JADE

Release v1.2.0

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JADE USER GUIDE:

Version: v1.2.0

JADE is a new tool for nuclear libraries V&V. Brought to you by NIER, University of Bologna (UNIBO) and Fusion For Energy (F4E).

JADE is an open-source software licensed under the *GNU GPLv3 License*. When using JADE for scientific publications you are kindly encouraged to cite the following papers:

- Davide Laghi et al, 2020, "JADE, a new software tool for nuclear fusion data libraries verification & validation", Fusion Engineering and Design, **161** 112075, doi: https://doi.org/10.1016/j.fusengdes.2020.112075.

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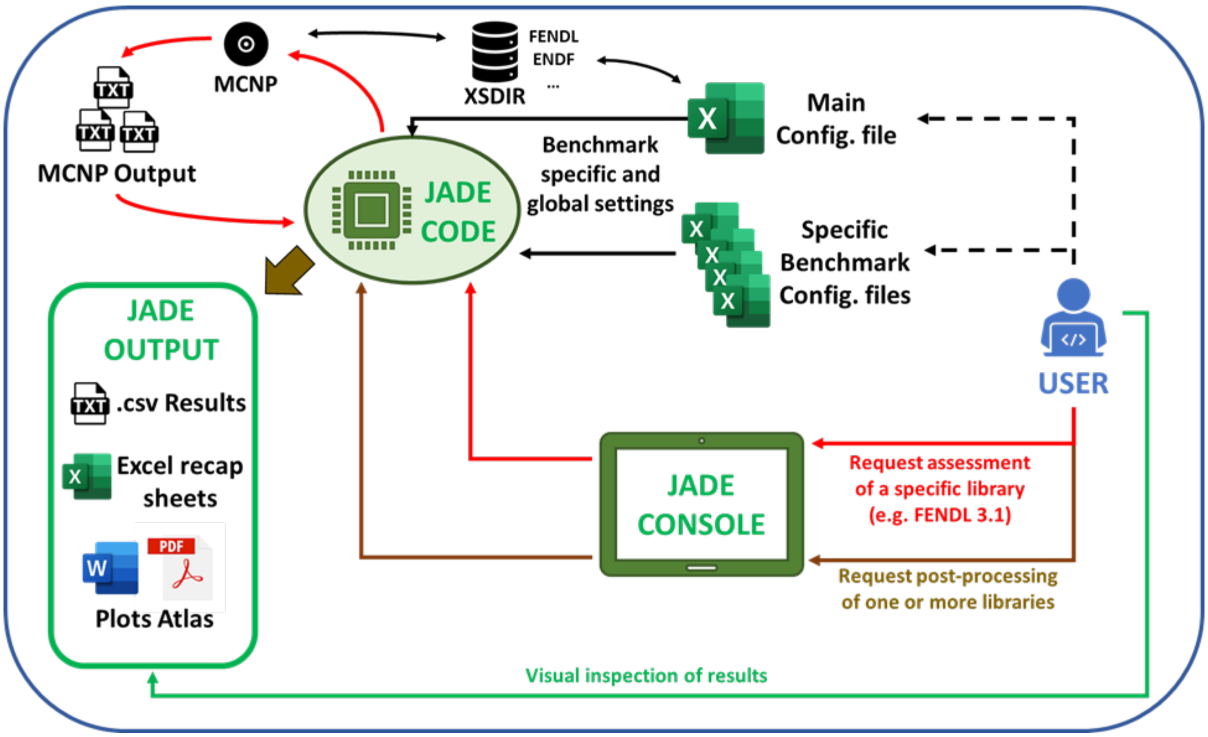
For additional information on future developments please check the issues list on the GitHub repository [link].

JADE IN A NUTSHELL



JADE is a new tool for nuclear libraries V&V. Brought to you by NIER, University of Bologna (UNIBO) and Fusion For Energy (F4E). JADE is an open source, Python 3 based software able to:

- automatically build a series of MCNP input file using different nuclear data libraries;
- automatically run simulations on such inputs;
- automatically parse and post-process all the generated MCNP outputs.

The benchmarks implemented by default are divided between computational and experimental benchmarks. The post-processing output includes:

- raw data in .csv files containing the entire tallied output from the simulations;
- formatted Excel recap files;
- Word and PDF atlas collecting the plots generated during the post-processing.

