$\mathrm{U}_W\mathrm{B}_1$ User's Manual

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Contents

Introduction

U_WB_1 fast nuclear fuel depletion code and its usage is described in this manual. U_WB_1 code is being developed as a part of burnable absorber research at University of West Bohemia, Pilsen, Czech Republic. Although the code is intended for fuel design optimization with burnable absorbers, it can be used to calculate other fuel depletion calculations.

The code's main features include burnup solver, parallelized Monte Carlo transport solver and 2sPC depletion scheme. Currently, arbitrary 2-D geometry described by concentric cylinders in square or triangular lattice is supported. Based on geometry and composition of the model, neutron flux and effective cross sections are calculated by Monte Carlo transport solver at the beginning and the end of fuel depletion, the rest of depletion time steps are estimated by nuclide-based interpolation scheme of 2sPC depletion scheme. Burnup solver uses matrix exponential method and CRAM approximation to calculate next-step inventory of selected geometric regions. The code is supplied with data libraries based on ENDF/B-VII.1 nuclear data library.

The code is able to calculate fuel inventory and multiplication factor during depletion. Multiplication factor progress during fuel depletion can be used to evaluate fuel design. Knowledge of fuel inventory may be used to calculate quantities based on fuel inventory, e.g. decay heat, radiation sources, activity and so on.

Instructions for installation of the code are supplied. Example input and output files are shown and commented. In case of problems, comments or suggestions, please contact us via e-mail lovecky@rice.zcu.cz.

Chapter 1

Installation

The chapter describes installation of $U_W B_1$ code. Recommended system settings are suggested.

1.1 Requirements

$U_W B_1$ code is written in Fortran language. In order to speed-up burnup solver, algebraic libraries BLAS[1] (BLAS , 2001) and MUMPS[2] (MUMPS , 2011) are used. Poor performance of $U_W B_1$ code with the algebraic libraries under Windows OS lead to the support of only Linux OS, however, the code was successfully tested on Mac OS. Relatively large internal variables require 64-bit OS.

The code is being developed under Ubuntu environment. The environment can be used either as native Linux environment or as Linux environment operated virtually under Windows machine. Virtual operating system is handled with virtualization software Oracle VM VirtualBox, other alternatives are possible (e.g. VMware Player). The code is developed mainly on system with Intel Core i7-3630QM processor and memory of 8 GB RAM under latest long-term Ubuntu version (14.10) that is running under Windows 7 Professional with help of VirtualBox. If VirtualBox is used, typical issues are:

1. setting 64-bit guest Linux in Windows host - be sure that virtualization option is enabled in BIOS
2. setting share folder between Linux and Windows - be sure to install VirtualBox's Guest Additions, shared folder with Windows location `C:\...\folder` appears on Linux as `/media/sf_folder`
3. accessing share folder in Ubuntu - be sure to add user into vboxsf group

Processor is not limiting parameter of $U_W B_1$ code, however, at least 2 GHz speed is recommended. Current version of the code runs in parallel mode. Only Monte Carlo solver, that account for the major part of calculation time, is parallelized by OpenMP interface, therefore, shared-memory multiprocessor platforms are supported.

Operating memory slightly depends on the number of geometry regions. For minimum number of 2 geometry regions, the code will allocate about 2.5 GB. Minimum of 4 GB RAM is required, however, 8 GM RAM is highly recommended.

Disc space is not an issue for $U_W B_1$ code, data libraries are less than 500 MB. Based on number of geometry regions and depletion interval, output file can typically require tens of MB space.

[1]Set of algebraic libraries (Fortran 90 and C) for the solution of linear systems of equations, linear least squares problems, eigenvalue problems and singular value problems.

[2]Set of algebraic libraries (Fortran 90 and C) for solving systems of linear equations where the matrix is a square sparse matrix. MUMPS implements a direct method based on Gaussian factorization and LU decomposition.

1.2 Compiling

U_WB_1 code is supplied as an executable file without source files, therefore, compilation should not be an issue. Standard compilation is performed with GNU Fortran (GFortran), required algebraic libraries are linked into executable file.

1.3 Installing

U_WB_1 code consists of two parts, executable file `uwb1` and data libraries folder `uwb1libs`. Since the code lack GUI, only executable file, data libraries, input and output files are objects to describe.

U_WB_1 executable file `uwb1` typically needs to be present in the folder where calculation is being performed. However, based on user's preferences, executable file can be moved into another location and/or be used as alias without the need to be present in the calculation folder. These options are described later in the next part of the manual. Because of the differences between Linux and Mac OS, separate executable files `uwb1_linux` and `uwb1_macosx` are available.

U_WB_1 data libraries folder `uwb1libs` needs be copied to an arbitrary location. Path to data libraries folder is part of U_WB_1 input file.

1.4 Running

Running U_WB_1 code is not different from running other software in Linux environment. Input and output file names are parameters of the code execution. Having executable file `uwb1`, running options are:

1. copy executable file `uwb1` into calculation folder and call calculation in terminal line by

   ```
   ./uwb1 <input> <output>
   ```

   For example,

   ```
   ./uwb1 vver50.inp vver50.out
   ```

2. copy executable file `uwb1` into software installation folder `folder` and use path to executable file in calculation call in terminal by

   ```
   /folder/uwb1 <input> <output>
   ```

   For example, copy executable file into folder `/home/lovecky` and run the code from calculation folder in terminal line by typing

   ```
   /home/lovecky/uwb1 vver50.inp vver50.out
   ```

3. set environmental variable for U_WB_1 and use it as an alias, user should edit its bashrc file (∼`/.bashrc`) and call calculation in terminal line by

   ```
   uwb1 <input> <output>
   ```

   For example

   ```
   uwb1 vver50.inp vver50.out
   ```

Users are encouraged to use U_WB_1 in batch calculation using bash script. Provide the list of calculation calls into executable script and tell your Linux OS that you are using bash script – include

```
#!/bin/bash
```

in the first line of the script.

Chapter 2

Version history

$U_W B_1$ code is under constant development, its weaknesses are continuously removed by introducing new versions of the code as performed calculations require. The chapter summarizes stable code releases. Code versions are labeled by the date of compilations, this date is the first information that $U_W B_1$ prints to screen output. Code development began in late 2012.

2.1 December 2012

Initial release of $U_W B_1$ code. Implementation of algebraic library BLAS/LAPACK(MUMPS , 2008) for general matrix calculations in burnup solver via CRAM method (Isotalo and Aarnio, 2011), (Pusa and Leppänen, 2010). Both Windows and Linux OS supported. Employs fuel depletion with flux depletion and precomputed libraries of 1-group or 2-group effective cross sections for various nuclear fuel types.

2.2 February 2013

LAPACK algebraic library replaced by PARDISO library for sparse matrices (Schenk et al., 2008), (Schenk et al., 2007). Improvement in the speed with no influence on the precision. No change in input files. Calculations published in Annals of Nuclear Energy (Lovecký et al., 2014a) and later on ICONE-22 (Prehradný et al., 2014), (Lovecký et al., 2014b).

2.3 January 2014

Unstable behavior of PARDISO sparse library lead to replacement by MUMPS library. Only Linux OS supported. Power depletion introduced, replacing flux depletion. Improvement both speed and precision of the code.

2.4 October 2014

Major improvement in the precision by introducing the Monte Carlo transport solver. Because of the improvements, data libraries folder containing general nuclear data is introduced. Arbitrary geometry available, precomputed effective cross sections no longer used. New input file structure. Monte Carlo solver currently under publication process in Annals of Nuclear Energy (Lovecký et al., 2015a).

2.5 December 2014

Two-step predictor-corrector method (2sPC) introduced. Improvement in the speed while having minimal influence on precision. No change in input files, ready for publication in Annals of Nuclear Energy (Lovecký et al., 2015b) and ICONE-23 (Prehradný et al., 2015), (Lovecký et al., 2015c).

2.6 February 2015

Improvements in precision and generalization. New geometry model with arbitrary number of concentric cylinders to better describe CANDU fuel, arbitrary number of power-depleted and flux-depleted regions. New description of thermal scattering cross section dependence on target velocities increase the precision. Minor changes in 2sPC burnup solver callings in order to speed-up the calculation. Minor changes in input file.

2.7 June 2015

Monte Carlo solver parallelized by OpenMP interface. Minor changes in random number generator stride. Minor changes in input file (added line that describes number of CPU threads).

2.8 September 2015

Improved accuracy - neutron direction description variables changed, rotation of direction cosines updated. No changes in input file.

Chapter 3

Data libraries

Data libraries contain mainly nuclear data such as cross sections, radioactive decay description and nuclide's properties. Very little input or deep library knowledge is required on the user in the area of nuclear data libraries. Data libraries containing nuclear data were prepared from ENDF/B-VII.1 library by $\mathrm{U}_W\mathrm{B}_1$ subroutines that are not supplied with the code, i.e. the user cannot change the base library (ENDF/B-VII.1).

Nuclide's description library `uwb1zaid0423to3820.txt`, like the rest of the libraries, is an ASCII free-format file library. Burnup solver handles 3820 nuclides from radioactive data library, transport solver handles 423 nuclides from neutron data library. Each nuclide has three ID numbers – position in 423 nuclides (first column of the library), position in 3820 nuclides (second column of the library) and ZAID (third column of the library). ZAID number is given by ZAID=10000*Z+10*A+m, for example, U-238 has ZAID designation 922380, while Am-242m is designated by 952421.

The rest of the libraries are described in Appendix A on page 41. Format or data stored in these libraries does not influence the creation of $\mathrm{U}_W\mathrm{B}_1$ input file.

Chapter 4

Code flowchart

The chapter describes the way $U_W B_1$ code works in order to describe nuclear fuel depletion. Coupling of burnup and transport solver as well as 2sPC depletion scheme are described.

4.1 Calculation stages

$U_W B_1$ execution is performed in 5 stages – initial, predictor, corrector, depletor and estimator. The main code flowchart is depicted in Figure 4.1. 2sPC depletion scheme with used equations in detail is described in (Lovecký et al., 2015b).

Initial stage is used to analyse initial state of calculated fuel model by Monte Carlo transport solver. Total macroscopic cross sections are calculated before MC simulation in order to speed-up neutron random walk. Transport solver then calculate multiplication factor and neutron flux in all geometry regions in 4308 energy groups. Support calculations for burnup solver, evaluation of fuel basis and relative region powers, are made. Estimation formula describes ratio of neutron production to absorption in the fuel model.

Predictor stage uses initial state variables, mainly effective cross sections, to estimate fuel model state at the end of fuel depletion without calling transport solver in the inner depletion steps. Burnup solver is called in two loops, inner depletion step loop and outer geometry regions loop. Order of the loops was changed for calculation speed-up that is significant in the case of multiple depleted regions because of calling transition matrix preparation subroutine is minimized. At the end of predictor stage, transport solver is called for the second time in the calculation, predicting final state variables.

Corrector stage works in identical way that predictor stage, the only difference is that initial state effective cross sections are used from predicted final state effective cross sections. The idea is that this way, predictor and corrector averaged values calculate final state composition with approximately averaged effective cross sections (i.e. mid-burnup effective cross sections). Corrector stage employs the third and final transport solver execution. Averages of predictor and corrector values (effective cross sections, relative region powers, multiplication factor estimates, transport multiplication values) are used as final state values for the second step of 2sPC method.

Depletor stage is used to calculate fuel composition and multiplication factor estimate during burnup. Similarly to predictor stage, depletor stage uses two loops over depletion steps and geometry regions. On the other hand, third loop over the second predictor-corrector step is added. In this innermost loop, both effective cross sections and fuel composition at the end of depletion step are predicted, corrected and averaged. No transport solver is called during depletor stage.

Estimator stage is used to compare initial and final state multiplication factors calculated by transport solver with multiplication factor estimates. It is assumed that estimator formula has a difference that is linearly dependent on burnup. Multiplication factor estimates are corrected for the expected differences and used in final output.

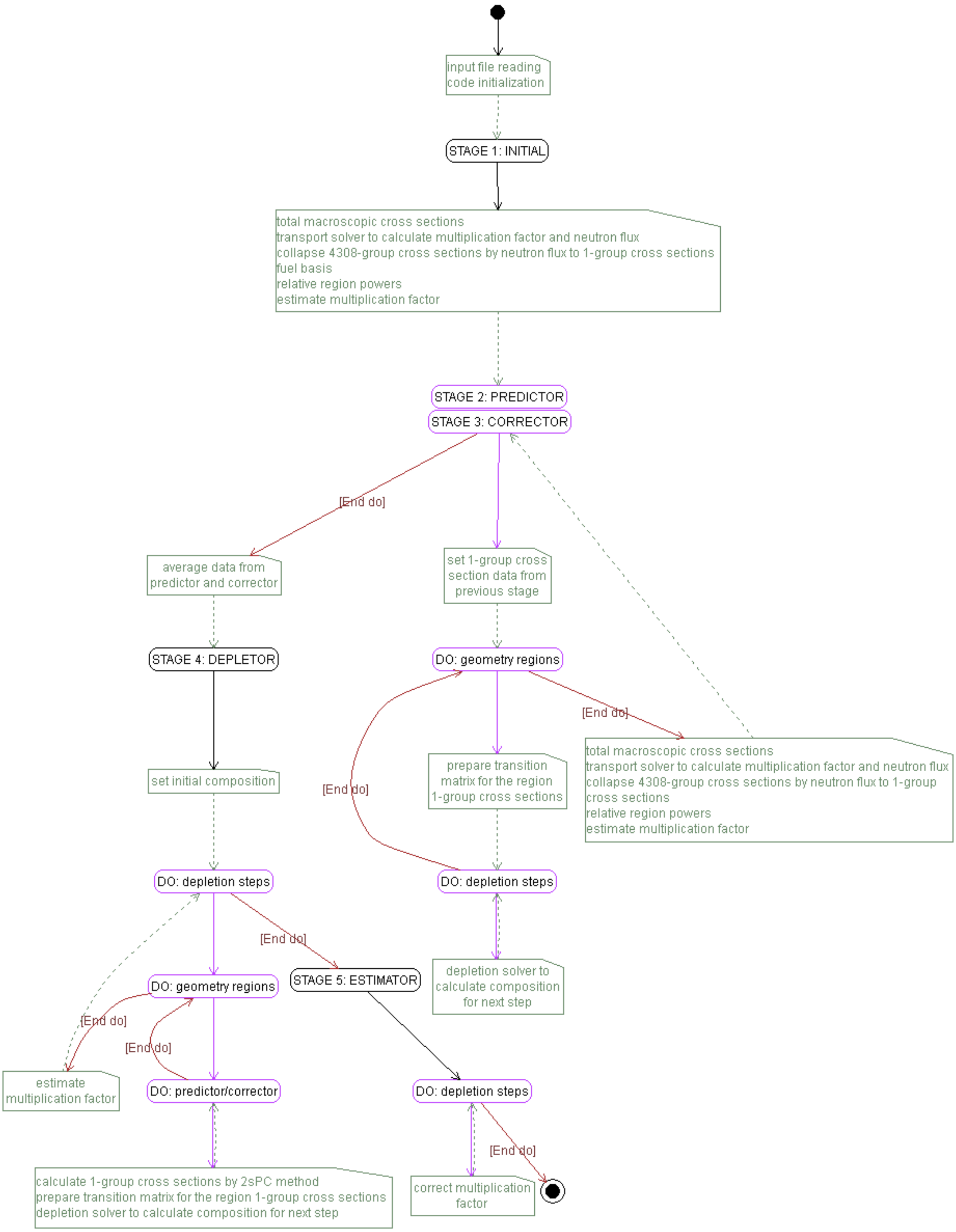

Figure 4.1: $U_W B_1$ flowchart.

Chapter 5

Input file

The chapter describes $U_W B_1$ input file and its options. Sample problems of CANDU, PWR, VVER and SFR fuel depletion are shown. $U_W B_1$ code reads only required numerical (integer or double real) or text data, both in free-format reading. The format allows different number formats and arbitrary separators between numbers. For example, number 1 is the same as 1.0 or 1.0E+00. First number in the line can be preceded by separators.

Comments at the end of lines are skipped during $U_W B_1$ execution. Comments are divided from data by at least one space, no other separators are necessary. Comments in sample cases contain basic information about the input, namely variable name and its short description.

5.1 Input file structure

Input file is divided into lines according to Table 5.1, no blank lines are allowed. The table summarizes $U_W B_1$ variables as they appear in input file. Integer numbers and arrays, double precision real numbers and arrays and characters of 200 length are used. Input file is read by Fortran's free format. Detailed description of input lines is summarized in Table 5.2.

