided every cycle into time steps of 26.25 days (every step thus accounts for an average burn-up of 1 GWd/tHM) for a total of 51 burn-up steps (48 constant power steps and 3 decay

steps). We have burned the fuel in the model as a single cell¹. For every burn-up step we have run a criticality calculation of 280 cycles (30 inactive and 250 active cycles) with 20000 neutron histories per cycle. The fractional absorption criterion has been set to 99.99 %. The average error on the total flux is 0.02 % for. The complete ALEPH input file for this problem can be found in appendix B.

Table 6.1: Relative differences (given in %) of WIMS8A and ALEPH 1.1.2 to APOLLO2 using JEF 2.2 data after 420, 870 and 1320 days of irradiation for the pin cell model.

Nuclide	EOC1 (420 days)		EOC2 (870 days)		EOC3 (1320 days)	
	WIMS	ALEPH	WIMS	ALEPH	WIMS	ALEPH
²³⁴ U	1.14	-0.21	2.13	-0.43	3.16	-0.61
²³⁵ U	0.22	0.20	0.48	0.26	0.86	0.21
²³⁶ U	-0.96	-1.02	-0.90	-0.83	-0.84	-0.80
²³⁸ U	-0.02	0.01	-0.04	0.02	-0.10	-0.02
²³⁸ Pu	0.13	0.24	0.46	0.55	1.01	1.01
²³⁹ Pu	0.88	-0.40	2.09	-0.83	3.73	-0.96
²⁴⁰ Pu	-1.04	0.22	-1.87	0.26	-2.60	-0.03
²⁴¹ Pu	1.84	0.65	2.78	1.37	3.40	1.89
²⁴² Pu	0.55	-0.44	1.13	-0.70	1.71	-0.66
²³⁷ Np	-8.83	14.38	-8.94	13.28	-9.13	12.26
²⁴¹ Am	1.06	0.31	2.12	0.81	3.16	1.17
^{242m} Am	-10.63	-3.53	-9.37	-3.00	-7.91	-2.45
²⁴³ Am	-3.16	0.93	-3.65	0.90	-3.97	0.94
²⁴² Cm	3.88	0.89	3.84	1.29	4.07	1.87
²⁴³ Cm	5.13	1.46	4.81	1.84	4.90	2.55
²⁴⁴ Cm	0.01	0.20	-0.64	0.30	-1.17	0.44
²⁴⁵ Cm	1.59	-2.05	1.11	-0.24	0.92	-0.11
⁹⁵ Mo	-0.04	0.02	-0.11	0.18	-0.21	0.37
⁹⁹ Tc	0.97	0.58	0.37	0.78	0.12	0.98
¹⁰¹ Ru	-0.64	-2.88	-0.64	-2.70	-0.66	-2.52
¹⁰³ Rh	-0.20	-3.00	-0.39	-3.45	-0.50	-3.83
¹⁰⁹ Ag	0.41	-3.05	0.38	-3.73	0.66	-4.46
¹³³ Cs	-0.08	1.40	-0.33	1.50	-0.45	1.62
¹⁴³ Nd	0.37	1.35	0.18	1.29	0.23	1.30
¹⁴⁵ Nd	-0.36	-0.48	-0.47	-0.25	-0.53	0.03
¹⁴⁷ Sm	-0.50	-0.62	-0.79	-0.39	-1.02	-0.30
¹⁴⁹ Sm	18.12	11.34	1.51	-6.52	2.47	-7.44
¹⁵⁰ Sm	-1.02	2.71	-1.29	3.69	-1.42	5.32
¹⁵¹ Sm	0.72	1.66	1.28	-3.11	2.01	-7.32
¹⁵² Sm	-1.43	-1.39	-1.68	-3.07	-1.93	-5.69
¹⁵³ Eu	-0.87	0.21	-1.22	-0.80	-1.59	-2.22
¹⁵⁵ Gd	3.58	-16.75	0.20	-10.30	-5.88	-3.42

¹To correctly take into account the rim-effect, we can also sub-divide the fuel cell in several separate concentric fuel cells.