Additional JADE features are:

- the possibility to implement user-defined benchmarks;

- operate on the material card of an MCNP input (e.g. create material mixtures or translate it to a different nuclear data library);
- print a recap of the material composition of an MCNP input.

When using JADE for scientific publications you are kindly encouraged to cite the following papers:

- Davide Laghi et al, 2020, "JADE, a new software tool for nuclear fusion data libraries verification & validation", Fusion Engineering and Design, **161** 112075, doi: https://doi.org/10.1016/j.fusengdes.2020.112075.

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CHAPTER

TWO

INSTALLATION

The procedure to install JADE is the following:

1. Install/update Anaconda, you can update all packages in your current environment using:

   ```
   conda update --all
   ```

   However, if bugs or problems are encountered, a fresh Anaconda re-installation may solve the issues.

2. Install additional packages. It may be necessary to activate the conda-forge channel. It can be done typing in an anaconda prompt shell:

   ```
   conda config --add channels conda-forge
   ```

   then use:

   ```
   conda install python-docx
   ```

   The second package that is needed is numjuggler for parsing of MCNP inputs. Unfortunately, this is not available for conda installation and pip should be used instead:

   ```
   pip install numjuggler
   ```

3. Extract the zip into a folder of choice (from now on <JADE_root>);

4. Rename the folder containing the Python scripts as 'Code' (<JADE_root>\Code);

5. Open the global configuration file: <JADE_root>\Code\Configuration\Config.xlsx; here you need to properly set the environment variables specified in the 'MAIN Config.' sheet (i.e. xsdir Path, and multithread options);

6. Open an anaconda prompt shell and change directory to <JADE_root>\Code. Then type:

   ```
   python main.py
   ```

7. On the first usage the rest of the folders architecture is initialized.

Important: A limitator has been inserted in the code in order to test it before using JADE for production (this will be eliminated when a proper function testing the installation will be produced). To remove it, open <JADE_root>\Code\testrun.py and comment out line 239 and 298 while de-commenting line 238 and 297.

CHAPTER THREE

FOLDER STRUCTURE

The following is a scheme of the JADE folder structure:

```
<JADE_root>
    |--------- Benchmark inputs
    |
    |--------- Code
    |            |----- Default Settings
    |            |----- docs
    |            |----- Installation Files
    |            |----- Templates
    |
    |--------- Configuration
    |                |----------- Benchmarks Configuration
    |                |----------- Config.xlsx
    |
    |--------- Experimental results
    |                    |------------ <Benchmark name 1>
    |                    |------------ [...]
    |
    |--------- [Quality]
    |
    |--------- Tests
    |            |--------- MCNP simulations
    |            |                 |----------- <Lib suffix 1>
    |            |                 |                  |---------- <Benchmark name 1>
    |            |                 |                  |---------- [...]
    |            |                 |----------- [...]
    |            |
    |            |--------- Post-Processing
    |                             |------------ Comparisons
    |                             |                  |-------- <lib 1>_Vs_<lib 2>_Vs..
↪..
    |                             |                  |                  |-------------
↪----- <Benchmark name 1>
    |                             |                  |                  |            ␣
↪                |----------- Atlas
    |                             |                  |                  |            ␣
↪                |----------- Excel
    |                             |                  |                  |
    |                             |                  |                  |-------------
↪----- [...]
    |                             |                  |
    |                             |                  |------- [...]
    |                             |
```