Input file is divided into three basic blocks that describes fuel depletion. In the first block, all input data excluding material composition are defined. The second block is used to list used data libraries, only few user inputs are required. The last block contain material composition at the beginning of fuel depletion for all geometry regions. The first line contain case label and it is copied to output file. The second line describes number of CPU threads used for Monte Carlo solver (`prl_threads`).

Transport solver requires Monte Carlo parameter, geometry and material input in order to calculate neutron fluxes in geometry regions.

Monte Carlo parameters are used to describe the number of neutrons that will be used in the MC simulation. These parameters include number of neutrons per generation (`npg`), number of skipped neutron generations (`nsng`) that will not be used for tallying (inactive generations) and total number of neutron generations (`tnng`) that are divided into inactive and active generations. Because two dimensional fuel cell geometry is used, relatively small number of neutrons are needed. Values used in the sample case are more than enough for fuel cell model, at least 1 inactive and 50 active generations should be used. A few thousand neutrons per generation are a minimum.

Geometry is described in four lines. For geometry dimensions (cm), radii of concentric cylinders (`rccregion`) and half pitch (`hpitch`) is required. Number of concentric cylinders (`n_ccregion`) defines total number of geometry regions (`n_ccregion`+1), the last geometry region is the region between the cylinder with largest radius and the lattice boundaries planes. The code assumes infinite lattice with periodic boundaries, either square (`lat`=1) or triangular lattice (`lat`=2) is available. The simplest available geometry is two regions, at least one cylinder region is required. For light water and fast reactors, three basic regions are required (fuel, cladding, moderator/coolant), for heavy water reactors, more regions that describe homogenized fuel bundle are required.

Material composition, used by both transport and burnup solvers, is read from line 36 to the end of input file. Material composition is required for each geometry region, even if the material is used in multiple regions. For each region, number of nuclides and their nuclear densities (atoms per barn-cm) needs to be assigned. Material input is divided into two parts, the first part contain number of nuclides in each region in separate lines, the second part contain nuclide description and nuclear density for all regions (each nuclide on a separate line). Nuclide description comprises of three ID numbers – position in transport library, position in burnup library and ZAID. These three identifiers are unique for each nuclide and their list is part of (`uwb1zaid0423to3820.txt`) library. For help with calculation nuclide densities, see the last section of the chapter.

Burnup solver requires depletion history and list of depleted regions in order to calculate fuel composition in depleted regions for each depletion steps. For each depletion interval/step (`idepl`), irradiation power (`depl_power(idepl)`) in MW and duration (`depl_time(idepl)`) in days are required. Integral of power and duration gives burnup (MWd/MTU) achieved by the fuel. Initial mass of heavy metals (MTU = metric tonnes of uranium, or more precisely MTHM = metric tonne of heavy metals) in each geometry region is calculated by the code. Irradiation power can be calculated by the total power of the reactor and initial heavy metal mass, for VVER-1000 sample case, reactor power 3000 MW is achieved by 163 fuel assemblies, each containing 0.467 MTU, therefore, irradiation power is slightly below 40 MW/MTU. Be sure to exclude oxygen mass in UO_2 when calculating the power. For each region, depletion is performed by power depletion option (`depl_type`=1), flux depletion option (`depl_type`=2), or the region is not depleted (`depl_type`=0). Fissile regions should be depleted by power depletion, important non-fissile regions (cladding with burnable absorber, highly absorbating regions) should be depleted by flux depletion option, however, power depletion is allowed. Structure materials and coolant region should not be depleted. Irradiation power is total power of all regions, relative powers are calculated by the code.

If the number of depletion time steps `idepl` is set to zero, only transport calculation of the input composition (step 0) is performed, i.e. criticality calculation instead of depletion calculation is performed.

Data libraries are part of lines 14-35 of the input file and describe nuclear data used in the calculation. Majority of them are case-independent. User should change input lines 14-16 and can change input lines 29-30 and 34-35. The path to data libraries (`folderpath`), enclosed by quotes, is used to read all listed libraries. Because cross sections depends on the temperature, different libraries should be used. The user has the option to use two transport libraries and two burnup libraries and choose which geometry region will use the first (`reg_libtype`=1) or the second library (`reg_libtype`=2). Only two libraries are used in order to decrease RAM demands. Currently, four different temperature-dependent data libraries are available (293 K, 600 K, 900 K, 1200 K). Thermal reactor fuels usually operates with 900 K library, fast reactor fuels with 1200 K. Moderator/coolant regions should use 293 K (heavy water reactors) or 600 K (light water reactors) libraries. Temperature effects include Doppler broadening and thermal motion of nuclei. The first effect is taken into account in data libraries, the second is handled by the code – the user should input temperatures (K) for all geometry regions (`maxwell_kelvin`) in line 15.

Table 5.1: $U_W B_1$ input variables.

Line	Variable	Type	User's concern
1	caselabel	character*200	arbitrary
2	prl_threads	integer*4	MC
3	npg	integer*4	MC
4	nsng	integer*4	MC
5	tnng	integer*4	MC
6	n_ccregion	integer*4	geometry
7	rccregion(n_ccregion)	real*8	geometry
8	hpitch	real*8	geometry
9	lat	integer*4	geometry
10	idepl	integer*4	depletion
11	depl_power(idepl)	real*8	depletion
12	depl_time(idepl)	real*8	depletion
13	depl_type(n_ccregion+1)	integer*4	depletion
14	reg_libtype(n_ccregion+1)	integer*4	library
15	maxwell_kelvin(n_ccregion+1)	real*8	library
16	folderpath	character*200	library
17	libpath(1)	character*200	none
18	libpath(2)	character*200	none
19	libpath(3)	character*200	none
20	libpath(4)	character*200	none
21	libpath(5)	character*200	none
22	libpath(6)	character*200	none
23	libpath(7)	character*200	none
24	libpath(8)	character*200	none
25	libpath(9)	character*200	none
26	libpath(10)	character*200	none
27	libpath(11)	character*200	none
28	libpath(12)	character*200	none
29	libpath(13)	character*200	library
30	libpath(14)	character*200	library
31	libpath(15)	character*200	none
32	libpath(16)	character*200	none
33	libpath(17)	character*200	none
34	libpath(18)	character*200	library
35	libpath(19)	character*200	library
36	libpath(20)	character*200	none
37+	n_nucl(n_ccregion+1)	integer*4	material
37++	pos0423_nucl(sum(n_nucl)), pos3820_nucl(sum(n_nucl)), zaid_nucl(sum(n_nucl)), ndens_nucl(sum(n_nucl))	integer*4, integer*4, integer*4, real*8	material

Table 5.2: $U_W B_1$ input description.

Line	Description	User's concern
1	case label	arbitrary
2	number of CPU threads	MC
3	number of neutrons per generation	MC
4	number of skipped neutron generations	MC
5	total number of neutron generations	MC
6	number of concentric cylinder regions	geometry
7	concentric cylinder region radii (cm)	geometry
8	half pitch (cm)	geometry
9	lattice type (1=square, 2=hexagonal)	geometry
10	number of depletion intervals	depletion
11	irradiation power (MW/MTU)	depletion
12	irradiation days (d)	depletion
13	regions depletion (0=no depletion, 1=power depletion, 2=flux depletion)	depletion
14	regions transport/burnup libraries position (1 or 2)	library
15	regions maxwell temperatures	library
16	folder with uwb1 libraries	library
17	position of transport nuclides in depletion nuclides	none
18	nuclide mass relative to neutron	none
19	qvalues for inelastic reactions	none
20	xs_n2n chi data library	none
21	xs_n3n chi data library	none
22	xs_fission chi data library	none
23	xs_inelastic_continuum chi data library	none
24	nubar data library	none
25	xs_elastic angular distribution data library	none
26	xs_inelastic_discrete angular distribution data library	none
27	xs_inelastic_continuum angular distribution data library	none
28	energy grid for xs data	none
29	xs data library no1	library
30	xs data library no2	library
31	transition matrix Aii, universal flux-independent part	none
32	transition data Fij, part of Aij, case-flux-dependent part	none
33	transition matrix Aij, universal flux-independent part	none
34	cross section library for depletion reactions no1	library
35	cross section library for depletion reactions no2	library
36	recoverable energy library for depletion reactions	none
37+	number of nuclides in regions	material
37++	nuclear densities in regions (at/bcm)	material

5.2 Sample input file 01 – VVER

Following sample input file describes VVER-1000 fuel criticality. Only criticality is performed, no depletion is assumed (`idepl`=0). If no depletion is required, power and time can be omitted (`depl_power(idepl)`, `depl_time(idepl)`), however, `depl_type` needs to be defined, although it is not used in the calculation. Fuel cell is modeled as two regions, the simplest geometry possible. Only selected nuclides are defined in the composition.

```
uwb1 vver50 criticality test
4                                    prl_threads - number of threads
10000                                npg - number of neutrons per generation
5                                    nsng - number of skipped neutron generations
105                                  tnng - total number of neutron generations
1                                    n_ccregion - number of concentric cylinder regions
0.38                                 rccregion - concentric cylinder region radii
0.6375                               hpitch - half pitch
2                                    lat - lattice type (1=square, 2=hexagonal)
0                                    idepl - number of depletion intervals
                                     depl_power - irradiation power
                                     depl_time - irradiation days
1 0                                  depl_type - regions depletion (0=no depletion, 1=power depletion, 2=flux depletion)
1 2                                  reg_libtype - regions transport/burnup libraries position
900.0 578.0                          maxwell_kelvin - regions maxwell temperatures
"/media/sf_xwork/uwb1libs/"          folder with uwb1 libraries
uwb1zaid0423to3820.txt               position of transport nuclides in depletion nuclides
uwb1nmass.txt                        nuclide mass relative to neutron
uwb1qvalues4mc.txt                   qvalues for inelastic reactions
uwb1chi16.txt                        xs_n2n chi data library
uwb1chi17.txt                        xs_n3n chi data library
uwb1chi18.txt                        xs_fission chi data library
uwb1chi91.txt                        xs_inelastic_continuum chi data library
uwb1nubar.txt                        nubar data library
uwb1angular02.txt                    xs_elastic angular distribution data library
uwb1angular51t90.txt                 xs_inelastic_discrete angular distribution data library
uwb1angular91.txt                    xs_inelastic_continuum angular distribution data library
uwb1egrid.txt                        energy grid for xs data
uwb1xscom0900k.txt                   xs data library no1
uwb1xscom0600k.txt                   xs data library no2
uwb1aiiuni.txt                       transition matrix Aii, universal flux-independent part
uwb1fijphi.txt                       transition data   Fij, part of Aij, case-flux-dependent part
uwb1aijuni.txt                       transition matrix Aij, universal flux-independent part
uwb1deplxscom0900k.txt               cross section library for depletion reactions no1
uwb1deplxscom0600k.txt               cross section library for depletion reactions no2
uwb1qvalues4depl.txt                 recoverable energy library for depletion reactions
2                                    number of nuclides in region  1 (fuel)
2                                    number of nuclides in region  2 (mod)
  362   3514   922350  1.16848E-03  nuclear densities in region   1 (fuel)
  365   3518   922380  2.19207E-02
    1      1    10010  5.01551E-02  nuclear densities in region   2 (mod)
   15     86    80160  2.50775E-02
eof
```

5.3 Sample input file 02 – VVER

Following sample input file describes VVER-1000 fuel criticality, the sample input is a generalization of the previous one. Fuel cell is modeled as fuel, cladding and moderator regions, the composition lists all nuclides for VVER-1000 nuclear fuel.

```
uwb1 vver50 criticality test
4                                   prl_threads - number of threads
10000                               npg - number of neutrons per generation
5                                   nsng - number of skipped neutron generations
105                                 tnng - total number of neutron generations
2                                   n_ccregion - number of concentric cylinder regions
0.38 0.455                          rccregion - concentric cylinder region radii
0.6375                              hpitch - half pitch
2                                   lat - lattice type (1=square, 2=hexagonal)
0                                   idepl - number of depletion intervals
                                    depl_power - irradiation power
                                    depl_time - irradiation days
1 0 0                               depl_type - regions depletion (0=no depletion, 1=power depletion, 2=flux depletion)
1 2 2                               reg_libtype - regions transport/burnup libraries position
900.0 625.0 578.0                   maxwell_kelvin - regions maxwell temperatures
"/media/sf_xwork/uwb1libs/"         folder with uwb1 libraries
uwb1zaid0423to3820.txt              position of transport nuclides in depletion nuclides
uwb1nmass.txt                       nuclide mass relative to neutron
uwb1qvalues4mc.txt                  qvalues for inelastic reactions
uwb1chi16.txt                       xs_n2n chi data library
uwb1chi17.txt                       xs_n3n chi data library
uwb1chi18.txt                       xs_fission chi data library
uwb1chi91.txt                       xs_inelastic_continuum chi data library
uwb1nubar.txt                       nubar data library
uwb1angular02.txt                   xs_elastic angular distribution data library
uwb1angular51t90.txt                xs_inelastic_discrete angular distribution data library
uwb1angular91.txt                   xs_inelastic_continuum angular distribution data library
uwb1egrid.txt                       energy grid for xs data
uwb1xscom0900k.txt                  xs data library no1
uwb1xscom0600k.txt                  xs data library no2
uwb1aiiuni.txt                      transition matrix Aii, universal flux-independent part
uwb1fijphi.txt                      transition data   Fij, part of Aij, case-flux-dependent part
uwb1aijuni.txt                      transition matrix Aij, universal flux-independent part
uwb1deplxscom0900k.txt              cross section library for depletion reactions no1
uwb1deplxscom0600k.txt              cross section library for depletion reactions no2
uwb1qvalues4depl.txt                recoverable energy library for depletion reactions
4                                   number of nuclides in region  1 (fuel)
12                                  number of nuclides in region  2 (clad)
4                                   number of nuclides in region  3 (mod)
   15     86    80160  4.60685E-02  nuclear densities in region   1 (fuel)
   16     87    80170  1.75478E-05
  362   3514   922350  1.16848E-03
  365   3518   922380  2.19207E-02
  117   1039   400900  2.19170E-02  nuclear densities in region   2 (clad)
  118   1041   400910  4.77956E-03
  119   1042   400920  7.30565E-03
  121   1044   400940  7.40363E-03
  123   1046   400960  1.19276E-03
  124   1081   410930  4.22623E-04
```

```
  304   2594   721740  1.05594E-08
  305   2596   721760  3.47139E-07
  306   2597   721770  1.22753E-06
  307   2600   721780  1.80037E-06
  308   2603   721790  8.98867E-07
  309   2606   721800  2.31514E-06
    1      1    10010  5.01551E-02  nuclear densities in region   3 (mod)
   10     41    50100  4.98826E-06
   11     42    50110  2.00784E-05
   15     86    80160  2.50775E-02
eof
```