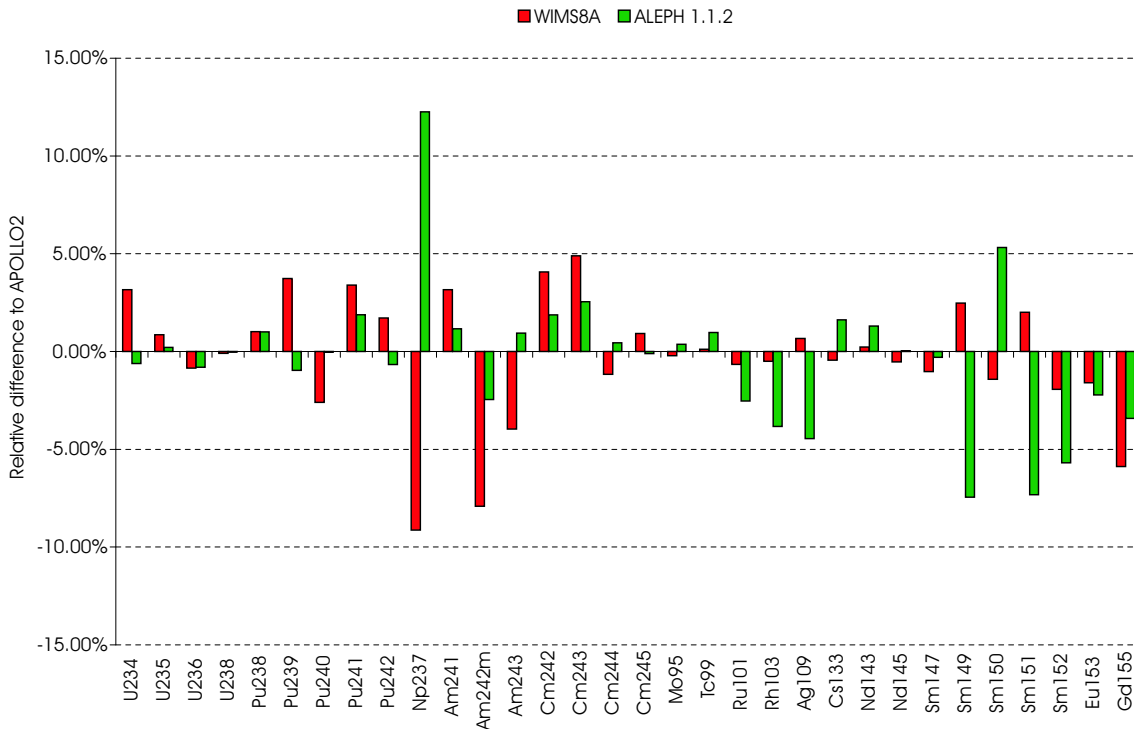


Figure 6.1: Relative differences (given in %) of WIMS8A and ALEPH 1.1.2 to APOLLO2 using JEF 2.2 data after 1320 days of irradiation for the pin cell model.

The data used in the calculation is JEF 2.2 (as the results given in the BUC benchmark are obtained with JEF 2.2 data). The fuel cell has a temperature of 900 K, the JEF 2.2 data at 900 K that we used can be found in ALEPH-LIB [20]. The cladding and moderator cell have a temperature of 620 and 575 K respectively. We used ALEPH-DLG to prepare the required data at these temperatures.

The calculation time was 280 hours (on a single Dual Xeon 3 GHz machine). Table 6.1 gives the relative difference of ALEPH 1.1.2 and WIMS8A [25] to APOLLO2 [26] after an irradiation of 420, 870 and 1320 days (the end of the three cycles - EOC1, EOC2 and EOC3). Figure 6.1 shows the results for the end of cycle 3.

Figure 6.1 and table 6.1 shows that ALEPH performs admirably well compared to APOLLO2 for the actinides. All U and Pu isotopes (except ^{238}Pu) have final compositions within 1.5 % of those of APOLLO. The ^{237}Np content is computed lower and higher respectively by WIMS and ALEPH, as compared to APOLLO. It should be noted that the ^{237}Np build-up is mainly linked to the (n,2n) reaction of ^{238}U for MOX fuel. As we showed before, the value for this reaction is in perfect agreement with MCNPX 2.5.f (see table tab:reactionratesu238comparisonmcnpx25e) so this is probably a data problem in the three codes. The Am and Cm isotopes are predicted within 1.5 to 4 % from the values given by APOLLO. In general, ALEPH performs better compared to WIMS for the actinide compositions except for ^{237}Np , ^{238}Pu and ^{245}Cm . In the case of ^{242m}Am , we can even speak of a major improvement.