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```
    |                              |------------ Single Libraries
    |                                                   |----------- <Lib suffix 1>
    |                                                   |                  |----------
↪<Benchmark name 1>
    |                                                   |                  |          ␣
↪        |----------- Atlas
    |                                                   |                  |          ␣
↪        |----------- Excel
    |                                                   |                  |          ␣
↪        |----------- Raw Data
    |                                                   |                  |
    |                                                   |                  |----------␣
↪[...]
    |                                                   |
    |                                                   |----------- [...]
    |
    |-------- Utilities
```

<JADE_root> is the root folder chosen by the user. As described in *Installation* section, the JADE GitHub repo should be renamed and placed inside the root directory as <JADE_root>\Code.

All folders parallel to the <JADE_root>\Code will be created after the first JADE run.

Hereafter, a general overview of the different JADE tree branches is presented.

3.1 Benchmark inputs

<JADE_root>\Benchmark inputs contains all the inputs of the default benchmarks avaialble in the JADE suite. This is the folder where eventual user defined benchmark inputs should be positioned. In case of benchmarks that are composed by more than one run, all the inputs are reunited in a sub-folder (e.g. <JADE_root>\Benchmark inputs\Oktavian.

3.2 Code

<JADE_root>\Code contains the JADE GitHub repo itself. All the source code is contained here toghether with the following subfolders:

Default Settings Contains all JADE default settings. On the first JADE instance these are copied to the <JADE_root>\Configuration folder. They can be restored by a dedicated utility function available from the main menu.

docs Contains all files related to this documentation. Here, local version of the documentations can be found.

Installation Files Contains files to be used during the first JADE run. They have not any appeal to the general user.

Templates Contains all the Microsoft Office and Word templates to be used during post-processing. In case of user-defined benchmarks that are based on specific templates, these need to be added here.

3.3 Configuration

`<JADE_root>\Configuration` stores the main JADE configuration file `Config.xlsx` and all benchmark-specific configuration files that are stored in `<JADE_root>\Code\Benchmarks Configuration`.

See also:

Configuration for additional description of the configuration files.

3.4 Experimental results

`<JADE_root>\Experimental results` stores all the experimental results needed for the post-processing of experimental benchmarks. In case of benchmarks that are composed by more than one run, all the inputs are reunited in a sub-folder (e.g. `<JADE_root>\Experimental results\Oktavian`.

3.5 Quality

NOT IMPLEMENTED

3.6 Tests

`<JADE_root>\Tests` reunites all the outputs of the benchmarks assessments.

MCNP simulations contains the results of the transport simulations.

Post-Processing contains all the results coming from the post-processing of results. These are divided between *Comparisons* and *Single Libraries*.

3.7 Utilities

`<JADE_root>\Tests` is where all outputs coming from the *Utilities* are reunited. Each utility generates a dedicated sub-folder when is used for the first time. Upon installation, the only sub-folder is `<JADE_root>\Tests\Log Files` that contains all log files produced by each JADE session.

CHAPTER

FOUR

CONFIGURATION

All configuration files are included in the `<JADE_root>\Configuration` directory. In principle, **the general user should only operate on the** *Main Configuration* **file**, while all other configuration files simply guarantee an additional level of personalization for the user.

Note: In case of user-defined benchmarks suitable *Benchmark run configuration* and *Benchmark post-processing configuration* files need to be produced.

4.1 Main Configuration

The most important configuration file is `<JADE_root>\Configuration\Config.xlsx`. This is **the only configuration file that the user must modify** before operating with JADE. Herafter, a description of the different sheets included in the file is given.

4.1.1 MAIN Config.

MAIN CONFIGURATION VARIABLES	
xsdir Path	C:\Users\d.laghi\Documents\MCNP\MCNP_DATA\xsdir_mcnp6.2
multithread	True
CPU	4

This sheet contains the JADE *ambient variables*:

xsdir Path Absolute path to the xsdir file that has been set to be used during MCNP simulations.

multithread Under Windows operative system, MCNP allows to run on multithread using the `tasks` keyword. Setting this variable to `True` enables this capability.