5.4 Sample input file 03 – VVER

Following sample input file describes VVER-1000 fuel depletion, only power and time is defined differently from the previous sample input. Fuel pin is modeled as a single region.

```
uwb1 vver50 depletion test
4                                    prl_threads - number of threads
10000                                npg - number of neutrons per generation
5                                    nsng - number of skipped neutron generations
105                                  tnng - total number of neutron generations
2                                    n_ccregion - number of concentric cylinder regions
0.38 0.455                           rccregion - concentric cylinder region radii
0.6375                               hpitch - half pitch
2                                    lat - lattice type (1=square, 2=hexagonal)
43                                   idepl - number of depletion intervals
4.00000E+01 4.00000E+01 4.00000E+01 4.00000E+01 4.00000E+01 4.00000E+01 4.00000E+01 4.00000E+01 4.00000E+01 4.00000E+01 4.00000E+01 4.00000E+01 4.00000E+01 4.00000E+01 4.00000E+01 4.00000E+01 4.00000E+01 4.00000E+01 4.00000E+01 4.00000E+01 4.00000E+01 4.00000E+01 4.00000E+01 4.00000E+01 4.00000E+01 4.00000E+01 4.00000E+01 4.00000E+01 4.00000E+01 4.00000E+01 4.00000E+01 4.00000E+01 4.00000E+01 4.00000E+01 4.00000E+01 4.00000E+01 4.00000E+01 4.00000E+01 4.00000E+01 4.00000E+01 4.00000E+01 4.00000E+01 4.00000E+01 depl_power - irradiation power
1.00000E+00 2.00000E+00 3.00000E+00 4.00000E+00 5.00000E+00 1.00000E+01 1.50000E+01 2.00000E+01 2.50000E+01 3.75000E+01 5.00000E+01 6.25000E+01 7.50000E+01 8.75000E+01 1.00000E+02 1.12500E+02 1.25000E+02 1.37500E+02 1.50000E+02 1.62500E+02 1.75000E+02 1.87500E+02 2.00000E+02 2.12500E+02 2.25000E+02 2.37500E+02 2.50000E+02 3.12500E+02 3.75000E+02 4.37500E+02 5.00000E+02 5.62500E+02 6.25000E+02 6.87500E+02 7.50000E+02 8.12500E+02 8.75000E+02 9.37500E+02 1.00000E+03 1.06250E+03 1.12500E+03 1.18750E+03 1.25000E+03 depl_time - irradiation days
1 0 0                                depl_type - regions depletion (0=no depletion, 1=power depletion, 2=flux depletion)
1 2 2                                reg_libtype - regions transport/burnup libraries position
900.0 625.0 578.0                    maxwell_kelvin - regions maxwell temperatures
"/media/sf_xwork/uwb1libs/"          folder with uwb1 libraries
uwb1zaid0423to3820.txt               position of transport nuclides in depletion nuclides
uwb1nmass.txt                        nuclide mass relative to neutron
uwb1qvalues4mc.txt                   qvalues for inelastic reactions
uwb1chi16.txt                        xs_n2n chi data library
uwb1chi17.txt                        xs_n3n chi data library
uwb1chi18.txt                        xs_fission chi data library
uwb1chi91.txt                        xs_inelastic_continuum chi data library
uwb1nubar.txt                        nubar data library
uwb1angular02.txt                    xs_elastic angular distribution data library
uwb1angular51t90.txt                 xs_inelastic_discrete angular distribution data library
uwb1angular91.txt                    xs_inelastic_continuum angular distribution data library
uwb1egrid.txt                        energy grid for xs data
uwb1xscom0900k.txt                   xs data library no1
uwb1xscom0600k.txt                   xs data library no2
uwb1aiiuni.txt                       transition matrix Aii, universal flux-independent part
uwb1fijphi.txt                       transition data   Fij, part of Aij, case-flux-dependent part
uwb1aijuni.txt                       transition matrix Aij, universal flux-independent part
uwb1deplxscom0900k.txt               cross section library for depletion reactions no1
uwb1deplxscom0600k.txt               cross section library for depletion reactions no2
uwb1qvalues4depl.txt                 recoverable energy library for depletion reactions
4                                    number of nuclides in region  1 (fuel)
12                                   number of nuclides in region  2 (clad)
```

```
4                                       number of nuclides in region  3 (mod)
    15      86     80160  4.60685E-02  nuclear densities in region   1 (fuel)
    16      87     80170  1.75478E-05
   362    3514    922350  1.16848E-03
   365    3518    922380  2.19207E-02
   117    1039    400900  2.19170E-02  nuclear densities in region   2 (clad)
   118    1041    400910  4.77956E-03
   119    1042    400920  7.30565E-03
   121    1044    400940  7.40363E-03
   123    1046    400960  1.19276E-03
   124    1081    410930  4.22623E-04
   304    2594    721740  1.05594E-08
   305    2596    721760  3.47139E-07
   306    2597    721770  1.22753E-06
   307    2600    721780  1.80037E-06
   308    2603    721790  8.98867E-07
   309    2606    721800  2.31514E-06
     1       1     10010  5.01551E-02  nuclear densities in region   3 (mod)
    10      41     50100  4.98826E-06
    11      42     50110  2.00784E-05
    15      86     80160  2.50775E-02
eof
```

5.5 Sample input file 04 – VVER

Following sample input file describes VVER-1000 fuel depletion. In contrast to the previous example, fuel pin is divided into 4 regions.

```
uwb1 vver50 depletion test
4                                    prl_threads - number of threads
10000                                npg - number of neutrons per generation
5                                    nsng - number of skipped neutron generations
105                                  tnng - total number of neutron generations
5                                    n_ccregion - number of concentric cylinder regions
0.1 0.2 0.3 0.38 0.455               rccregion - concentric cylinder region radii
0.6375                               hpitch - half pitch
2                                    lat - lattice type (1=square, 2=hexagonal)
43                                   idepl - number of depletion intervals
4.00000E+01 4.00000E+01 4.00000E+01 4.00000E+01 4.00000E+01 4.00000E+01 4.00000E+01 4.00000E+01 4.00000E+01 4.00000E+01 4.00000E+01 4.00000E+01 4.00000E+01 4.00000E+01 4.00000E+01 4.00000E+01 4.00000E+01 4.00000E+01 4.00000E+01 4.00000E+01 4.00000E+01 4.00000E+01 4.00000E+01 4.00000E+01 4.00000E+01 4.00000E+01 4.00000E+01 4.00000E+01 4.00000E+01 4.00000E+01 4.00000E+01 4.00000E+01 4.00000E+01 4.00000E+01 4.00000E+01 4.00000E+01 4.00000E+01 4.00000E+01 4.00000E+01 4.00000E+01 4.00000E+01 4.00000E+01 4.00000E+01 depl_power - irradiation power
1.00000E+00 2.00000E+00 3.00000E+00 4.00000E+00 5.00000E+00 1.00000E+01 1.50000E+01 2.00000E+01 2.50000E+01 3.75000E+01 5.00000E+01 6.25000E+01 7.50000E+01 8.75000E+01 1.00000E+02 1.12500E+02 1.25000E+02 1.37500E+02 1.50000E+02 1.62500E+02 1.75000E+02 1.87500E+02 2.00000E+02 2.12500E+02 2.25000E+02 2.37500E+02 2.50000E+02 3.12500E+02 3.75000E+02 4.37500E+02 5.00000E+02 5.62500E+02 6.25000E+02 6.87500E+02 7.50000E+02 8.12500E+02 8.75000E+02 9.37500E+02 1.00000E+03 1.06250E+03 1.12500E+03 1.18750E+03 1.25000E+03 depl_time - irradiation days
1 1 1 1 0 0                          depl_type - regions depletion (0=no depletion, 1=power depletion, 2=flux depletion)
1 1 1 1 2 2                          reg_libtype - regions transport/burnup libraries position
900.0 900.0 900.0 900.0 625.0 578.0 maxwell_kelvin - regions maxwell temperatures
"/media/sf_xwork/uwb1libs/"          folder with uwb1 libraries
uwb1zaid0423to3820.txt               position of transport nuclides in depletion nuclides
uwb1nmass.txt                        nuclide mass relative to neutron
uwb1qvalues4mc.txt                   qvalues for inelastic reactions
uwb1chi16.txt                        xs_n2n chi data library
uwb1chi17.txt                        xs_n3n chi data library
uwb1chi18.txt                        xs_fission chi data library
uwb1chi91.txt                        xs_inelastic_continuum chi data library
uwb1nubar.txt                        nubar data library
uwb1angular02.txt                    xs_elastic angular distribution data library
uwb1angular51t90.txt                 xs_inelastic_discrete angular distribution data library
uwb1angular91.txt                    xs_inelastic_continuum angular distribution data library
uwb1egrid.txt                        energy grid for xs data
uwb1xscom0900k.txt                   xs data library no1
uwb1xscom0600k.txt                   xs data library no2
uwb1aiiuni.txt                       transition matrix Aii, universal flux-independent part
uwb1fijphi.txt                       transition data   Fij, part of Aij, case-flux-dependent part
uwb1aijuni.txt                       transition matrix Aij, universal flux-independent part
uwb1deplxscom0900k.txt               cross section library for depletion reactions no1
uwb1deplxscom0600k.txt               cross section library for depletion reactions no2
uwb1qvalues4depl.txt                 recoverable energy library for depletion reactions
4                                    number of nuclides in region  1 (fuel)
4                                    number of nuclides in region  2 (fuel)
```

```
4                                   number of nuclides in region  3 (fuel)
4                                   number of nuclides in region  4 (fuel)
12                                  number of nuclides in region  5 (clad)
4                                   number of nuclides in region  6 (mod)
   15     86    80160  4.60685E-02  nuclear densities in region   1 (fuel)
   16     87    80170  1.75478E-05
  362   3514   922350  1.16848E-03
  365   3518   922380  2.19207E-02
   15     86    80160  4.60685E-02  nuclear densities in region   2 (fuel)
   16     87    80170  1.75478E-05
  362   3514   922350  1.16848E-03
  365   3518   922380  2.19207E-02
   15     86    80160  4.60685E-02  nuclear densities in region   3 (fuel)
   16     87    80170  1.75478E-05
  362   3514   922350  1.16848E-03
  365   3518   922380  2.19207E-02
   15     86    80160  4.60685E-02  nuclear densities in region   4 (fuel)
   16     87    80170  1.75478E-05
  362   3514   922350  1.16848E-03
  365   3518   922380  2.19207E-02
  117   1039   400900  2.19170E-02  nuclear densities in region   5 (clad)
  118   1041   400910  4.77956E-03
  119   1042   400920  7.30565E-03
  121   1044   400940  7.40363E-03
  123   1046   400960  1.19276E-03
  124   1081   410930  4.22623E-04
  304   2594   721740  1.05594E-08
  305   2596   721760  3.47139E-07
  306   2597   721770  1.22753E-06
  307   2600   721780  1.80037E-06
  308   2603   721790  8.98867E-07
  309   2606   721800  2.31514E-06
    1      1    10010  5.01551E-02  nuclear densities in region   6 (mod)
   10     41    50100  4.98826E-06
   11     42    50110  2.00784E-05
   15     86    80160  2.50775E-02
eof
```

5.6 Sample input file 05 – CANDU

Following sample input file describes homogenized CANDU 37-element fuel bundle depletion. No burnable absorbers are assumed.

```
uwb1 candu depletion
4                                    prl_threads - number of threads
10000                                npg - number of neutrons per generation
5                                    nsng - number of skipped neutron generations
205                                  tnng - total number of neutron generations
18                                   n_ccregion - number of concentric cylinder regions
0.609000 0.650460 1.062133 1.114754 1.862246 1.914867 2.434083 2.488561 3.262439 3.316917 3.890841 3.945102 4.715898 4.770159 5.15 5.59308 6.4478 6.5875  rccregion - concentric cylinder region radii
14.2875                              hpitch - half pitch
1                                    lat - lattice type (1=square, 2=hexagonal)
42                                   idepl - number of depletion intervals
3.29080E+01 3.29080E+01 3.29080E+01 3.29080E+01 3.29080E+01 3.29080E+01 3.29080E+01 3.29080E+01 3.29080E+01 3.29080E+01 3.29080E+01 3.29080E+01 3.29080E+01 3.29080E+01 3.29080E+01 3.29080E+01 3.29080E+01 3.29080E+01 3.29080E+01 3.29080E+01 3.29080E+01 3.29080E+01 3.29080E+01 3.29080E+01 3.29080E+01 3.29080E+01 3.29080E+01 3.29080E+01 3.29080E+01 3.29080E+01 3.29080E+01 3.29080E+01 3.29080E+01 3.29080E+01 3.29080E+01 3.29080E+01 3.29080E+01 3.29080E+01 3.29080E+01 3.29080E+01 3.29080E+01 3.29080E+01  depl_power - irradiation power
2.00000E-01 4.50000E-01 8.50000E-01 1.45000E+00 2.45000E+00 4.45000E+00 8.45000E+00 1.44500E+01 2.24500E+01 3.04500E+01 3.94500E+01 5.14500E+01 6.74500E+01 8.74500E+01 1.07450E+02 1.27450E+02 1.47450E+02 1.67450E+02 1.87450E+02 2.07450E+02 2.27450E+02 2.47450E+02 2.67450E+02 2.87450E+02 3.07450E+02 3.27450E+02 3.47450E+02 3.67450E+02 3.87450E+02 4.07450E+02 4.27450E+02 4.47450E+02 4.67450E+02 4.87450E+02 5.07450E+02 5.27450E+02 5.47450E+02 5.67450E+02 5.87450E+02 6.07450E+02 6.27450E+02 6.47450E+02  depl_time - irradiation days
1 0 0 0 1 0 0 0 1 0 0 0 1 0 0 0 0 0 0  depl_type - regions depletion (0=no depletion, 1=power depletion, 2=flux depletion)
1 2 2 2 1 2 2 2 1 2 2 2 1 2 2 2 2 2 2  reg_libtype - regions transport/burnup libraries position
1011.0 561.66 561.66 561.66 1011.0 561.66 561.66 561.66 1011.0 561.66 561.66 561.66 1011.0 561.66 561.66 561.66 450.41 339.16 339.16  maxwell_kelvin - regions maxwell temperatures
"/media/sf_xwork/uwb1libs/"          folder with uwb1 libraries
uwb1zaid0423to3820.txt               position of transport nuclides in depletion nuclides
uwb1nmass.txt                        nuclide mass relative to neutron
uwb1qvalues4mc.txt                   qvalues for inelastic reactions
uwb1chi16.txt                        xs_n2n chi data library
uwb1chi17.txt                        xs_n3n chi data library
uwb1chi18.txt                        xs_fission chi data library
uwb1chi91.txt                        xs_inelastic_continuum chi data library
uwb1nubar.txt                        nubar data library
uwb1angular02.txt                    xs_elastic angular distribution data library
uwb1angular51t90.txt                 xs_inelastic_discrete angular distribution data library
uwb1angular91.txt                    xs_inelastic_continuum angular distribution data library
uwb1egrid.txt                        energy grid for xs data
uwb1xscom0900k.txt                   xs data library no1
uwb1xscom0293k.txt                   xs data library no2
uwb1aiiuni.txt                       transition matrix Aii, universal flux-independent part
uwb1fijphi.txt                       transition data   Fij, part of Aij, case-flux-dependent part
uwb1aijuni.txt                       transition matrix Aij, universal flux-independent part
uwb1deplxscom0900k.txt               cross section library for depletion reactions no1
uwb1deplxscom0293k.txt               cross section library for depletion reactions no2
```

```
uwb1qvalues4depl.txt                 recoverable energy library for depletion reactions
4                                    number of nuclides in region  1 (fuel)
17                                   number of nuclides in region  2 (sheath)
4                                    number of nuclides in region  3 (coolant)
17                                   number of nuclides in region  4 (sheath)
4                                    number of nuclides in region  5 (fuel)
17                                   number of nuclides in region  6 (sheath)
4                                    number of nuclides in region  7 (coolant)
17                                   number of nuclides in region  8 (sheath)
4                                    number of nuclides in region  9 (fuel)
17                                   number of nuclides in region 10 (sheath)
4                                    number of nuclides in region 11 (coolant)
17                                   number of nuclides in region 12 (sheath)
4                                    number of nuclides in region 13 (fuel)
17                                   number of nuclides in region 14 (sheath)
4                                    number of nuclides in region 15 (coolant)
18                                   number of nuclides in region 16 (pressure tube)
2                                    number of nuclides in region 17 (gap)
17                                   number of nuclides in region 18 (calandria tube)
4                                    number of nuclides in region 19 (moderator)
   15     86    80160  4.68703E-02  fuel
  361   3513   922340  1.28868E-06
  362   3514   922350  1.68695E-04
  365   3518   922380  2.32599E-02
   10     41    50100  2.32687E-07  sheath for no BA case
   54    463   240500  3.26559E-06
   55    465   240520  6.29740E-05
   56    466   240530  7.13996E-06
   57    467   240540  1.77750E-06
   59    523   260540  8.67033E-06
   60    525   260560  1.34788E-04
   61    526   260570  3.08615E-06
   62    527   260580  4.11481E-07
   66    587   280580  3.34828E-06
   68    589   280600  1.28006E-06
   71    593   280640  4.46306E-08
  117   1039   400900  2.16399E-02
  118   1041   400910  4.71910E-03
  119   1042   400920  7.21317E-03
  121   1044   400940  7.30989E-03
  123   1046   400960  1.17763E-03
    1      1    10010  4.38240E-04  coolant
    2      2    10020  4.88020E-02
   15     86    80160  2.46110E-02
   16     87    80170  9.35570E-06
   10     41    50100  2.32687E-07  sheath for no BA case
   54    463   240500  3.26559E-06
   55    465   240520  6.29740E-05
   56    466   240530  7.13996E-06
   57    467   240540  1.77750E-06
   59    523   260540  8.67033E-06
   60    525   260560  1.34788E-04
   61    526   260570  3.08615E-06
   62    527   260580  4.11481E-07
   66    587   280580  3.34828E-06
   68    589   280600  1.28006E-06
   71    593   280640  4.46306E-08
  117   1039   400900  2.16399E-02
```