We also observe a global agreement between WIMS and APOLLO2 for the fission products in the three cases, especially for the Sm isotopes. The fact that ALEPH doesn't perform as well on the fission products (the compositions show differences of 0.5 to 10 % with APOLLO) as with the actinides is probably caused by the fact that the version of ALEPH used for these calculations still uses the original fission yield values from the ORIGEN library. A newer version of ALEPH will also update these yield values.

6.2 Problem summary

The first part of the ALEPH output file consists of the ALEPH input instructions and the MCNP(X) input file. This is followed by the problem summary. This is an overview of some important calculation parameters such as the number of groups used and the upper and lower energy considered in the calculation. The problem summary also gives an overview of the burnable and variable materials that are being used in the problem. For every material, the composition in g cm^{-3} will be given. For burnable materials that are being burned or for variable materials that are being used in the beginning, an overview of the cells, volumes and temperature will also be given.

The problem summary for the single pin problem looks like this:

Problem summary

Group Structure:

43000 groups
E_min = 1e-05 eV
E_max = 2e+07 eV

Burnable materials:

1 materials being burned in 1 different cells
0 materials currently not present
0 materials currently undergoing decay

Material 1 - currently being burned

Cells = 1
Volume = 52.810 cm3
Temperature = 7.756E-08 eV
Density = 10.450 g/cm3

Composition

8016 1.23735E+00 g/cm3
92234 1.00860E-04 g/cm3
92235 2.11885E-02 g/cm3
92238 8.45426E+00 g/cm3
94238 1.84248E-02 g/cm3
94239 4.03154E-01 g/cm3
94240 1.92357E-01 g/cm3
94241 7.00149E-02 g/cm3
94242 5.30620E-02 g/cm3

6.3 Burn-up step output

6.3.1 Calculation output

For every burn-up step, ALEPH prints out a lot of information to the standard output screen. If the user has set the appropriate option on the OUTkeyword, ALEPH will also print all of that information to the output file. First, ALEPH will indicate for which points the spectra will be used (in the example given below the spectrum is used for calculating the composition up to

point 1). After running MCNP(X) and reading the spectra, ALEPH will start calculating the new ORIGEN libraries. At this point, ALEPH will write out data on every ENDF file used. Because multiple temperatures are possible, ALEPH will do this for every temperature used for burnable materials (in this case, it is only done for 900 K). When the new libraries have been prepared, ALEPH will run ORIGEN and accumulate the burn-up of every material. For the single pin model, this part of the output file looks like this (parts of the output were left out due to space restrictions):

```
Calculating spectra for point 1

  Preparing MCNPX input file

  Running MCNPX

  Performing file clean up

  Reading spectra

  Calculating ORIGEN libraries for materials with temperature T = 7.756e-08

    Processing ENDF cross section file ... for nuclide 10010

      Calculating multigroup cross section for ENDF MT-number 102

    Processing ENDF cross section file ... for nuclide 10020

      Calculating multigroup cross section for ENDF MT-number 16
      Calculating multigroup cross section for ENDF MT-number 102

    ...

    Processing ENDF cross section file ... for nuclide 922350

      Calculating multigroup cross section for ENDF MT-number 16
      Calculating multigroup cross section for ENDF MT-number 17
      Calculating multigroup cross section for ENDF MT-number 18
      Calculating multigroup cross section for ENDF MT-number 102

    ...

    Processing ENDF cross section file ... for nuclide 982530

      Calculating multigroup cross section for ENDF MT-number 18
      Calculating multigroup cross section for ENDF MT-number 102

    Processing ENDF cross section file ... for nuclide 992530

      Calculating multigroup cross section for ENDF MT-number 102

  Performing evolution calculation for point 1

    Processing irradiation history

    Calculating material composition for material 1

    Accumulating burn up
```

6.3.2 Calculated cross section values

Whenever asked by the user, ALEPH will print out the one group cross section values and branching ratios used by ORIGEN to perform the depletion calculation. The overview consists of 8 columns (total (n,γ) , total $(n,2n)$, $(n,3n)$, fission, (n,α) , (n,p) and the (n,γ) and $(n,2n)$ branching ratio) for every nuclide considered. To provide an easy overview, one group cross section values that are zero have simply been left blank in the table. All cross section values are expressed in barn.