CPU When **multithread** is set to `True`, **CPU** sets the argument that will be passed to `tasks` during MCNP runs.

4.1.2 Computational benchmarks

Computational benchmark additional options							
Default Benchmarks							
Description	**File Name**	**OnlyInput**	**Run**	**Post-Processing**	**NPS cut-off**	**CTME cut-off**	**Relative Error cut-off**
Sphere Leakage Test	Sphere.i	false	false	false	1.00E+04		
ITER 1D (by M. Sawan)	ITER_1D.i	false	false	false	1.00E+04		
Helium Cooled Pebble Bed Test Blanket Module (1D)	HCPB_TBM_1D.i	false	false	false	1.00E+03		
Water Cooled Lithium Lead Test Blanket Module (1D)	WCLL_TBM_1D.i	false	false	false	1.00E+03		
C-Model R181031 rev190715	C_Model.i	true	false	true	1.00E+03		

This table collects allows to personalize which *computational benchmarks* should be included in the JADE assessment. Each row controls a different benchmark, where the following options (columns) are available:

Description this is the extended name of the benchmark, this name will appear in specific outputs of the post-processing.

File Name name of the reference MCNP input file. These need to be placed in `<JADE root>\Benchmarks inputs`.

OnlyInput when this field is set to `True` the benchmark input is only generated but not run. This can be useful when the user wants to run the benchmark on a different hardware with respect to the one where JADE is being used.

See also:

External Run of a benchmark

Run the benchmark will be run during an assessment only if this field is set to `True`. This allows to customize the selection of benchmarks to be run during an assessment or avoid to re-run benchmarks that were already simulated in the past.

Post-Processing this field works exactly as the `Run` one but for the post-processing operations.

The last three options available for each benchmark control the MCNP STOP card parameters that help regulating the simulation lenght:

NPS cut-off this is equivalent to the `NPS` entry in the MCNP STOP card. It sets a maximum amount of histories to be simulated. Only integers are allowed.

CTME cut-off this is equivalent to the `CTME` entry in the MCNP STOP card. It sets a maximum computer time after which the simulation will be interrupted. Only integers are allowed.

Relative Error cut-off this is equivalent to the `F` entry in the MCNP STOP card. The sintax of this entry is:

F<*k*>-<*e*> (example: F16-0.0005)

This stops the calculation when the tally fluctuation chart of tally *k* has reached a relative error lower than *e*.

Note: All three STOP parameters can be simultaneously defined during a simulation. The first cut-off criteria reached will be the one triggering the end of the calculation.

4.1.3 Experimental benchmarks

Computational benchmark additional options							
Default Benchmarks							
Description	File Name	OnlyInput	Run	Post-Processing	NPS cut-off	CTME cut-off	Relative Error cut-off
Oktavian Experiment	Oktavian	false	true	true	1.00E+06		

The structure of the sheet is exactly the same as the *Computational benchmarks* one. Nevertheless, in this table are indicated the settings for the experimental benchmarks.

4.1.4 Libraries

Suffix	Name	Default
21c	FENDL 2.1c	
30c	FENDL 3.0	
31c	FENDL 3.1d	
32c	FENDL 3.2 beta	
70c	ENDF VII	
00c	ENDF VIII	yes

This table simply consists of a glossary where the user can associate more explicit names to the nuclear data libraries suffixes available in the xsdir file. This allows for a clearer post-processing output.

4.2 Benchmark run configuration

TBD

These are used only for *Sphere Leakage* and cannot be generalized.

4.3 Benchmark post-processing configuration

It is possible to control (to some extent) the post-processing of each benchmark via its specific configuration file. These files are located in the `<JADE_root>\Configuration\Benchmarks Configuration` folder and their name must be identical to the one used in the `File Name` field in the main configuration file (using the .xlsx extension instead of the .i). These files are available only for computational benchmarks, since the high degree of customization needed for an experimental benchmark makes quite difficult to standardize them. While computational benchmarks can be added to the JADE suite without the need for additional coding, this is not true also for experimental one.

The files contain two main sheets, that respectively regulate the Excel and the Word/PDF post-processing output.

4.3.1 Excel

Tally	x	x name	y	y name	cut Y
4	Energy	Energy [MeV]	Cells	Cell	20
14	Energy	Energy [MeV]	Cells	Cell	20
6	Cells	Cell	tally	Value	
16	Cells	Cell	tally	Value	
26	Cells	Cell	tally	Value	
24	Cells	Cell	tally	Value	
34	Cells	Cell	tally	Value	
44	Cells	Cell	tally	Value	
54	Cells	Cell	tally	Value	
64	Cells	Cell	tally	Value	
74	Cells	Cell	tally	Value	
84	Cells	Cell	tally	Value	
94	Cells	Cell	tally	Value	