94	118	1041	400910	4.71910E-03	
95	119	1042	400920	7.21317E-03	
96	121	1044	400940	7.30989E-03	
97	123	1046	400960	1.17763E-03	
98	15	86	80160	4.68703E-02	fuel
99	361	3513	922340	1.28868E-06	
100	362	3514	922350	1.68695E-04	
101	365	3518	922380	2.32599E-02	
102	10	41	50100	2.32687E-07	sheath for no BA case
103	54	463	240500	3.26559E-06	
104	55	465	240520	6.29740E-05	
105	56	466	240530	7.13996E-06	
106	57	467	240540	1.77750E-06	
107	59	523	260540	8.67033E-06	
108	60	525	260560	1.34788E-04	
109	61	526	260570	3.08615E-06	
110	62	527	260580	4.11481E-07	
111	66	587	280580	3.34828E-06	
112	68	589	280600	1.28006E-06	
113	71	593	280640	4.46306E-08	
114	117	1039	400900	2.16399E-02	
115	118	1041	400910	4.71910E-03	
116	119	1042	400920	7.21317E-03	
117	121	1044	400940	7.30989E-03	
118	123	1046	400960	1.17763E-03	
119	1	1	10010	4.38240E-04	coolant
120	2	2	10020	4.88020E-02	
121	15	86	80160	2.46110E-02	
122	16	87	80170	9.35570E-06	
123	10	41	50100	2.32687E-07	sheath for no BA case
124	54	463	240500	3.26559E-06	
125	55	465	240520	6.29740E-05	
126	56	466	240530	7.13996E-06	
127	57	467	240540	1.77750E-06	
128	59	523	260540	8.67033E-06	
129	60	525	260560	1.34788E-04	
130	61	526	260570	3.08615E-06	
131	62	527	260580	4.11481E-07	
132	66	587	280580	3.34828E-06	
133	68	589	280600	1.28006E-06	
134	71	593	280640	4.46306E-08	
135	117	1039	400900	2.16399E-02	
136	118	1041	400910	4.71910E-03	
137	119	1042	400920	7.21317E-03	
138	121	1044	400940	7.30989E-03	
139	123	1046	400960	1.17763E-03	
140	15	86	80160	4.68703E-02	fuel
141	361	3513	922340	1.28868E-06	
142	362	3514	922350	1.68695E-04	
143	365	3518	922380	2.32599E-02	
144	10	41	50100	2.32687E-07	sheath for no BA case
145	54	463	240500	3.26559E-06	
146	55	465	240520	6.29740E-05	
147	56	466	240530	7.13996E-06	
148	57	467	240540	1.77750E-06	
149	59	523	260540	8.67033E-06	
150	60	525	260560	1.34788E-04	
151	61	526	260570	3.08615E-06	

```
  62   527  260580  4.11481E-07
  66   587  280580  3.34828E-06
  68   589  280600  1.28006E-06
  71   593  280640  4.46306E-08
 117  1039  400900  2.16399E-02
 118  1041  400910  4.71910E-03
 119  1042  400920  7.21317E-03
 121  1044  400940  7.30989E-03
 123  1046  400960  1.17763E-03
   1     1   10010  4.38240E-04  coolant
   2     2   10020  4.88020E-02
  15    86   80160  2.46110E-02
  16    87   80170  9.35570E-06
  10    41   50100  2.32687E-07  sheath for no BA case
  54   463  240500  3.26559E-06
  55   465  240520  6.29740E-05
  56   466  240530  7.13996E-06
  57   467  240540  1.77750E-06
  59   523  260540  8.67033E-06
  60   525  260560  1.34788E-04
  61   526  260570  3.08615E-06
  62   527  260580  4.11481E-07
  66   587  280580  3.34828E-06
  68   589  280600  1.28006E-06
  71   593  280640  4.46306E-08
 117  1039  400900  2.16399E-02
 118  1041  400910  4.71910E-03
 119  1042  400920  7.21317E-03
 121  1044  400940  7.30989E-03
 123  1046  400960  1.17763E-03
  15    86   80160  4.68703E-02  fuel
 361  3513  922340  1.28868E-06
 362  3514  922350  1.68695E-04
 365  3518  922380  2.32599E-02
  10    41   50100  2.32687E-07  sheath for no BA case
  54   463  240500  3.26559E-06
  55   465  240520  6.29740E-05
  56   466  240530  7.13996E-06
  57   467  240540  1.77750E-06
  59   523  260540  8.67033E-06
  60   525  260560  1.34788E-04
  61   526  260570  3.08615E-06
  62   527  260580  4.11481E-07
  66   587  280580  3.34828E-06
  68   589  280600  1.28006E-06
  71   593  280640  4.46306E-08
 117  1039  400900  2.16399E-02
 118  1041  400910  4.71910E-03
 119  1042  400920  7.21317E-03
 121  1044  400940  7.30989E-03
 123  1046  400960  1.17763E-03
   1     1   10010  4.38240E-04  coolant
   2     2   10020  4.88020E-02
  15    86   80160  2.46110E-02
  16    87   80170  9.35570E-06
  10    41   50100  9.51420E-08  pressure_tube
  54   463  240500  2.64856E-07
  55   465  240520  5.10750E-06
```

```
    56    466   240530  5.79086E-07
    57    467   240540  1.44164E-07
    59    523   260540  1.93680E-06
    60    525   260560  3.01092E-05
    61    526   260570  6.89386E-07
    62    527   260580  9.19170E-08
    66    587   280580  1.67880E-06
    68    589   280600  6.41810E-07
    71    593   280640  2.23774E-08
   117   1039   400900  2.15082E-02
   118   1041   400910  4.69038E-03
   119   1042   400920  7.16921E-03
   121   1044   400940  7.26535E-03
   123   1046   400960  1.17046E-03
   124   1081   410930  1.08824E-03
    12     55    60120  1.62580E-05  gap
    15     86    80160  3.27948E-05
    10     41    50100  2.32997E-07  calandria_tube
    54    463   240500  3.26994E-06
    55    465   240520  6.30577E-05
    56    466   240530  7.14946E-06
    57    467   240540  1.77986E-06
    59    523   260540  5.58121E-06
    60    525   260560  8.67645E-05
    61    526   260570  1.98659E-06
    62    527   260580  2.64875E-07
    66    587   280580  2.63430E-05
    68    589   280600  1.00710E-05
    71    593   280640  3.51136E-07
   117   1039   400900  2.16747E-02
   118   1041   400910  4.72669E-03
   119   1042   400920  7.22473E-03
   121   1044   400940  7.32163E-03
   123   1046   400960  1.17952E-03
     1      1    10010  1.96150E-05  moderator
     2      2    10020  6.53650E-02
    15     86    80160  3.26800E-02
    16     87    80170  1.24230E-05
eof
```

5.7 Sample input file 06 – CANDU

Following sample input file describes homogenized CANDU 37-element fuel bundle depletion. Burnable absorber (150 mg Gd_2O_3 + 300 mg Eu_2O_3) is added into sheath regions.

```
uwb1 candu depletion
4                                   prl_threads - number of threads
10000                               npg - number of neutrons per generation
5                                   nsng - number of skipped neutron generations
205                                 tnng - total number of neutron generations
18                                  n_ccregion - number of concentric cylinder regions
0.609000 0.650460 1.062133 1.114754 1.862246 1.914867 2.434083 2.488561 3.262439 3.316917
    3.890841 3.945102 4.715898 4.770159 5.15 5.59308 6.4478 6.5875  rccregion - concentric
    cylinder region radii
14.2875                             hpitch - half pitch
1                                   lat - lattice type (1=square, 2=hexagonal)
42                                  idepl - number of depletion intervals
3.29080E+01 3.29080E+01 3.29080E+01 3.29080E+01 3.29080E+01 3.29080E+01 3.29080E+01 3.29080E
    +01 3.29080E+01 3.29080E+01 3.29080E+01 3.29080E+01 3.29080E+01 3.29080E+01 3.29080E+01
    3.29080E+01 3.29080E+01 3.29080E+01 3.29080E+01 3.29080E+01 3.29080E+01 3.29080E+01
    3.29080E+01 3.29080E+01 3.29080E+01 3.29080E+01 3.29080E+01 3.29080E+01 3.29080E+01
    3.29080E+01 3.29080E+01 3.29080E+01 3.29080E+01 3.29080E+01 3.29080E+01 3.29080E+01
    3.29080E+01 3.29080E+01 3.29080E+01 3.29080E+01 3.29080E+01 3.29080E+01  depl_power -
    irradiation power
2.00000E-01 4.50000E-01 8.50000E-01 1.45000E+00 2.45000E+00 4.45000E+00 8.45000E+00 1.44500E
    +01 2.24500E+01 3.04500E+01 3.94500E+01 5.14500E+01 6.74500E+01 8.74500E+01 1.07450E+02
    1.27450E+02 1.47450E+02 1.67450E+02 1.87450E+02 2.07450E+02 2.27450E+02 2.47450E+02
    2.67450E+02 2.87450E+02 3.07450E+02 3.27450E+02 3.47450E+02 3.67450E+02 3.87450E+02
    4.07450E+02 4.27450E+02 4.47450E+02 4.67450E+02 4.87450E+02 5.07450E+02 5.27450E+02
    5.47450E+02 5.67450E+02 5.87450E+02 6.07450E+02 6.27450E+02 6.47450E+02  depl_time -
    irradiation days
1 2 0 2 1 2 0 2 1 2 0 2 1 2 0 0 0 0 0  depl_type - regions depletion (0=no depletion, 1=
    power depletion, 2=flux depletion)
1 2 2 2 1 2 2 2 1 2 2 2 1 2 2 2 2 2 2  reg_libtype - regions transport/burnup libraries
    position
1011.0 561.66 561.66 561.66 1011.0 561.66 561.66 561.66 1011.0 561.66 561.66 561.66 1011.0
    561.66 561.66 561.66 450.41 339.16 339.16  maxwell_kelvin - regions maxwell temperatures
"/media/sf_xwork/uwb1libs/"         folder with uwb1 libraries
uwb1zaid0423to3820.txt              position of transport nuclides in depletion nuclides
uwb1nmass.txt                       nuclide mass relative to neutron
uwb1qvalues4mc.txt                  qvalues for inelastic reactions
uwb1chi16.txt                       xs_n2n chi data library
uwb1chi17.txt                       xs_n3n chi data library
uwb1chi18.txt                       xs_fission chi data library
uwb1chi91.txt                       xs_inelastic_continuum chi data library
uwb1nubar.txt                       nubar data library
uwb1angular02.txt                   xs_elastic angular distribution data library
uwb1angular51t90.txt                xs_inelastic_discrete angular distribution data library
uwb1angular91.txt                   xs_inelastic_continuum angular distribution data library
uwb1egrid.txt                       energy grid for xs data
uwb1xscom0900k.txt                  xs data library no1
uwb1xscom0293k.txt                  xs data library no2
uwb1aiiuni.txt                      transition matrix Aii, universal flux-independent part
uwb1fijphi.txt                      transition data   Fij, part of Aij, case-flux-dependent
    part
uwb1aijuni.txt                      transition matrix Aij, universal flux-independent part
uwb1deplxscom0900k.txt              cross section library for depletion reactions no1
uwb1deplxscom0293k.txt              cross section library for depletion reactions no2
```

```
uwb1qvalues4depl.txt                 recoverable energy library for depletion reactions
4                                    number of nuclides in region  1 (fuel)
27                                   number of nuclides in region  2 (sheath)
4                                    number of nuclides in region  3 (coolant)
27                                   number of nuclides in region  4 (sheath)
4                                    number of nuclides in region  5 (fuel)
27                                   number of nuclides in region  6 (sheath)
4                                    number of nuclides in region  7 (coolant)
27                                   number of nuclides in region  8 (sheath)
4                                    number of nuclides in region  9 (fuel)
27                                   number of nuclides in region 10 (sheath)
4                                    number of nuclides in region 11 (coolant)
27                                   number of nuclides in region 12 (sheath)
4                                    number of nuclides in region 13 (fuel)
27                                   number of nuclides in region 14 (sheath)
4                                    number of nuclides in region 15 (coolant)
18                                   number of nuclides in region 16 (pressure tube)
2                                    number of nuclides in region 17 (gap)
17                                   number of nuclides in region 18 (calandria tube)
4                                    number of nuclides in region 19 (moderator)
   15    86   80160  4.68703E-02  fuel
  361  3513  922340  1.28868E-06
  362  3514  922350  1.68695E-04
  365  3518  922380  2.32599E-02
   10    41   50100  2.32686E-07  sheath for CANLUB homogenized sheath case, annular 01
   15    86   80160  7.62177E-06
   54   463  240500  3.26558E-06
   55   465  240520  6.29738E-05
   56   466  240530  7.13994E-06
   57   467  240540  1.77749E-06
   59   523  260540  8.67030E-06
   60   525  260560  1.34788E-04
   61   526  260570  3.08614E-06
   62   527  260580  4.11480E-07
   66   587  280580  3.34827E-06
   68   589  280600  1.28006E-06
   71   593  280640  4.46304E-08
  117  1039  400900  2.16398E-02
  118  1041  400910  4.71908E-03
  119  1042  400920  7.21314E-03
  121  1044  400940  7.30987E-03
  123  1046  400960  1.17763E-03
  267  2168  631510  1.63505E-06
  269  2172  631530  1.78566E-06
  274  2210  641520  3.32093E-09
  276  2212  641540  3.61979E-08
  277  2213  641550  2.45749E-07
  278  2215  641560  3.39896E-07
  279  2216  641570  2.59862E-07
  280  2217  641580  4.12458E-07
  281  2219  641600  3.62976E-07
    1     1   10010  4.38240E-04  coolant
    2     2   10020  4.88020E-02
   15    86   80160  2.46110E-02
   16    87   80170  9.35570E-06
   10    41   50100  2.32686E-07  sheath for CANLUB homogenized sheath case, annular 02
   15    86   80160  7.80275E-06
   54   463  240500  3.26558E-06
```

94	55	465	240520	6.29738E-05	
95	56	466	240530	7.13993E-06	
96	57	467	240540	1.77749E-06	
97	59	523	260540	8.67030E-06	
98	60	525	260560	1.34788E-04	
99	61	526	260570	3.08614E-06	
100	62	527	260580	4.11480E-07	
101	66	587	280580	3.34827E-06	
102	68	589	280600	1.28006E-06	
103	71	593	280640	4.46304E-08	
104	117	1039	400900	2.16398E-02	
105	118	1041	400910	4.71908E-03	
106	119	1042	400920	7.21314E-03	
107	121	1044	400940	7.30986E-03	
108	123	1046	400960	1.17763E-03	
109	267	2168	631510	1.67388E-06	
110	269	2172	631530	1.82806E-06	
111	274	2210	641520	3.39978E-09	
112	276	2212	641540	3.70575E-08	
113	277	2213	641550	2.51585E-07	
114	278	2215	641560	3.47967E-07	
115	279	2216	641570	2.66032E-07	
116	280	2217	641580	4.22252E-07	
117	281	2219	641600	3.71595E-07	
118	15	86	80160	4.68703E-02	fuel
119	361	3513	922340	1.28868E-06	
120	362	3514	922350	1.68695E-04	
121	365	3518	922380	2.32599E-02	
122	10	41	50100	2.32686E-07	sheath for CANLUB homogenized sheath case, annular 03
123	15	86	80160	7.52032E-06	
124	54	463	240500	3.26558E-06	
125	55	465	240520	6.29738E-05	
126	56	466	240530	7.13994E-06	
127	57	467	240540	1.77749E-06	
128	59	523	260540	8.67030E-06	
129	60	525	260560	1.34788E-04	
130	61	526	260570	3.08614E-06	
131	62	527	260580	4.11480E-07	
132	66	587	280580	3.34827E-06	
133	68	589	280600	1.28006E-06	
134	71	593	280640	4.46305E-08	
135	117	1039	400900	2.16398E-02	
136	118	1041	400910	4.71908E-03	
137	119	1042	400920	7.21315E-03	
138	121	1044	400940	7.30987E-03	
139	123	1046	400960	1.17763E-03	
140	267	2168	631510	1.61329E-06	
141	269	2172	631530	1.76189E-06	
142	274	2210	641520	3.27672E-09	
143	276	2212	641540	3.57161E-08	
144	277	2213	641550	2.42478E-07	
145	278	2215	641560	3.35372E-07	
146	279	2216	641570	2.56403E-07	
147	280	2217	641580	4.06968E-07	
148	281	2219	641600	3.58145E-07	
149	1	1	10010	4.38240E-04	coolant
150	2	2	10020	4.88020E-02	
151	15	86	80160	2.46110E-02	