For the first point of the single pin calculation, the following values were used by ORIGEN (the $(n,3n)$, fission and (n,α) columns were left out due to lack of space):

Cross section values used in evolution calculation for material 1 for point 1

	n, gamma	n, 2n	...	n, p	n, g BR	n, 2n BR
10010	7.32792E-03		...			
10020	1.45761E-05	2.35605E-03	...			
10030		8.32168E-05	...			
20030			...	1.17128E+02		
30060	8.54820E-04		...	1.61288E-03		
30070	8.10438E-04	2.31914E-05	...			
40090	2.44718E-04		...	3.36593E-08		
50100	1.10028E-02		...	3.27360E-03		
50110	1.35484E-04	2.40301E-06	...	7.48990E-07		
...						
110230	1.46639E-02	3.08755E-06	...	7.10060E-04	4.04840E-01	
130270	6.45261E-03	2.14205E-06	...	1.72824E-03		
150310	4.36780E-03	2.58941E-06	...	1.41911E-02		
160320	1.25646E-02	1.07506E-08	...	2.70882E-02		
160330	8.10124E-03	1.28321E-04	...	2.42587E-02		
...						
922340	1.81934E+01	8.59481E-04	...			
922350	4.57342E+00	5.71103E-03	...			
922360	9.09639E+00	4.19806E-03	...			
922370	1.35042E+01	1.14287E-02	...			
922380	8.13424E-01	6.15924E-03	...			
932370	2.14749E+01	1.31837E-03	...			7.41493E-01
932380	4.66131E+00	7.30583E-03	...			
932390	1.25471E+01	1.85385E-03	...		1.15044E-01	
...						
982520	1.69042E+00	4.21989E-03	...			
982530	1.52449E+01		...			
992530	1.25686E+02		...		4.10005E-01	

6.4 Final output

6.4.1 Burn-up history

When the entire calculation is done, ALEPH will print out the final output. This starts with a detailed overview of the final irradiation history used by ALEPH. This overview will indicate material changes (both to burnable and variable materials), geometry changes, ... This overview will also give the power or flux levels as calculated by ALEPH and used by ORIGEN 2.2 for every burnable material that was being burned.

For our single pin problem, this summary looks like this:

Burn up history overview

```

Step 1
  IRP 0.000350955 MW/cm3 26.25 d
...
Step 16
  IRP 0.000350955 MW/cm3 26.25 d
...
Step 17
  DEC 30 d
...
Step 18
  IRP 0.000350955 MW/cm3 26.25 d
...
Step 50
  IRP 0.000350955 MW/cm3 26.25 d
...
Step 51
  DEC 5 y

```

6.4.2 Accumulated burn-up

An important quantity in depletion calculations is the burn-up accumulated by a material during the irradiation. Burn-up is usually expressed as GWd/ton initial heavy metal or MWd/kg initial heavy metal. We prefer to use this last unit. So, in the case of an irradiation step with constant power P_j the burn up BU_j accumulated by material j will be given by:

$$BU_j = 10^6 \frac{P_j t}{\rho_{a,j} V_j} \quad (6.4.1)$$

where $\rho_{a,j}$ is the density (in g/cm^3) of the actinides initially present in the material and t is the irradiation period in days. V_j is the volume of the cells containing the material j .

For a step with constant flux irradiation of material j with flux ϕ_j , this becomes:

$$BU_j = 10^6 \frac{P_{0,j} t \phi_j}{\rho_{a,j} V_j \phi_{0,j}} \quad (6.4.2)$$

where $P_{0,j}$ is the specific normalisation power of material j and $\phi_{0,j}$ is a measure of the total flux in the material j (in fact, MCNP(X) will provide us with $\phi_{0,j} V_j$ per source particle for every material that we are burning), see equation 2.8.1.

For the single pin model, this burn-up summary looks like this:

Accumulated burn-up summary - MWd/kg initial HM

	point 1	point 2	...	point 51	total burn-up
1	1.00000E-00	1.00000E-00	...	0.00000E+00	4.80000E+01

6.4.3 Material composition

The most important part of the output consists of the material compositions. For every burnable material an overview of the evolution of every nuclide is given. For the single pin problem, this look like:

Evolution of individual nuclides for material 1 - g/cm3

	point 0	point 1	...	point 50	point 51
10010	0.00000E+00	7.98349E-10	...	4.22820E-08	4.22820E-08
10020	0.00000E+00	3.95773E-15	...	1.21228E-11	1.21228E-11
10030	0.00000E+00	2.08759E-08	...	9.12884E-07	6.89493E-07
...					
922350	2.11885E-02	2.09231E-02	...	1.05881E-02	1.06173E-02
922360	0.00000E+00	6.69858E-05	...	2.29681E-03	2.38345E-03
...					
922380	8.45426E+00	8.44889E+00	...	8.16957E+00	8.16957E+00
...					
942380	1.84248E-02	1.82784E-02	...	1.57764E-02	1.66780E-02
942390	4.03154E-01	3.96673E-01	...	2.05135E-01	2.05846E-01
942400	1.92357E-01	1.92442E-01	...	1.65372E-01	1.66953E-01
942410	7.00149E-02	7.14086E-02	...	9.50976E-02	7.47551E-02
942420	5.30620E-02	5.30168E-02	...	6.07010E-02	6.07028E-02
...					
992540	0.00000E+00	0.00000E+00	...	1.20236E-14	1.21903E-16
992541	0.00000E+00	0.00000E+00	...	3.07651E-16	0.00000E+00
992550	0.00000E+00	0.00000E+00	...	3.75551E-17	3.01101E-31

6.4.4 Timing report

The final part of the output file is the timing report. It is a summary of the time that it took ALEPH to perform the calculation. In this summary, the MCNP(X) calculation time (this is wall time), the time required to read the spectra from the tally file, the time to calculate the new libraries and the time to run ORIGEN is given for every point in the irradiation history. All these times are given in seconds. At the end of this summary, ALEPH indicates the total calculation time in seconds minutes and hours.

ALEPH timing report

Reading ALEPH and MCNP(X) input files: 1 s

ALEPH calculation time per point:

	Running MCNPX	Reading spectra	Calculate libraries	Running ORIGEN	Total time
0	6.31600E+03		3.40000E+01	2.00000E+00	6.35200E+03
1	1.12870E+04		3.10000E+01	2.00000E+00	1.13200E+04
...					
49	2.49460E+04		3.10000E+01	2.00000E+00	2.49790E+04
50				1.00000E+00	1.00000E+00

Total calculation time: 1.00824e+06 s

Total calculation time: 16804 min

Total calculation time: 280.066 h

Appendix A

Version history

ALEPH version 1.0.0 (January 2005)

- Initial release

ALEPH version 1.0.1 (May 2005)

- Minor fixes: some input options were rewritten and new ones were added to simplify the ALEPH input and especially the MCNP(X) input file.

The keywords `MCN` for the MCNP(X) executable and `MMC` for the fractional absorption criterion were replaced by `MCNP` and `ABS`. This is just a cosmetic change, the meaning of the keywords didn't change.

The keywords `APL` to specify the activation products library number, `ACL` to specify the actinide library number, `FPL` to specify the fission products library number and `PHL` to specify the photon library were merged into a single keyword `LIB`. This keyword is also used to specify the name of the `ORIGEN` library file and the name of the decay library file. The `ORIGEN` library name no longer needs to be specified on the ALEPH command line as before.

The keyword `ORI` is now used to specify the path and executable name of `ORIGEN 2.2`, similar to the `MCNP` keyword for the MCNP(X) executable (but without the parallel options of course).

The `DAT` keyword is now used to specify the data path to the ENDF files used by ALEPH. This allows for a greater flexibility for the nuclear data compared to the now obsolete option based keyword (`-1` for JEF 2.2, `-2` for JEFF 3.0, ...). The `xmdiraleph` file has been introduced to specify the individual ENDF files for every isotope and library number on the `MAT` keyword.

The temperatures on the temperature keyword `TMP` have now to be specified in eV and not in K as before. This was changed because temperatures are specified in eV in MCNP(X).

The `NGR` keyword used to specify the number of groups in the group structure has been replaced by the `EGS` keyword for specifying the entire group structure using a constant lethargy approach. The group structure does no longer have to be included in the MCNP(X) input file, which shortens the input file considerably. The `ERG` keyword to specify the begin energy of the group structure is now obsolete (this has been set to 10^{-11} MeV by default).

The `NSP` keyword that was used to specify the number of burnable material is now replaced by the `BURN` keyword. The `BURN` keyword is used to specify the number of materials that are burned at any given time along with all the burnable material numbers. A similar keyword called `VAR` has to be used to declare the variable material numbers.

The new keyword `VOL` has now to be used to specify the volumes of the cells containing burnable materials (using the same order as on the `BURN` keyword). These volumes no longer have to be specified in comment lines in the `MCNP(X)` input file.

Due to the previous two changes, the comment labels `VARCELL`, `BURNCELL`, `VARMAT` and `BURNMAT` along with the required parameters (volumes, index, ...) no longer have to be used. Only the density of burnable and variable materials has still to be specified using a `$`-style comment in the `MCNP(X)` input file.