152	16	87	80170	9.35570E-06	
153	10	41	50100	2.32686E-07	sheath for CANLUB homogenized sheath case, annular 04
154	15	86	80160	7.70555E-06	
155	54	463	240500	3.26558E-06	
156	55	465	240520	6.29738E-05	
157	56	466	240530	7.13993E-06	
158	57	467	240540	1.77749E-06	
159	59	523	260540	8.67030E-06	
160	60	525	260560	1.34788E-04	
161	61	526	260570	3.08614E-06	
162	62	527	260580	4.11479E-07	
163	66	587	280580	3.34827E-06	
164	68	589	280600	1.28006E-06	
165	71	593	280640	4.46304E-08	
166	117	1039	400900	2.16398E-02	
167	118	1041	400910	4.71908E-03	
168	119	1042	400920	7.21314E-03	
169	121	1044	400940	7.30986E-03	
170	123	1046	400960	1.17763E-03	
171	267	2168	631510	1.65303E-06	
172	269	2172	631530	1.80529E-06	
173	274	2210	641520	3.35743E-09	
174	276	2212	641540	3.65959E-08	
175	277	2213	641550	2.48451E-07	
176	278	2215	641560	3.43633E-07	
177	279	2216	641570	2.62719E-07	
178	280	2217	641580	4.16992E-07	
179	281	2219	641600	3.66967E-07	
180	15	86	80160	4.68703E-02	fuel
181	361	3513	922340	1.28868E-06	
182	362	3514	922350	1.68695E-04	
183	365	3518	922380	2.32599E-02	
184	10	41	50100	2.32686E-07	sheath for CANLUB homogenized sheath case, annular 05
185	15	86	80160	7.56216E-06	
186	54	463	240500	3.26558E-06	
187	55	465	240520	6.29738E-05	
188	56	466	240530	7.13994E-06	
189	57	467	240540	1.77749E-06	
190	59	523	260540	8.67030E-06	
191	60	525	260560	1.34788E-04	
192	61	526	260570	3.08614E-06	
193	62	527	260580	4.11480E-07	
194	66	587	280580	3.34827E-06	
195	68	589	280600	1.28006E-06	
196	71	593	280640	4.46304E-08	
197	117	1039	400900	2.16398E-02	
198	118	1041	400910	4.71908E-03	
199	119	1042	400920	7.21314E-03	
200	121	1044	400940	7.30987E-03	
201	123	1046	400960	1.17763E-03	
202	267	2168	631510	1.62227E-06	
203	269	2172	631530	1.77169E-06	
204	274	2210	641520	3.29495E-09	
205	276	2212	641540	3.59148E-08	
206	277	2213	641550	2.43827E-07	
207	278	2215	641560	3.37238E-07	
208	279	2216	641570	2.57830E-07	
209	280	2217	641580	4.09232E-07	

```
  281   2219   641600  3.60138E-07
    1      1    10010  4.38240E-04  coolant
    2      2    10020  4.88020E-02
   15     86    80160  2.46110E-02
   16     87    80170  9.35570E-06
   10     41    50100  2.32686E-07  sheath for CANLUB homogenized sheath case, annular 06
   15     86    80160  7.66532E-06
   54    463   240500  3.26558E-06
   55    465   240520  6.29738E-05
   56    466   240530  7.13993E-06
   57    467   240540  1.77749E-06
   59    523   260540  8.67030E-06
   60    525   260560  1.34788E-04
   61    526   260570  3.08614E-06
   62    527   260580  4.11480E-07
   66    587   280580  3.34827E-06
   68    589   280600  1.28006E-06
   71    593   280640  4.46304E-08
  117   1039   400900  2.16398E-02
  118   1041   400910  4.71908E-03
  119   1042   400920  7.21314E-03
  121   1044   400940  7.30986E-03
  123   1046   400960  1.17763E-03
  267   2168   631510  1.64440E-06
  269   2172   631530  1.79586E-06
  274   2210   641520  3.33990E-09
  276   2212   641540  3.64048E-08
  277   2213   641550  2.47153E-07
  278   2215   641560  3.41838E-07
  279   2216   641570  2.61347E-07
  280   2217   641580  4.14815E-07
  281   2219   641600  3.65050E-07
   15     86    80160  4.68703E-02  fuel
  361   3513   922340  1.28868E-06
  362   3514   922350  1.68695E-04
  365   3518   922380  2.32599E-02
   10     41    50100  2.32686E-07  sheath for CANLUB homogenized sheath case, annular 07
   15     86    80160  7.57165E-06
   54    463   240500  3.26558E-06
   55    465   240520  6.29738E-05
   56    466   240530  7.13994E-06
   57    467   240540  1.77749E-06
   59    523   260540  8.67030E-06
   60    525   260560  1.34788E-04
   61    526   260570  3.08614E-06
   62    527   260580  4.11480E-07
   66    587   280580  3.34827E-06
   68    589   280600  1.28006E-06
   71    593   280640  4.46305E-08
  117   1039   400900  2.16398E-02
  118   1041   400910  4.71908E-03
  119   1042   400920  7.21315E-03
  121   1044   400940  7.30987E-03
  123   1046   400960  1.17763E-03
  267   2168   631510  1.62430E-06
  269   2172   631530  1.77391E-06
  274   2210   641520  3.29909E-09
  276   2212   641540  3.59599E-08
```

```
  277   2213   641550  2.44133E-07
  278   2215   641560  3.37661E-07
  279   2216   641570  2.58153E-07
  280   2217   641580  4.09746E-07
  281   2219   641600  3.60590E-07
    1      1    10010  4.38240E-04  coolant
    2      2    10020  4.88020E-02
   15     86    80160  2.46110E-02
   16     87    80170  9.35570E-06
   10     41    50100  9.51420E-08  pressure_tube
   54    463   240500  2.64856E-07
   55    465   240520  5.10750E-06
   56    466   240530  5.79086E-07
   57    467   240540  1.44164E-07
   59    523   260540  1.93680E-06
   60    525   260560  3.01092E-05
   61    526   260570  6.89386E-07
   62    527   260580  9.19170E-08
   66    587   280580  1.67880E-06
   68    589   280600  6.41810E-07
   71    593   280640  2.23774E-08
  117   1039   400900  2.15082E-02
  118   1041   400910  4.69038E-03
  119   1042   400920  7.16921E-03
  121   1044   400940  7.26535E-03
  123   1046   400960  1.17046E-03
  124   1081   410930  1.08824E-03
   12     55    60120  1.62580E-05  gap
   15     86    80160  3.27948E-05
   10     41    50100  2.32997E-07  calandria_tube
   54    463   240500  3.26994E-06
   55    465   240520  6.30577E-05
   56    466   240530  7.14946E-06
   57    467   240540  1.77986E-06
   59    523   260540  5.58121E-06
   60    525   260560  8.67645E-05
   61    526   260570  1.98659E-06
   62    527   260580  2.64875E-07
   66    587   280580  2.63430E-05
   68    589   280600  1.00710E-05
   71    593   280640  3.51136E-07
  117   1039   400900  2.16747E-02
  118   1041   400910  4.72669E-03
  119   1042   400920  7.22473E-03
  121   1044   400940  7.32163E-03
  123   1046   400960  1.17952E-03
    1      1    10010  1.96150E-05  moderator
    2      2    10020  6.53650E-02
   15     86    80160  3.26800E-02
   16     87    80170  1.24230E-05
eof
```

5.8 Sample input file 07 – PWR

Following sample input file describes PWR fuel depletion.

```
uwb1 pwr depletion
4                                   prl_threads - number of threads
10000                               npg - number of neutrons per generation
5                                   nsng - number of skipped neutron generations
205                                 tnng - total number of neutron generations
2                                   n_ccregion - number of concentric cylinder regions
0.4025 0.4750                       rccregion - concentric cylinder region radii
0.6295                              hpitch - half pitch
1                                   lat - lattice type (1=square, 2=hexagonal)
34                                  idepl - number of depletion intervals
4.000E+01 4.000E+01 4.000E+01 4.000E+01 4.000E+01 4.000E+01 4.000E+01 4.000E+01 4.000E+01
    4.000E+01 4.000E+01 4.000E+01 4.000E+01 4.000E+01 4.000E+01 4.000E+01 4.000E+01 4.000E
    +01 4.000E+01 4.000E+01 4.000E+01 4.000E+01 4.000E+01 4.000E+01 4.000E+01 4.000E+01
    4.000E+01 4.000E+01 4.000E+01 4.000E+01 4.000E+01 4.000E+01 4.000E+01 4.000E+01
    depl_power - irradiation power
1.000E+00 2.000E+00 3.000E+00 4.000E+00 5.000E+00 1.000E+01 1.500E+01 2.000E+01 2.500E+01
    5.000E+01 7.500E+01 1.000E+02 1.250E+02 1.500E+02 1.750E+02 2.000E+02 2.250E+02 2.500E
    +02 3.125E+02 3.750E+02 4.375E+02 5.000E+02 5.625E+02 6.250E+02 6.875E+02 7.500E+02
    8.125E+02 8.750E+02 9.375E+02 1.000E+03 1.063E+03 1.125E+03 1.188E+03 1.250E+03
    depl_time - irradiation days
1 0 0                               depl_type - regions depletion (0=no depletion, 1=power
    depletion, 2=flux depletion)
1 2 2                               reg_libtype - regions transport/burnup libraries position
900.0 600.0 600.0                   maxwell_kelvin - regions maxwell temperatures
"/media/sf_xwork/uwb1libs/"         folder with uwb1 libraries
uwb1zaid0423to3820.txt              position of transport nuclides in depletion nuclides
uwb1nmass.txt                       nuclide mass relative to neutron
uwb1qvalues4mc.txt                  qvalues for inelastic reactions
uwb1chi16.txt                       xs_n2n chi data library
uwb1chi17.txt                       xs_n3n chi data library
uwb1chi18.txt                       xs_fission chi data library
uwb1chi91.txt                       xs_inelastic_continuum chi data library
uwb1nubar.txt                       nubar data library
uwb1angular02.txt                   xs_elastic angular distribution data library
uwb1angular51t90.txt                xs_inelastic_discrete angular distribution data library
uwb1angular91.txt                   xs_inelastic_continuum angular distribution data library
uwb1egrid.txt                       energy grid for xs data
uwb1xscom0900k.txt                  xs data library no1
uwb1xscom0600k.txt                  xs data library no2
uwb1aiiuni.txt                      transition matrix Aii, universal flux-independent part
uwb1fijphi.txt                      transition data   Fij, part of Aij, case-flux-dependent
    part
uwb1aijuni.txt                      transition matrix Aij, universal flux-independent part
uwb1deplxscom0900k.txt              cross section library for depletion reactions no1
uwb1deplxscom0600k.txt              cross section library for depletion reactions no2
uwb1qvalues4depl.txt                recoverable energy library for depletion reactions
4                                   number of nuclides in region  1 (fuel)
29                                  number of nuclides in region  2 (cladding)
4                                   number of nuclides in region  3 (moderator)
  15     86    80160  4.63000E-02   nuclear densities in region   1 (fuel)
  16     87    80170  1.76360E-05
 362   3514   922350  1.17435E-03
 365   3518   922380  2.20309E-02
  54    463   240500  3.30121E-06   nuclear densities in region   2 (cladding)
```

```
   55   465   240520  6.36606E-05
   56   466   240530  7.21860E-06
   57   467   240540  1.79686E-06
   59   523   260540  8.68307E-06
   60   525   260560  1.36306E-04
   61   526   260570  3.14789E-06
   62   527   260580  4.18926E-07
  117  1039   400900  2.18865E-02
  118  1041   400910  4.77292E-03
  119  1042   400920  7.29551E-03
  121  1044   400940  7.39335E-03
  123  1046   400960  1.19110E-03
  170  1531   501120  4.68066E-06
  172  1534   501140  3.18478E-06
  173  1535   501150  1.64064E-06
  174  1536   501160  7.01616E-05
  175  1537   501170  3.70592E-05
  176  1539   501180  1.16872E-04
  177  1540   501190  4.14504E-05
  178  1542   501200  1.57212E-04
  179  1545   501220  2.23417E-05
  181  1548   501240  2.79392E-05
  304  2594   721740  3.54138E-09
  305  2596   721760  1.16423E-07
  306  2597   721770  4.11686E-07
  307  2600   721780  6.03806E-07
  308  2603   721790  3.01460E-07
  309  2606   721800  7.76449E-07
    1     1    10010  4.83495E-02  nuclear densities in region   3 (moderator)
   10    41    50100  4.80869E-06
   11    42    50110  1.93556E-05
   15    86    80160  2.41747E-02
eof
```

5.9 Sample input file 08 – SFR

Following sample input file describes SFR fuel depletion.

```
uwb1 sfr depletion
4                                   prl_threads - number of threads
10000                               npg - number of neutrons per generation
5                                   nsng - number of skipped neutron generations
205                                 tnng - total number of neutron generations
2                                   n_ccregion - number of concentric cylinder regions
0.28 0.33                           rccregion - concentric cylinder region radii
0.42                                hpitch - half pitch
2                                   lat - lattice type (1=square, 2=hexagonal)
74                                  idepl - number of depletion intervals
1.30000E+02 1.30000E+02 1.30000E+02 1.30000E+02 1.30000E+02 1.30000E+02 1.30000E+02 1.30000E
    +02 1.30000E+02 1.30000E+02 1.30000E+02 1.30000E+02 1.30000E+02 1.30000E+02 1.30000E+02
    1.30000E+02 1.30000E+02 1.30000E+02 1.30000E+02 1.30000E+02 1.30000E+02 1.30000E+02
    1.30000E+02 1.30000E+02 1.30000E+02 1.30000E+02 1.30000E+02 1.30000E+02 1.30000E+02
    1.30000E+02 1.30000E+02 1.30000E+02 1.30000E+02 1.30000E+02 1.30000E+02 1.30000E+02
    1.30000E+02 1.30000E+02 1.30000E+02 1.30000E+02 1.30000E+02 1.30000E+02 1.30000E+02
    1.30000E+02 1.30000E+02 1.30000E+02 1.30000E+02 1.30000E+02 1.30000E+02 1.30000E+02
    1.30000E+02 1.30000E+02 1.30000E+02 1.30000E+02 1.30000E+02 1.30000E+02 1.30000E+02
    1.30000E+02 1.30000E+02 1.30000E+02 1.30000E+02 1.30000E+02 1.30000E+02 1.30000E+02
    1.30000E+02 1.30000E+02 1.30000E+02 1.30000E+02 1.30000E+02 1.30000E+02 1.30000E+02
    1.30000E+02 1.30000E+02 1.30000E+02  depl_power - irradiation power
3.07692E-01 6.15385E-01 9.23077E-01 1.23077E+00 1.53846E+00 3.07692E+00 4.61538E+00 6.15385E
    +00 7.69231E+00 1.53846E+01 2.30769E+01 3.07692E+01 3.84615E+01 4.61538E+01 5.38462E+01
    6.15385E+01 6.92308E+01 7.69231E+01 9.61538E+01 1.15385E+02 1.34615E+02 1.53846E+02
    1.73077E+02 1.92308E+02 2.11538E+02 2.30769E+02 2.50000E+02 2.69231E+02 2.88462E+02
    3.07692E+02 3.26923E+02 3.46154E+02 3.65385E+02 3.84615E+02 4.03846E+02 4.23077E+02
    4.42308E+02 4.61538E+02 4.80769E+02 5.00000E+02 5.19231E+02 5.38462E+02 5.57692E+02
    5.76923E+02 5.96154E+02 6.15385E+02 6.34615E+02 6.53846E+02 6.73077E+02 6.92308E+02
    7.11538E+02 7.30769E+02 7.50000E+02 7.69231E+02 7.88462E+02 8.07692E+02 8.26923E+02
    8.46154E+02 8.65385E+02 8.84615E+02 9.03846E+02 9.23077E+02 9.42308E+02 9.61538E+02
    9.80769E+02 1.00000E+03 1.01923E+03 1.03846E+03 1.05769E+03 1.07692E+03 1.09615E+03
    1.11538E+03 1.13462E+03 1.15385E+03  depl_time - irradiation days
1 0 0                               depl_type - regions depletion (0=no depletion, 1=power
    depletion, 2=flux depletion)
1 2 2                               reg_libtype - regions transport/burnup libraries position
1200.0 600.0 600.0                  maxwell_kelvin - regions maxwell temperatures
"/media/sf_xwork/uwb1libs/"         folder with uwb1 libraries
uwb1zaid0423to3820.txt              position of transport nuclides in depletion nuclides
uwb1nmass.txt                       nuclide mass relative to neutron
uwb1qvalues4mc.txt                  qvalues for inelastic reactions
uwb1chi16.txt                       xs_n2n chi data library
uwb1chi17.txt                       xs_n3n chi data library
uwb1chi18.txt                       xs_fission chi data library
uwb1chi91.txt                       xs_inelastic_continuum chi data library
uwb1nubar.txt                       nubar data library
uwb1angular02.txt                   xs_elastic angular distribution data library
uwb1angular51t90.txt                xs_inelastic_discrete angular distribution data library
uwb1angular91.txt                   xs_inelastic_continuum angular distribution data library
uwb1egrid.txt                       energy grid for xs data
uwb1xscom1200k.txt                  xs data library no1
uwb1xscom0600k.txt                  xs data library no2
uwb1aiiuni.txt                      transition matrix Aii, universal flux-independent part
uwb1fijphi.txt                      transition data   Fij, part of Aij, case-flux-dependent
    part
```

```
uwb1aijuni.txt                     transition matrix Aij, universal flux-independent part
uwb1deplxscom1200k.txt             cross section library for depletion reactions no1
uwb1deplxscom0600k.txt             cross section library for depletion reactions no2
uwb1qvalues4depl.txt               recoverable energy library for depletion reactions
4                                  number of nuclides in region  1 (fuel)
4                                  number of nuclides in region  2 (cladding)
1                                  number of nuclides in region  3 (moderator)
  15     86    80160  4.63522E-02  nuclear densities in region   1 (fuel)
  16     87    80170  1.76558E-05
 362   3514   922350  3.52253E-03
 365   3518   922380  1.97089E-02
   59   523   260540  4.97940E-03  nuclear densities in region   2 (cladding)
   60   525   260560  7.81660E-02
   61   526   260570  1.80519E-03
   62   527   260580  2.40238E-04
   19   141   110230  2.30515E-02  nuclear densities in region   3 (coolant)
eof
```

Chapter 6

Output file

The chapter describes U_WB_1 output file and its sections. Parts of sample problem of VVER-1000 fuel depletion output is shown.