It is no longer necessary to end a burn-up step using the `END` keyword and it is no longer necessary to specify the total number of steps on the `HIS` keyword and the step number on the `STP` keyword.

- New feature: a third output option has been added to the `OUT` keyword: write the screen output to the output file.

ALEPH version 1.1.0 (June 2005)

- New feature: material compositions can now be entered in atom fractions and densities can be entered as atoms $\text{barn}^{-1} \text{cm}^{-1}$ as well. Previously, the compositions had to be entered as weight fractions and densities in g cm^{-3} . As is the case in `MCNP(X)`, both representation can also be interchanged (compositions in weight fraction and density in atoms $\text{barn}^{-1} \text{cm}^{-1}$ and vice versa are allowed).

Material compositions are now stored internally as atoms $\text{barn}^{-1} \text{cm}^{-1}$ and no longer in g cm^{-3} . In order to recalculate the compositions to this representation, ALEPH requires the isotopes file that should be located in the directory given by the data path specified using the `DAT` keyword. We have decided to update the atomic mass values from `MCNP(X)` by using the Atomic Mass Evaluation 2003 included into `NUBASE` [21] from the Atomic Mass Data Center. These values can be found in the isotopes file and they are also included in the `xmdir` files provided with `ALEPH-LIB`.

- New feature: to allow for easier geometry changes, the `CHTR` change keyword has been added. This keyword allows a user to change the transformation card number on a surface card during an irradiation step. Previously, geometry changes were only possible by using the `CHCM` card where a cell's material was replaced by another. A disadvantage of this method was that every cell that took part in the geometry change had to be modeled separately, something which is not the case with the surface transformation.

ALEPH version 1.1.1 (August 2005)

- Minor bug fix: due to an indexing error in the calculation of multi-group cross sections, it was possible to have negative cross sections when the upper energy limit of the linearized cross section is smaller than the upper energy of the group structure. This has been corrected.

ALEPH version 1.1.2 (November 2005)

- Minor bug fix: when adding tallies to the MCNP(X) input file other than the tally for the calculation of the spectra for the reaction rate calculation, ALEPH stopped with a segmentation fault when starting to calculate the ORIGEN libraries. This was due to a problem when reading the tally output file that contained multiple tallies. This has been corrected.
- Minor bug fix: under some circumstances, the total composition of a burnable material that was placed into a cell again when it had been taken out in a previous step produced some anomalies (impossible nuclide identification numbers, ...). This was due to a test that was missing when assigning the correct library numbers. This has been corrected.
- Minor fix: rewrote some of the error and warning messages to be more clear to the user.
- New feature: a fourth output option has been added to the OUT keyword: write the ORIGEN output file for every ORIGEN calculation to a separate output file. This has been added to allow the user access to ORIGEN data other than compositions (such as toxicities, ...).
- New feature: in the ENDF format, the (n,2n), (n,p) and (n, α) reactions can be represented using a summation cross section, discrete levels, and a continuum in the same way that inelastic scattering is represented. For (n,2n) this is mt16 and mt875-891, for (n,p) this is mt103 and mt600-649 and for (n, α) this is mt107 and mt800-849. The fission reaction is also defined as a summation cross section (mt18) with partials (mt19-21 and mt38 for first, second, third and fourth chance fission).

The ENDF format states clearly that the summation cross section should always be given if any partials are present for the fission, (n,p) and (n, α) reaction (in other words: mt18, mt103 and mt107 should always be present). This is not the case for (n,2n). For ^9Be from JEFF 3.1 only the partials of the (n,2n) reaction are given. In order to correct problems like this, ALEPH will now first check if the summation cross sections are present and if they are not ALEPH will look for the partials and use those - should they exist.