6.1 Output structure

Depletion scheme of U_WB_1 code couples transport and burnup solver in 2sPC scheme. Screen output tells user currently solver step, after each transport and burnup solver, main output data are written into output file. Burnup solver output is supressed in predictor and corrector stage. At the end of fuel depletion, estimator output is written.

6.2 Transport solver output

Transport solver is called three times, for the initial composition (depletion step 0) and predicted and corrected final composition (depletion step `idepl`). Following output example for sample case shows output data that comprises of multiplication factor details and neutron flux details. Multiplication factor for each simulated generation is written, average multiplication factor during the simulation and its uncertainty is also reported. Three dots in the example are used to shorted large data lines, however, neutron flux is calculated and printed for all 4308 energy groups. Upper energy group boundary and neutron flux for each geometry region is tabulated.

```
transport calculation for depletion step    0 /  43
k-eff values during MC simulation:         1.30490   1.33590   ...   1.31980   1.32720
k-eff averages during MC simulation:       0.00000   0.00000   ...   1.32132   1.32138
k-eff uncertainty during MC simulation:    0.00000   0.00000   ...   0.00080   0.00080
final k-eff:    1.32138   0.00080
energy grid:                               1.02563E-05 ... 1.96802E+07 2.00000E+07
neutron flux in region    1:               0.00000E+00 ... 0.00000E+00 0.00000E+00
neutron flux in region    2:               0.00000E+00 ... 0.00000E+00 0.00000E+00
neutron flux in region    3:               1.36566E-08 ... 0.00000E+00 0.00000E+00
```

6.3 Burnup solver output

Burnup solver writes output for initial composition and end-of-step composition during depletor stage. Fuel burnup is reported, followed by nuclide identifications and their nuclear densities in all geometry regions (even if the regions are not depleted). Following example for sample case shows output data for the last calling of burnup solver.

```
depletion calculation for depletion step   43 /  43
```

```
fuel burnup:    50000.0 MWd/MTU
nuclide positions:                          1            2  ...         3819         3820
zaid identifiers:                       10010        10020  ...      1102791      1112720
region   1 inventory:         9.10639E-07 4.50389E-09  ...  0.00000E+00 0.00000E+00
region   2 inventory:         0.00000E+00 0.00000E+00  ...  0.00000E+00 0.00000E+00
region   3 inventory:         5.01551E-02 0.00000E+00  ...  0.00000E+00 0.00000E+00
```

6.4 Estimator output

Estimator writes table of multiplication factor dependency on burnup.

```
burnup (MWd/MTU)  k-eff (-)
            0.00    1.32138
           40.00    1.30450
           80.00    1.30096
          120.00    1.29996
          160.00    1.29920
          200.00    1.29854
          400.00    1.29665
          600.00    1.29491
          800.00    1.29340
         1000.00    1.29192
         1500.00    1.28897
         2000.00    1.28478
         2500.00    1.28005
         3000.00    1.27494
         3500.00    1.26956
         4000.00    1.26400
         4500.00    1.25832
         5000.00    1.25257
         5500.00    1.24680
         6000.00    1.24104
         6500.00    1.23531
         7000.00    1.22963
         7500.00    1.22400
         8000.00    1.21843
         8500.00    1.21294
         9000.00    1.20752
         9500.00    1.20217
        10000.00    1.19690
        12500.00    1.17749
        15000.00    1.15355
        17500.00    1.13113
        20000.00    1.11089
        22500.00    1.09189
        25000.00    1.07280
        27500.00    1.05202
        30000.00    1.03240
        32500.00    1.01484
        35000.00    0.99910
        37500.00    0.98478
        40000.00    0.97162
        42500.00    0.95927
        45000.00    0.94751
        47500.00    0.93637
        50000.00    0.92586
```

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Appendix A

Data libraries

Data libraries contain mainly nuclear data such as cross sections, radioactive decay description and nuclide's properties. Very little input or deep library knowledge is required on the user in the area of nuclear data libraries. Data libraries containing nuclear data were prepared from ENDF/B-VII.1 library by $U_W B_1$ subroutines that are not supplied with the code, i.e. the user cannot change the base library (ENDF/B-VII.1).

A.1 Algebraic libraries

Algebraic libraries account for 5 out of 33 data libraries. They are used for CRAM method in burnup solver to calculated matrix exponential that is approximated by the sum of inverse matrices. Linear system that is described by a complex sparse matrix is solved by BLAS and MUMPS libraries. BLAS library is contained in the file `blas_LINUX.a`, compiled from BLAS March 2007 source files (http://www.netlib.org/blas/blas.tgz). MUMPS library uses BLAS library and is part of 4 files `libmpiseq.a`, `libmumps_common.a`, `libpord.a` and `libzmumps.a`. MUMPS version 4.10.0 from 2011 was used. Both libraries were tested on Ubuntu 13.10 under Windows 7 and on Red Hat Enterprise Linux 6.5, giving the same results. If executable file $\mathtt{U}_W\mathtt{B}_1$ is supplied, algebraic libraries are not used but rather linked into the executable file.

A.2 Nuclide's description library

Nuclide's description library `uwb1zaid0423to3820.txt`, like the rest of the libraries, is an ASCII free-format file library. Burnup solver handles 3820 nuclides from radioactive data library, transport solver handles 423 nuclides from neutron data library. Each nuclide has three ID numbers – position in 423 nuclides (first column of the library), position in 3820 nuclides (second column of the library) and ZAID (third column of the library). ZAID number is given by ZAID=10000*Z+10*A+m, for example, U-238 has ZAID designation 922380, while Am-242m is designated by 952421.

A.3 Burnup solver libraries

Burnup solver libraries account for 8 out of 33 data libraries. The purpose of the libraries is the numerical evaluation of transition matrix used in depletion calculations. Transition matrix can be divided into four streams, diagonal and non-diagonal elements and flux-dependent and flux-independent elements.

The diagonal elements of the transition matrix represents radioactive decay and the disappearance rate due to all nuclear reactions. Separation of the diagonal elements into two parts is a result of data dependency on neutron flux that is not known a priori. The non-diagonal elements of the transition matrix represents radioactive decay and the nuclear reaction transition between the nuclides. Similar to the diagonal elements, non-diagonal matrix elements are stored in two separate streams (flux-dependent and flux-independent).

`uwb1aiiuni.txt` library contains diagonal flux-indepedent elements of transition matrix that describe radioactive decay. Data were prepared for $U_W B_1$ from radioactive decay library ENDF/B-VII.1. First description line is followed by arbitrary number of three-column lines. The first two columns are nuclide description (position in 3820 burnup nuclides, ZAID number), the last column is the value of transition matrix element (negative real numbers, because the elements describe nuclide disappearance rate). For example, Cs-137 line

```
1799  551370 -7.30203E-10
```

shows that Cs-137 (1799th nuclide out of 3820) disappears with decay constant 7.30203E-10 s^{-1} (half-life of slightly over 30 years).

`uwb1fijphi.txt` library contains non-diagonal flux-dependent elements of transition matrix that describe disappearance rate due to nuclear reactions. Seven-column data format follows two description lines

```
i, j, zaid i, zaid j, fij, pos0423, reac30
107331 number of entries in Fij library
```

The second description line defines number of lines that will be read by the code, the first line contains basic description of the data. The first and second column contain row and column index of transition matrix that has the order or 3820. The third and fourth column designated ZAID of i-th and j-th nuclides. The fifth column is the transition matrix factor F_{ij}, the factor is the transition fraction covering decay schemes, multiplicity of daughter nuclides, and fission yields. The sixth column is the position of j-th nuclide in transport nuclides (out of 423) k, the last column is the position of the reaction (out of 30 burnup reactions) m. Note that the transition matrix factor F_{ij} depends on 4 variables (row index, column index, nuclide, nuclear reaction). The transition matrix element A_{ij} represent a rate of transition of the j-th nuclide into the i-th nuclide. The transition matrix element A_{ij} is therefore calculated by summing over all nuclides and all nuclear reactions that describe the disappearance that leads to creation of i-th nuclide by the relationship $A_{ij} = \varphi \sum_{km} F_{ij}\sigma_{km}$. Effective cross sections σ_{km} are described in the following paragraph. For example, line

```
 3519 3518   922390   922380   1.00000E+00   365    18
```

describes radiation capture reaction U-238(n,γ)U-239 that eventually leads to Pu-239 build-up, (n,γ) is reaction 18/30 in $U_W B_1$ burnup solver. Another example, line

```
 1799 3514   551370   922350   5.99988E-04   362     4
```

describes U-235 fission with Cs-137 fission product with independent fission product yield 5.99988E-04, (n,f) is reaction 4/30 in $U_W B_1$ burnup solver.

`uwb1deplxscom0293k.txt`, `uwb1deplxscom0600k.txt`, `uwb1deplxscom0900k.txt`, `uwb1deplxscom1200k.txt` libraries contain cross sections of 30 nuclear reactions used in $U_W B_1$ burnup solver and 423 nuclides that have non-zero cross section data. The data are supplied for four Doppler-broadened temperatures 293 K, 600 K, 900 K (typical for thermal reactor fuel) and 1200 K (typical for fast reactor fuel). The 4308-group cross section data are stored in compressed format to avoid storing large number of zeroes, however, in order to handle them fast in $U_W B_1$ execution, variables are stored in uncompressed way. Data are stored in 423 blocks, one block for each nuclide sorted by their position in the transport nuclides (first data for H-1, lastly data for Fm-255). First line of each nuclide block describes the position of the nuclide, ZAID of nuclide and number of non-zero cross sections. For example, line

```
       362     922350           6
```

is the first line of U-235 block, U-235 has 6 non-zero nuclear reactions. After the first line follows data lines for each nuclear reactions, each reaction is stored on separate line. The first number is the nuclear reaction ID in $U_W B_1$ burnup reactions, the second number is the MT number of ENDF-6 format reaction (all data are from ENDF/B-VII.1 library), the third number is the first energy group with non-zero cross section, the fourth number if the number of non-zero energy groups, the rest of the line are actual cross section data (barns) in $U_W B_1$ energy grid (4308 energy groups). Following example of U-235 for 900 K shows that of 6 reactions, the dominant are fission (MT=18) and radioactive capture (MT=102). List of nuclear reactions in $U_W B_1$ burnup solver (all available reactions that leads to change of the nuclide) is part of Table A.1.

```
 1    4    2101    2208   1.20700E-07 ...
 2   16    4239      70   3.40753E-03 ...
 3   17    4279      30   5.00382E-05 ...
 4   18       1    4308   3.11441E+04 ...
14   37    4303       6   5.14348E-05 ...
18  102       1    4308   5.91243E+03 ...
```

Table A.1: Nuclear reactions in $U_W B_1$ burnup solver.

i	MT	Reaction	Output nuclide(s)	i	MT	Reaction	Output nuclide(s)
1	4	(n,n)	A,Z,M+1	16	44	(n,n2p)	A-2,Z-2
2	16	(n,2n)	A-1,Z	17	45	(n,npα)	A-5,Z-3
3	17	(n,3n)	A-2,Z	18	102	(n,γ)	A+1,Z
4	18	(n,f)	FP	19	103	(n,p)	A,Z-1
5	22	(n,nα)	A-4,Z-2	20	104	(n,d)	A-1,Z-1
6	23	(n,n3α)	A-12,Z-6	21	105	(n,t)	A-2,Z-1
7	24	(n,2nα)	A-5,Z-2	22	106	(n,^{3}He)	A-2,Z-2
8	25	(n,3nα)	A-6,Z-2	23	107	(n,α)	A-3,Z-2
9	28	(n,np)	A-1,Z-1	24	108	(n,2α)	A-7,Z-4
10	29	(n,n2α)	A-8,Z-4	25	111	(n,2p)	A-1,Z-2
11	32	(n,nd)	A-2,Z-1	26	112	(n,pα)	A-4,Z-3
12	33	(n,nt)	A-3,Z-1	27	113	(n,t2α)	A-10,Z-5
13	34	(n,n^{3}He)	A-3,Z-2	28	115	(n,pd)	A-2,Z-2
14	37	(n,4n)	A-3,Z	29	116	(n,pt)	A-3,Z-2
15	41	(n,2np)	A-2,Z-1	30	117	(n,dα)	A-5,Z-3

`uwb1aijuni.txt` library contains non-diagonal flux-indepedent elements of transition matrix that describe radioactive decay. Data file provides decay scheme information as well as multiplication and spontaneous fission yield data. Data format is similar to diagonal data library. First description line is followed by arbitrary number of five-column lines. The first four columns are nuclide description (i-th and j-th position in 3820 burnup nuclides, i-th and j-th ZAID number), the last column is the value of transition matrix element (positive real numbers, because the elements describe nuclide creation rate). For example, Cs-137 lines

```
1846 1799  561370  551370  3.87048E-11
1847 1799  561371  551370  6.91498E-10
```

shows that Cs-137 (1799th nuclide out of 3820) decay with effective decay constant 3.87048E-11 s^{-1} to Ba-137 (1846th nuclide) and with effective decay constant 6.91498E-10 s^{-1} to Ba-137m (1847th nuclide). Each possible radioactive decay mode from Table A.2 and ENDF/B-VII.1 radioactive data library is stored in $U_W B_1$.

`uwb1qvalues4depl.txt` library contains reaction Q-values (recoverable energy) that are used in power depletion to transform power to flux. First description line is followed by 423-column data format. The first two columns are nuclide identification (position in transport nuclides, ZAID number), followed by 423 columns of Q-values (eV) for the burnup reactions. Typical Q-values are around 200 MeV for fission and 5 MeV for radioactive capture. For example, U-235 data line

```
362   922350  0.00000E+00  0.00000E+00  0.00000E+00  1.93405E+08  0.00000E+00  0.00000E+00
    0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E
    +00  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  6.54520E+06  0.00000E+00
    0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E
    +00  0.00000E+00  0.00000E+00  0.00000E+00  0.00000E+00
```

shows that 193.405 MeV is recoverable energy from fission, while only 6.545 MeV for radioactive capture. Recoverable energies for radioactive capture became dominant in non-fissile regions like fuel cladding. Values in the library are used by burnup solver, transport solver uses another library with different format and different nuclear reactions.

Table A.2: Radioactive modes in $U_W B_1$.

i	RTYP	Reaction	Output nuclide(s)
1	1.0	β decay	A,Z+1,m
2	2.0	Electron capture and/or positron emission	A,Z-1,m
3	3.0	iIsomeric transition	A,Z,m-1
4	4.0	α decay	A-4,Z-2,m
5	5.0	Neutron emission	A-1,Z,m
6	6.0	Spontaneous fission	FP
7	7.0	Proton emission	A-1,Z-1,m
8	1.1	Double β decay	A,Z+2,m
9	1.4	β decay followed by α emission	A-4,Z-1,m
10	1.5	β decay followed by neutron emission	A-1,Z+1,m
11	1.55	β decay followed by 2 neutron emissions	A-2,Z+1,m
12	1.555	β decay followed by 3 neutron emissions	A-3,Z+1,m
13	1.5555	β decay followed by 4 neutron emissions	A-4,Z+1,m
14	2.4	Positron decay followed by α emission	A-4,Z-3,m
15	2.6	Positron decay followed by SF	FP of daughter
16	2.7	Positron decay followed by proton emission	A-1,Z-2,m
17	2.77	Positron decay followed by 2 proton emissions	A-2,Z-3,m
18	5.5	Double neutron emission	A-2,Z,m
19	7.7	Double proton emission	A-2,Z-2,m

A.4 Transport solver libraries

Monte Carlo transport solver libraries account for 19 out of 33 data libraries. The purpose of the libraries is to supply data needed to Monte Carlo simulation. Based on available nuclear data from ENDF/B-VII.1 data library, burnup and transport solvers use different set of nuclear reactions and nuclides. Transport solver handle 423 nuclides with known neutron cross section data and 46 nuclear reactions that are necessary for a description of a neutron transport via Monte Carlo simulation. Burnup solver handle 3820 nuclides with known radioactive properties and 30 nuclear reactions that describe transition between the nuclides.