Appendix B

NEA-BUC MOX pin cell input

```
TIT NEA Burn-up Credit Criticality Benchmark - single cell

c nuclear data
DAT /xs_aleph/aleph xsdiraleph22_900      $ data is JEF2.2 at 900 K
TMP 7.756E-08                             $ temperature set to 900 K = 7.756E-08 eV

c spectra information
BURN 1 1                                  $ burn material 1
VOL 52.8101725
EGS 1000 1e-10 1000 1e-9 1000 1e-8 1000 1e-7 1000 1e-6 4000 1e-5 4000 1e-4 10000 1e-3
    10000 1e-2 4000 1e-1 4000 1e+0 1000 1e+1 1000 2e+1 $ the group structure

c ORIGEN information
ORI O2_THERM
LIB buc.lib 701 702 703 GXUO2BRM.LIB DECA.Y.LIB

c MCNPX information
ABS 0.9999                                $ produce material composition, responsible for 99.99% absorption
TAL 4                                      $ the tally number that contains all the spectra
MCNP mcnp250_lfc -1 $ use MCNPX 2.5.0

c weigh the multigroup cross sections
GWS -1                                    $ use constant flux weighing

c output
OUT 1 1 1

HIS
STP 1
  IRP -1 1.853398E-02 4 26.25
STP 1
  IRP -1 1.853398E-02 4 26.25
STP 1
  IRP -1 1.853398E-02 4 26.25
STP 1
  IRP -1 1.853398E-02 4 26.25
STP 1
  IRP -1 1.853398E-02 4 26.25
STP 1
  IRP -1 1.853398E-02 4 26.25
STP 1
  IRP -1 1.853398E-02 4 26.25
STP 1
  IRP -1 1.853398E-02 4 26.25
STP 1
  IRP -1 1.853398E-02 4 26.25
```


STP 1
IRP -1 1.853398E-02 4 26.25
STP 1
IRP -1 1.853398E-02 4 26.25
STP 1
IRP -1 1.853398E-02 4 26.25
STP 1
IRP -1 1.853398E-02 4 26.25
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IRP -1 1.853398E-02 4 26.25
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IRP -1 1.853398E-02 4 26.25
STP 1
IRP -1 1.853398E-02 4 26.25
STP 1
IRP -1 1.853398E-02 4 26.25
STP 1
IRP -1 1.853398E-02 4 26.25
STP 1
IRP -1 1.853398E-02 4 26.25
STP 0
DEC 5 5

c the material list

MAT

10010 09c
10020 09c
10030 09c
20030 09c
30060 09c
30070 09c
40090 09c
50100 09c
50110 09c
70140 09c
70150 09c
80160 09c
80170 09c
90190 09c
110220 -09c
110230 09c
130270 09c
150310 09c
160320 09c
160330 09c
160340 09c
160360 09c
180360 -09c
180380 -09c
180400 -09c

240500 09c
240520 09c
240530 09c
240540 09c
250550 09c
260540 09c
260560 09c
260570 09c
260580 09c
270580 -09c
270581 -79c
270590 09c
280580 09c
280590 -09c
280600 09c
280610 09c
280620 09c
280640 09c
300640 -09c
320720 09c
320730 09c
320740 09c
320760 09c
330750 09c
340740 09c
340760 09c
340770 09c
340780 09c
340800 09c
340820 09c
350790 09c
350810 09c
360780 09c
360800 09c
360820 09c
360830 09c
360840 09c
360850 09c
360860 09c
370850 09c
370860 09c
370870 09c
380840 09c
380860 09c
380870 09c
380880 09c
380890 09c
380900 09c
390890 09c
390900 09c
390910 09c
400900 09c
400910 09c
400920 09c
400930 09c
400940 09c
400950 09c
400960 09c

410930 09c
410940 09c
410950 09c
420920 09c
420940 09c
420950 09c
420960 09c
420970 09c
420980 09c
420990 09c
421000 09c
430990 09c
440960 09c
440980 09c
440990 09c
441000 09c
441010 09c
441020 09c
441030 09c
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451050 09c
461020 09c
461040 09c
461050 09c
461060 09c
461070 09c
461080 09c
461100 09c
471070 09c
471090 09c
471110 09c
481060 09c
481100 09c
481110 09c
481120 09c
481130 09c
481140 09c
481151 79c
481160 09c
491130 09c
491150 09c
501120 -09c
501140 09c
501150 09c
501160 09c
501170 09c
501180 09c
501190 09c
501200 09c
501220 09c
501230 09c
501240 09c
501250 09c
501260 09c
511210 09c

511230 09c
511240 09c
511250 09c
511260 09c
521200 09c
521220 09c
521230 09c
521240 09c
521250 09c
521260 09c
521271 79c
521280 09c
521291 79c
521300 09c
521320 09c
531270 09c
531290 09c
531300 09c
531310 09c
531350 09c
541240 09c
541260 09c
541280 09c
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551370 09c
561340 09c
561350 09c
561360 09c
561370 09c
561380 09c
561400 09c
571390 09c
571400 09c
581400 09c
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601440 09c
601450 09c
601460 09c
601470 09c