Nuclear reactions considered in neutron transport are divided into the following groups:

1. Elastic scattering (MT=2), neutron loses energy. ($U_W B_1$ transport reaction number 1)
2. Inelastic scattering to the continuum (MT=16, MT=17, MT=91), neutron loses energy and its weight is changed. ($U_W B_1$ transport reaction numbers 2, 3 and 45)
3. Fission (MT=18), neutron dies, neutron transport is ended and information about the fission is stored into neutron bank. ($U_W B_1$ transport reaction number 4)
4. Inelastic scattering to discrete nucleus states (MT=51 to MT=90), neutron loses energy and its weight is changed. A different description of the reaction than at scattering to continuum. ($U_W B_1$ transport reaction numbers 5 to 44)
5. Sum of reactions with zero outgoing neutrons (MT=102 to 117, a sum equivalent to MT=101), death of neutron, neutron transport ends. ($U_W B_1$ transport reaction number 46)

`uwb1angular02.txt` library contains angular distribution for elastic scattering (MT=2). Cosine of the scattering angle in center-of-mass system is stored in the library that is divided into blocks, each block describe different nuclide. The first line of each block is nuclide description (position in library, ZAID number), then follows 76x21 matrix of data. The first column of data matrix is dedicated to energy grid of angular distribution (energy of ingoing neutron in laboratory system). Energy grid is fixed do 76 values that focuses mainly on higher energy regions above 1.0E+05 eV. The next 20 columns contain actual angular distribution data for a fixed number of 20 equiprobable bins. For example, first H-1 data line

```
1.00000E-05 -9.00000E-01 -8.00000E-01 -7.00000E-01 -6.00000E-01 -5.00000E-01 -4.00000E-01
    -3.00000E-01 -2.00000E-01 -1.00000E-01  0.00000E+00  1.00000E-01  2.00000E-01  3.00000E
```

```
-01  4.00000E-01  5.00000E-01  6.00000E-01  7.00000E-01  8.00000E-01  9.00000E-01
1.00000E+00
```

describes angular distribution for energy 1.0E-05 eV, upper boundaries of the equiprobable bins in this example are equal to an isotropic distribution. The library is stored in un-compressed format, i.e. isotropic distributions are not handled differently from other distributions.

`uwb1angular51t90.txt` library contains angular distribution for inelastic scattering to discrete nucleus states (MT=51 to MT=90). Cosine of the scattering angle in center-of-mass system is stored, the same as in the case of elastic scattering. The same 76 point energy grid for angular distribution is also used. However, because of large number of reactions, library is stored in compressed format. The compressed format have two parts. In the first part, block of nuclides with data matrices are present. First column of data matrices store energy grid (energy of ingoing neutron in laboratory system). The next 40 columns store position of angular distribution of each of the 40 nuclear reactions. The angular distribution is then stored in the second part of the library. Zero position means isotropic distribution (88 % of number of reactions). Number of non-zero positions is stored in the first line of the second part of library that follows by angular distribution data (at each line, position of angular distribution and 20 equiprobable bins are available). For example, third U-238 line

```
 1.00000E+05   13713        0        0        0        0        0        0        0        0
     0        0        0        0        0        0        0        0        0        0        0
           0        0        0        0        0        0        0        0        0        0
     0        0        0        0        0        0        0        0        0        0
```

shows that for ingoing neutron energy 1.0E+05 eV, inelastic scattering to only first nucleus states is not isotropic, actual data are stored later on line

```
13713 -8.74013E-01 -7.58021E-01 -6.50025E-01 -5.47026E-01 -4.48026E-01 -3.52024E-01
    -2.58021E-01 -1.66017E-01 -7.50125E-02  1.49925E-02  1.04997E-01  1.96002E-01
    2.87006E-01  3.79011E-01  4.73013E-01  5.69453E-01  6.69015E-01  7.73013E-01  8.83008
    E-01  1.00000E+00
```

showing that the distribution is not far from the isotropic one.

`uwb1angular91.txt` library contains angular distribution for inelastic scattering to the continuum (MT=91). Cosine of the scattering angle in laboratory system is stored, opposite to center-of-mass system for previous reactions. Otherwise, data format is the same as for inelastic scattering to discrete nucleus states from `uwb1angular51t90.txt`, in compressed format for only 1 reaction instead of 40. Zero position means isotropic distribution (85 % of number of reactions).

`uwb1egrid.txt` library contains energy grid definition for transport solver. The whole data library is showed below. 4308 energy groups (called subgroups in the source code) are divided into 14 intervals (called groups in the source code), each interval is divided in uniform lethargy width.

```
4308 number of uwb1 energy subgroups
14 number of groups
1.00E-05  1.00E-04    91
1.00E-04  1.00E-03   100
1.00E-03  1.00E-02    99
1.00E-02  1.00E-01    84
1.00E-01  1.00E+00   100
1.00E+00  1.00E+01   100
1.00E+01  1.00E+02   391
1.00E+02  1.00E+03   663
1.00E+03  1.00E+04  1340
1.00E+04  2.00E+04   997
2.00E+04  1.00E+05   100
1.00E+05  1.00E+06   100
1.00E+06  1.00E+07   100
1.00E+07  2.00E+07    43
```

`uwb1chi16.txt` library contains secondary particle energy distribution for neutron scattering reaction (n,2n)

(MT=16). Secondary particle energy distribution (eV) is stored in fixed number of 1000 equiprobable bins. The library is divided into two parts. The first part describes ingoing neutron energy grid, the second part contain actual data of secondary particle energy distribution. For (n,2n) reaction, ingoing neutron energy grid is fixed to two energies that are different for each nuclide. The first part of the library have four columns – nuclide position, nuclide ZAID, ingoing neutron energy value #1 and ingoing neutron energy value #2. For example, U-238 line

```
  365   922380    7.00000E+06  2.00000E+07
```

shows that 7 MeV and 20 MeV were selected for linear interpolation. The second part of the library have two 425x1000 matrices containing distribution data for ingoing energy grid values for 423 nuclides (first two columns are nuclide identification) and 1000 equiprobable bins. For example, U-238 lines

```
  365   922380    4.05420E+03  ...  8.18500E+05
  365   922380    1.59240E+04  ...  1.36640E+07
```

means that upper equiprobable bin boundaries from 4 keV to 819 keV for ingoing 7 MeV neutron and 159 keV to 1366 keV for ingoing 20 MeV neutron are used in transport calculation.

`uwb1chi17.txt` library contains secondary particle energy distribution for neutron scattering reaction (n,3n) (MT=17). Secondary particle energy distribution (eV) is stored in fixed number of 1000 equiprobable bins. The library have the same format as the rest of secondary particle energy distribution data libraries, only number of ingoing neutron energy grid point differ. For (n,3n) reaction, only 1 energy grid point is assumed, therefore, the first part of the library is omitted. For example, U-238 line

```
365   922380    1.33180E+04  ...  6.22720E+06
```

means that upper equiprobable bin boundaries from 13 keV to 6 MeV are used in transport calculation.

`uwb1chi18.txt` library contains secondary particle energy distribution for neutron fission (n,f) (MT=18). For (n,f) reaction, only 1 energy grid point is assumed, therefore, the first part of the library is omitted. For example, U-238 line

```
  365   922380    1.83540E+04  ...  1.30320E+07
```

means that upper equiprobable bin boundaries from 18 keV to 13 MeV are used in transport calculation.

`uwb1chi91.txt` library contains secondary particle energy distribution for inelastic scattering to the continuum (MT=91). For MT=91 reaction, ingoing neutron energy grid is fixed to three energies that are different for each nuclide. For example, U-238 line

```
  365   922380    1.50000E+06  5.00000E+06  2.00000E+07
```

shows that 1.5 MeV, 5 MeV and 20 MeV were selected for linear interpolation. For example, 5 MeV U-238 line

```
  365   922380    1.12560E+04  ...  3.08520E+06
```

means that upper equiprobable bin boundaries from 11 keV to 3 MeV are used in transport calculation.

`uwb1maxwell0293k.txt`, `uwb1maxwell0600k.txt`, `uwb1maxwell0900k.txt`, `uwb1maxwell1200k.txt` libraries contain Maxwell-Boltzmann distribution data for thermal motion treatment. Target nucleus velocity is sampled from Maxwell-Boltzmann distribution that is tabulated for an arbitrary number of equiprobable bins. The data are supplied for four temperatures 293 K, 600 K, 900 K (typical for thermal reactor fuel) and 1200 K (typical for fast reactor fuel). The first line of the library contains number of equiprobable bins (40 was chosen) followed by the data – first two columns for nuclide identification (position, ZAID) followed by columns for each equiprobable bin. For example, H-1 (600 K) line

```
    1    10010  1.03365E+03  ..  7.49385E+03
```

means that upper equiprobable bin boundaries from 1034 m/s to 7494 m/s are used. Similarly for U-238 line

```
365   922380  6.73500E+01  ..  4.87650E+02
```

boundaries from 67 m/s to 488 m/s are used. Weakness of this approach is low precision in sampling low-probability target velocities at the edges of the distribution and fixed values of temperature. Therefore, these data libraries were replaced by different approach that samples target velocity directly during neutron transport, moreover, arbitrary temperatures are allowed in input file. Maxwell-Boltzmann data libraries are not needed for $U_W B_1$ version February 2015 and later.

`uwb1nmass.txt` library contains nuclide masses. These masses are used in fissile mass calculation, power distribution evaluation and mainly in the treatment of neutron scattering reactions where nuclide mass relative to neutron is important. After the first description line, three-column data are provided. The first two columns are used for nuclide identification, the third column store the nuclide mass relative to neutron mass. For example, H-1 line

```
  1     10010  9.99167E-01
```

shows that hydrogen (proton) mass is slighly lower than neutron mass.

`uwb1nubar.txt` library contains fission neutron multiplicities. The first column contain nuclide ZAID, the first line contain fission neutron energy, the inner matrix contain fission neutron multiplicities. The data are stored for a fixed number of 40 energies that works with linear interpolation to preserve the precision. For example, U-235 line

```
922350  2.43670E+00  ..  5.20985E+00
```

means that average number of 2.44 to 5.21 neutrons per fission are sampled.

`uwb1qvalues4mc.txt` library contains reaction Q-values that are used in the treatment of inelastic scattering reactions. The format is the same as for `uwb1qvalues4depl.txt` library containing similar data for burnup solver. The difference is in the list of reactions, for transport solver, scattering reactions (n,2n), (n,3n) and inelastic scattering reactions MT=51 to MT=90 are stored column-wise. Since Q-values are stored, negative sign of the data appears. For example, U-238 line

```
365   922380 -6.15280E+06 -1.12786E+07 -4.49000E+04 ... -3.90900E+06
```

means that 6 MeV for (n,2n) and 11 MeV for (n,3n) reactions is used, inelastic scattering Q-values increase from 45 keV to 4 MeV.

`uwb1xscom0293k.txt`, `uwb1xscom0600k.txt`, `uwb1xscom0900k.txt`, `uwb1xscom1200k.txt` libraries contain cross section for transport reactions. The data are stored in compressed format that is the same as for burnup solver cross section libraries. Following cut of 900 K U-238 data shows that for U-238, all 46 available reactions are non-zero. After the description line (nuclide position, nuclide ZAID, number of non-zero reactions), the first column stores $U_W B_1$ transport reaction number, the second column MT reaction number (used only for better visualization), the third one position of first non-zero energy group, the fourth the number of non-zero energy groups, data from the fifth column represent actual cross sections in barns.

```
     365    922380        46
 1     2         1    4308   6.02926E+01 5.95493E+01 ...
 2    16    4246        63   4.26574E-02 1.07807E-01 ...
 3    17    4274        35   3.03789E-04 4.07109E-03 ...
 4    18         1    4308   8.37628E-04 8.27087E-04 ...
 5    51    4017       292   1.16193E-02 2.35265E-02 ...
 6    52    4084       225   4.31701E-04 8.46727E-04 ...
 7    53    4115       194   1.26598E-21 3.49982E-21 ...
 8    54    4138       171   4.52360E-06 9.89050E-06 ...
 9    55    4150       159   4.91972E-02 9.01127E-02 ...
```

10	56	4153	156	2.29515E-02	4.70981E-02	...
11	57	4156	153	1.31175E-05	2.29783E-05	...
12	58	4158	151	8.40772E-04	2.24284E-03	...
13	59	4163	146	1.36336E-02	3.16144E-02	...
14	60	4164	145	4.26386E-02	6.70619E-02	...
15	61	4164	145	1.44892E-02	3.91035E-02	...
16	62	4165	144	2.10604E-05	4.82161E-05	...
17	63	4165	144	2.80598E-02	6.07946E-02	...
18	64	4166	143	9.43815E-03	2.39091E-02	...
19	65	4167	142	2.16936E-02	3.52403E-02	...
20	66	4168	141	2.11722E-02	4.71334E-02	...
21	67	4169	140	7.76012E-03	1.56075E-02	...
22	68	4169	140	1.46025E-02	3.11909E-02	...
23	69	4169	140	2.03498E-02	4.41864E-02	...
24	70	4170	139	1.10120E-05	2.11062E-05	...
25	71	4171	138	1.41216E-02	2.81133E-02	...
26	72	4174	135	3.01293E-04	4.93107E-04	...
27	73	4176	133	2.74499E-03	7.01193E-03	...
28	74	4183	126	7.53507E-04	1.23993E-03	...
29	75	4187	122	3.61916E-04	6.73170E-04	...
30	76	4191	118	4.47955E-04	8.35651E-04	...
31	77	4193	116	2.36368E-04	5.74515E-04	...
32	78	4196	113	5.76322E-04	9.89702E-04	...
33	79	4200	109	9.19763E-04	1.68332E-03	...
34	80	4203	106	1.28180E-03	2.25546E-03	...
35	81	4205	104	1.23864E-04	2.02920E-04	...
36	82	4206	103	1.43708E-03	3.60947E-03	...
37	83	4214	95	2.59229E-03	4.18266E-03	...
38	84	4217	92	1.95693E-03	3.53563E-03	...
39	85	4220	89	1.76516E-03	2.93510E-03	...
40	86	4222	87	8.34672E-04	1.30886E-03	...
41	87	4223	86	8.62864E-04	1.40116E-03	...
42	88	4224	85	7.91413E-04	1.32771E-03	...
43	89	4225	84	4.45724E-04	7.65716E-04	...
44	90	4226	83	4.68671E-04	8.33725E-04	...
45	91	4171	138	1.72438E-03	8.44953E-03	...
46	101	1	4308	1.33601E+02	1.31920E+02	...

Appendix B

Nuclear density calculation

The basic equation for nuclear density is

$$N_i = \frac{\rho w_{f,i} N_A}{A_{w,i}} \tag{B.1}$$

where N_i (at/bcm) is nuclear density of i-th nuclide/element in volume $V = 1.0E + 24\text{cm}^3$, ρ (g/cm^3) is mass density of the material, $w_{f,i}$ (-) is weight fraction of i-th nuclide/element in the material, $N_A = 0.602214199$ (at/mol*cm^2/b] Avogadro number and $A_{w,i}$ (g/mol) atomic weight of i-th nuclide/element.

In the case that atomic fraction $A_{f,i}$ (-) of i-th nuclide/element in the material is known, nuclear density of i-th nuclide is calculated by

$$N_i = A_{f,i} N \tag{B.2}$$

where N_i is nuclear density of i-th nuclide/element in the material with total nuclear density N.