601480 09c
601500 09c
611470 09c
611480 09c
611481 79c
611490 09c
611510 09c
621440 09c
621470 09c
621480 09c
621490 09c
621500 09c
621510 09c
621520 09c
621530 09c
621540 09c
631510 09c
631520 09c
631530 09c
631540 09c
631550 09c
631560 09c
631570 09c
641540 09c
641550 09c
641560 09c
641570 09c
641580 09c
641600 09c
651590 09c
651600 09c
661600 09c
661610 09c
661620 09c
661630 09c
661640 09c
671650 09c
681660 09c
681670 09c
711750 09c
711760 09c
721740 09c
721760 09c
721770 09c
721780 09c
721790 09c
721800 09c
731810 09c
731820 09c
741820 09c
741830 09c
741840 09c
741860 09c
751850 09c
751870 09c
791970 09c
832090 09c
902300 09c

902320 09c
 912310 09c
 912330 09c
 922320 09c
 922330 -09c
 922340 09c
 922350 09c
 922360 09c
 922370 09c
 922380 09c
 932370 09c
 932380 09c
 932390 09c
 942360 09c
 942370 09c
 942380 09c
 942390 09c
 942400 09c
 942410 09c
 942420 09c
 942430 09c
 942440 09c
 952410 09c
 952420 09c
 952421 79c
 952430 09c
 962410 09c
 962420 09c
 962430 09c
 962440 09c
 962450 09c
 962460 09c
 962470 09c
 962480 09c
 972490 09c
 982490 09c
 982500 09c
 982510 09c
 982520 09c
 982530 09c
 992530 -09c

END

MESSAGE: xsdir=xmdir22

TITLE: Benchmark BUC Phase IV-B : MOX fuels

c Case 5: first recycle MOX (case A) Pincell [Pu/U+Pu = 8% (5.136% fissile)]

c -----

c exterior worls

5 0 1 imp:n=0

c -----

c interior world

4 0 -1 imp:n=1 fill=3

c -----

c fuel pin

c fuel (900K)

1 1 6.987923E-02 -2 imp:n=1 u=3 tmp=7.756E-08

```

c   cladding (620K)
2   2 3.885870E-02 2 -3   imp:n=1 u=3   tmp=5.343E-08
c   moderator (575K)
3   3 7.265121E-02 3     imp:n=1 u=3   tmp=4.955E-08
c -----

c   surface cards
c
*1   rpp -0.65635 0.65635 -0.65635 0.65635 -50.0 50.0 $ pitch 1.3127
2   cz 0.410 $ MOX pellet radius
3   cz 0.475 $ cladding outer radius
c -----

c   data cards
c   average MOX
c   Nat=6.987923E-02
m1  nlib=01c $ 6.987923E-02
    92234 2.5952E-7 $ -2 0
    92235 5.4287E-5 $ -2 0
    92238 2.1387E-2 $ -2 0
    94238 4.6610E-5 $ -2 0
    94239 1.0156E-3 $ -2 0
    94240 4.8255E-4 $ -2 0
    94241 1.7491E-4 $ -2 0
    94242 1.3201E-4 $ -2 0
    8016 4.6586E-2 $ -1 0
c -----

c   Zr-2
c   Nat=3.885870E-02
m2  nlib=03c
    40090 1.9889E-02
    40091 4.3373E-03
    40092 6.6297E-03
    40094 6.7186E-03
    40096 1.0824E-03
    26054 7.8068E-06
    26056 1.2244E-04
    26057 2.8291E-06
    26058 3.7366E-07
    24050 2.9690E-06
    24052 5.7190E-05
    24053 6.4841E-06
    24054 1.6108E-06
c -----

c   water
c   Nat=7.265121E-02
m3  nlib=05c
    001001 4.8414E-2
    008016 2.4213E-2
    005010 4.7896E-6
    005011 1.9424E-5
mt3  lwtr.62t
c -----

c   tallies
c
fc4  flux
f4:n 1
sd4  1.0

```

```
fq4 E F
fm4
      (1.0)          $flux
c
c
print -85 -128
PRDMP 0 0 1 0 0
kcode 20000 1.16 30 280
totnu
sdef erg=d1 axs=0 0 1 rad=d2 ext=d3
sp1 -3 0.988 2.249
si2 0 0.410
si3 -50.0 50.0
```

OK

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