Atomic weight A_w of the material consisting of nuclides/elements with atomic fractions $A_{f,j}$ and atomic masses $A_{w,j}$ is given by

$$A_w = \sum_j A_{f,j} A_{w,j} \tag{B.3}$$

Atomic weight A_w of the material consisting of nuclides/elements with weight fractions $w_{f,j}$ and atomic masses $A_{w,j}$ is given by

$$\frac{1}{A_w} = \sum_j \frac{w_{f,j}}{A_{w,j}} \tag{B.4}$$

Combination the relations (B.1), (B.2) and (B.3), it is possible to calculate nuclear density of i-th nuclide/element in the material consisting of nuclides/elements j

$$N_i = A_{f,i} \frac{\rho N_A}{\sum_j \frac{A_{f,j}}{A_{w,j}}} \tag{B.5}$$

If the weight fraction of j-th nuclide/element $w_{f,j}$ is known, atomic fraction $A_{f,j}$ for previous relationship could be found by

$$A_{f,j} = \frac{\frac{w_{f,j}}{A_{w,j}}}{\sum_k \frac{w_{f,k}}{A_{w,k}}} = \frac{w_{f,j}}{A_{w,j}} A_w \tag{B.6}$$

Appendix C

Output data visualization

Output data was visualized for sample input 03 – VVER-1000 fuel depletion. Graphical representation of the multiplication factor progress during Monte Carlo simulation in the transport solver is depicted in Figure C.1. Graphical representation of the neutron flux is depicted in Figure C.2. Graphical representation of the fuel inventory data (region 1) is depicted in Figure C.3. Graphical representation of the estimator output (multiplication factor durign fuel depletion) is depicted in Figure C.4.

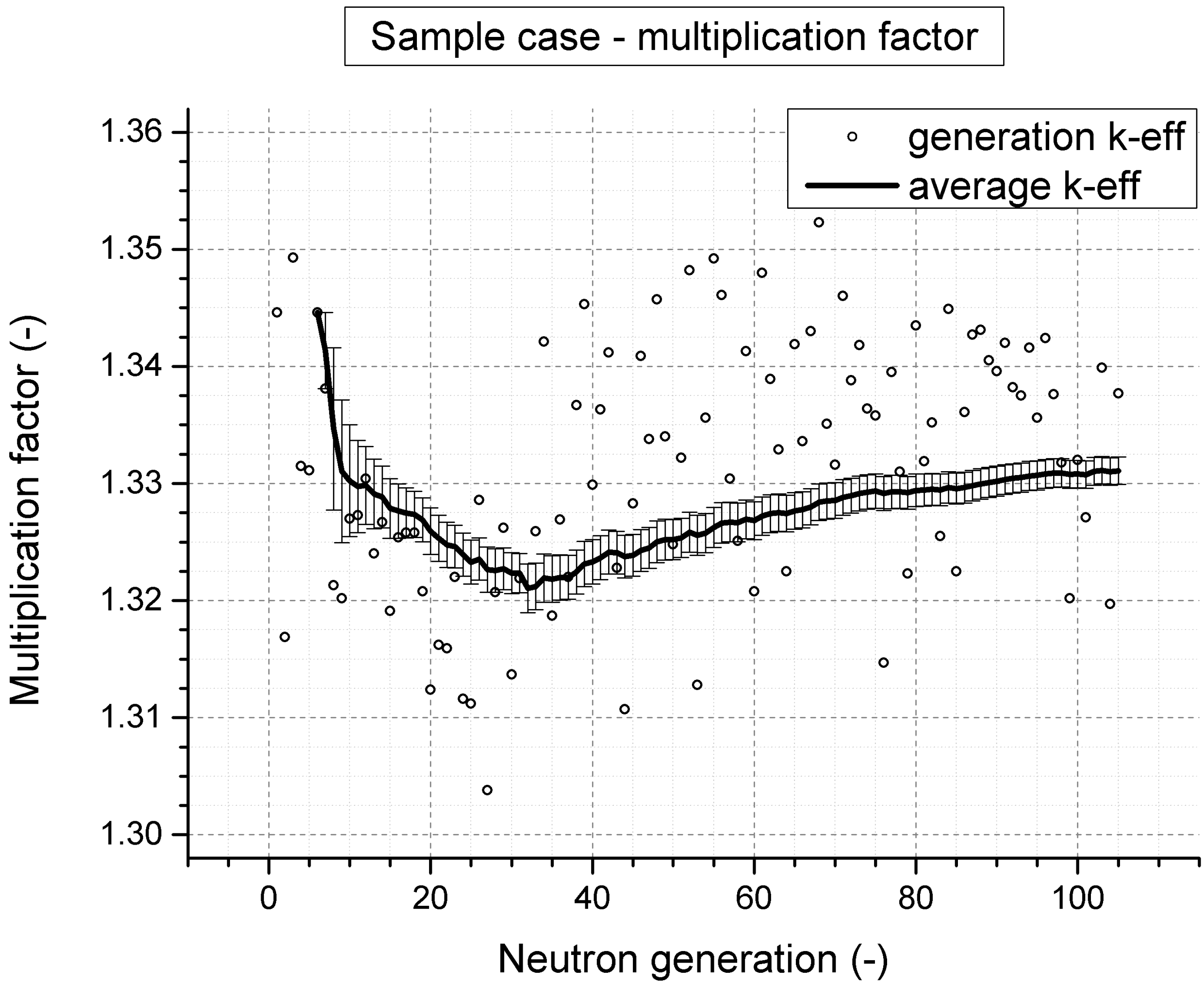

Figure C.1: $U_W B_1$ transport solver output - multiplication factor.

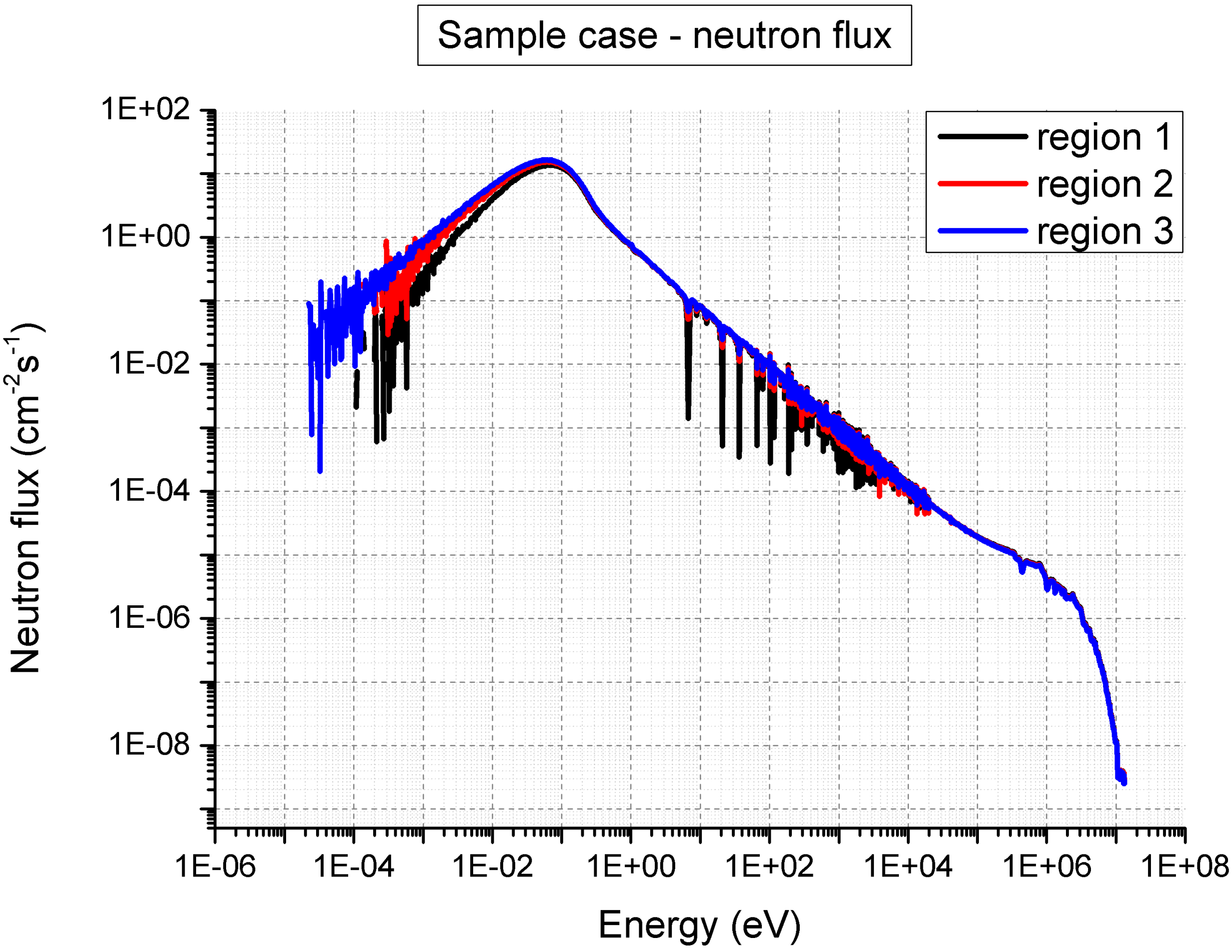

Figure C.2: $U_W B_1$ transport solver output - neutron flux.

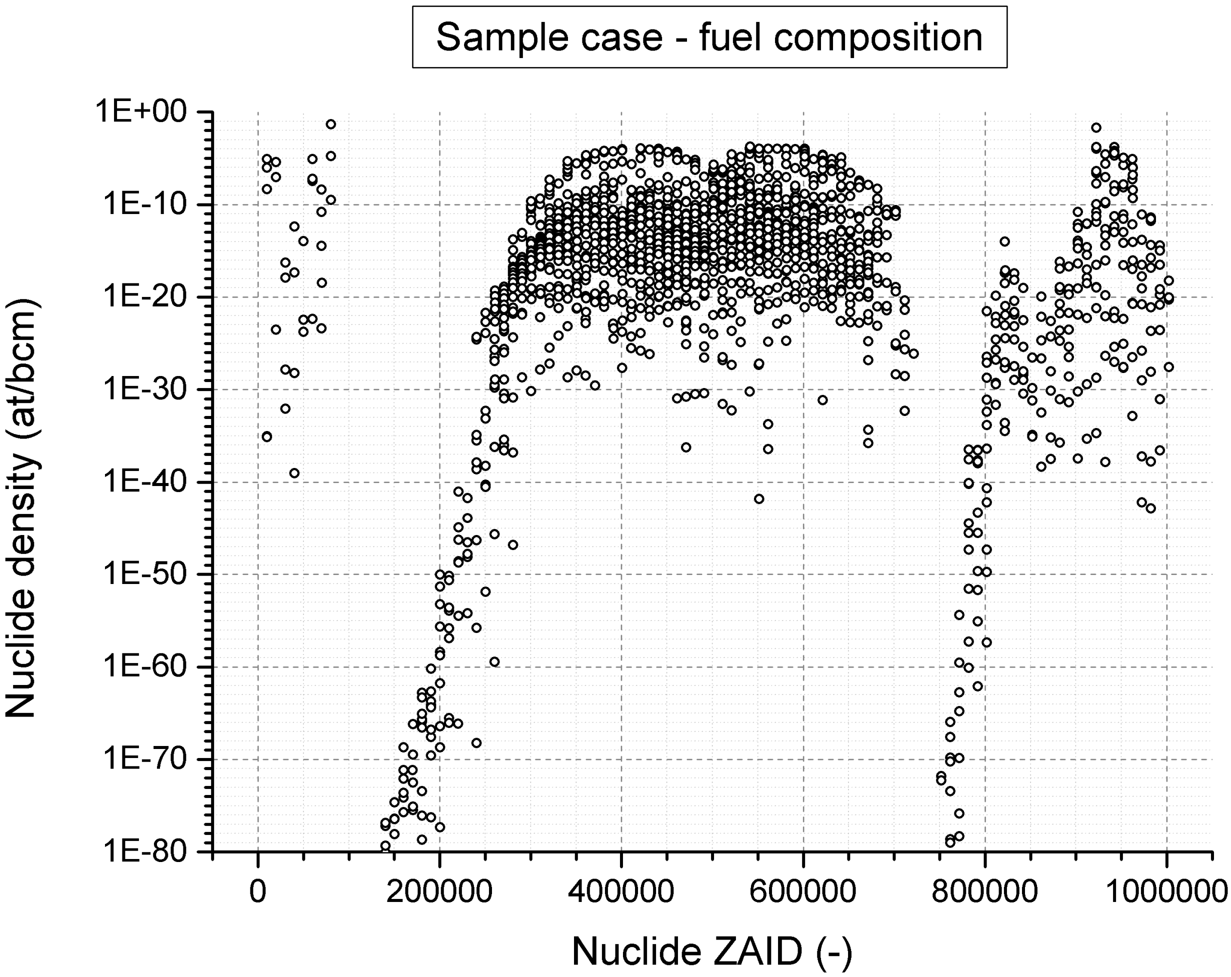

Figure C.3: $U_W B_1$ burnup solver output - fuel composition.

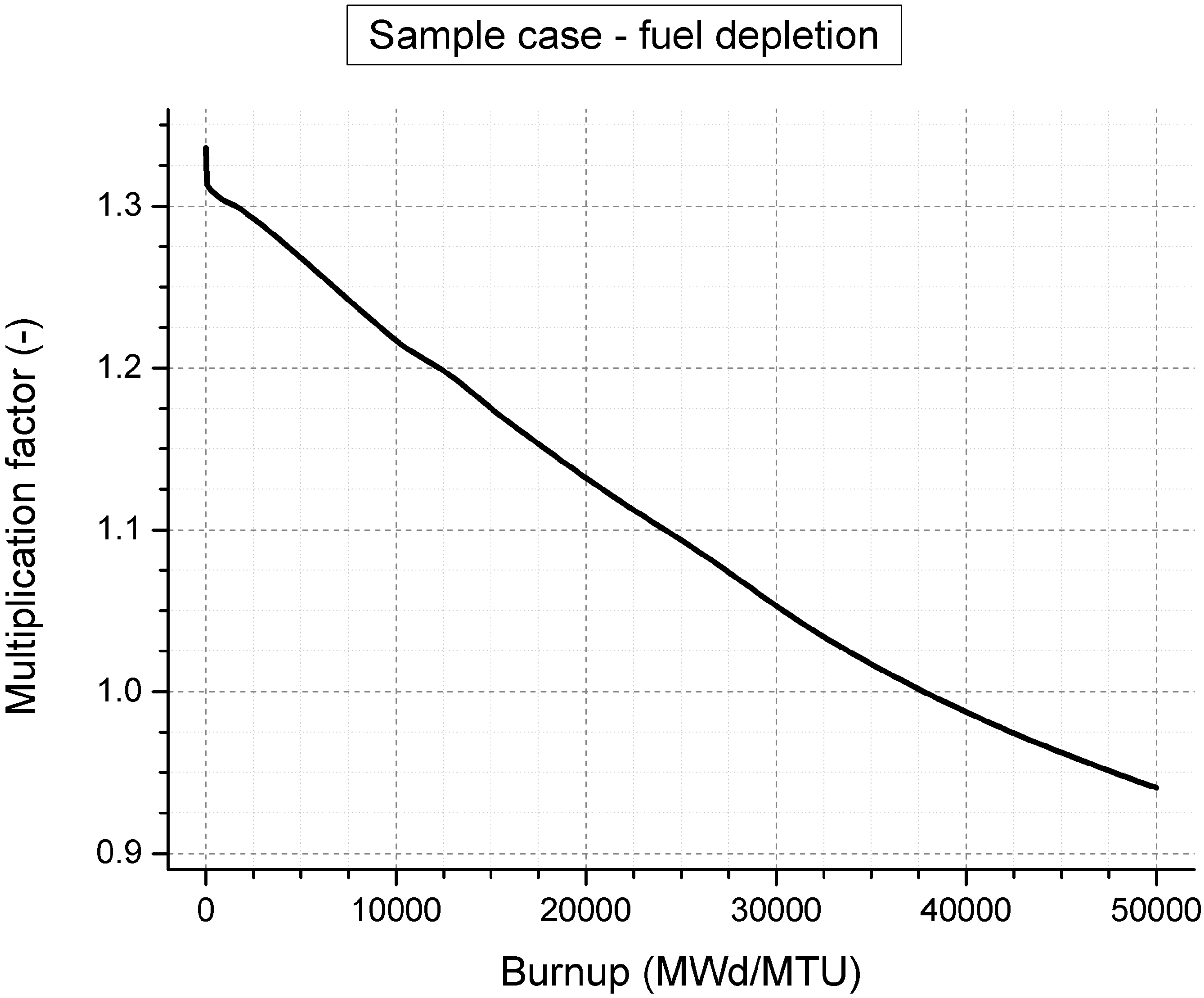

Figure C.4: $U_W B_1$ estimator output - multiplication factor.