104	Cells	Cell	tally	Value	
114	Cells	Cell	tally	Value	
124	Cells	Cell	tally	Value	
134	Cells	Cell	tally	Value	
144	Cells	Cell	tally	Value	
154	Cells	Cell	tally	Value	
164	Cells	Cell	tally	Value	
174	Energy	Energy [MeV]	Cells	Cell	20
204	Cells	Cell	tally	Value	
214	Cells	Cell	tally	Value	

This sheet regulates the Excel output derived from the benchmark. It consists of a table where each row regulates the output of a single tally present in the MCNP input.

Hereinafter a description of the available fields is reported.

Tally tally number according to MCNP input file.

x, y select the binnings to be used for the presentation of the excel results of the specific tally. Clearly, the binning should have been coherently defined in the MCNP input too. MCNP allows different types of tally binning, they can be accessed using the tags reported in the table below.

Table 1: Allowed binnings

Admissible **x** and **y**
Energy
Cells
time
tally
Dir
User
Segments
Multiplier
Cosine
Cor A
Cor B
Cor C

As a result of the selcted **x** and **y** option, the results of the post-processed tally will be display in a matrix format. In case only a single binning is defined in the MCNP input, the `tally` keyword should be used to signal to JADE to just to print the results in a column format.

Important: The main direction of an Excel file is considered to be the vertical one, which is the preferred scrolling direction. For this reason, the **x** direction is associated with the vertical direction in an Excel file and the **y** with the horizontal one.

Warning: No more than two binnings should be defined for a single MCNP tally due to the limitation of having to represent 2-D output. JADE may be able to to handle tallies with more than 2 binnings if some of them are constant values.

Tip: If a 1D FMESH is defined in the MCNP input, JADE will automatically transform it to a "binned" tally and handle it as any other tally using the `Cor A`, `Cor B` or `Cor C` field.

x name, y name These will be the names associated to the **x** and **y** axis printed in the excel file.

cut Y The idea behind JADE is to produce outputs that are easy to investigate simply by scrolling and concentrate on the main results highlighted through colors. Having a high number of bins both in the x and y axis may cause a problem in this sense, forcing the user to scroll on both axis. For this reason, a maximum number of columns can be set to solve this issue. This will cause the tally results not to be printed as a unique matrix but as sequential blocks each with a number of columns equal to **cut Y**.

4.3.2 Atlas

Tally	Quantity	Unit	Binned graph	Ratio graph
4	Neutron Flux	#/cm^2	True	False
14	Photon Flux	#/cm^2	True	False
6	Total Nuclear Heating	W/g	False	True
16	Neutron Heating	W/g	False	True
26	Photon Heating	W/g	False	True
24	DPA in Fe	dpa/FPY	False	False
34	Helium production in SS316	appm/FPY	False	False
44	Hydrogen production in SS316	appm/FPY	False	False
54	Tritium production in SS316	appm/FPY	False	False
64	DPA in Cu	dpa/FPY	False	False
74			False	False
84			False	False
94			False	False
104			False	False
114			False	False
124			False	False
134			False	False
144			False	False
154			False	False
164			False	False
174			False	False
204	Neutron Flux	#/cm^2	False	True
214	Photon Flux	#/cm^2	False	True

This sheet regulates the Atlas output (Word/PDF) derived from the benchmark. It consists of a table where each row regulates the output of a single tally present in the MCNP input. Hereinafter a description of the available fields is reported.

Tally tally number according to MCNP input file.

Quantity Physical quantity that will be plotted on the y-axis of the plot. For the x-axis the one specified in the Excel sheet under **x** will be considered. The quantity selected for plotting will always be the tallied quantity.

> **Important:** when two binnings are specified in the Excel sheet, a different plot for each of the **y** bins will be produced. For example, let's consider a neutron flux tally binned both in energy (selected as **x**) and cells (selected as **y**). Then, a plot showing the neutron flux as a function of energy will be produced for each cell indicated in the tally.

Unit Unit associated to the Quantity.

<Graph type> Different columns can be added where it can be specified if a plot in the style indicated by the column name should be generated (`true`) or not (`false`). The available plot styles are *Binned graph*, *Ratio Graph*, *Experimental points* and *Grouped bars*.

See also:

Plots Atlas for an additional description of the available plot styles.

CHAPTER

FIVE

USAGE

Once JADE is correctly configured (for additional details see *Configuration*), the application can be started from the 'Code' folder with:

`python main.py`

The main menu is loaded at this point:

```
***********************************************
            Welcome to JADE v1.1.0
     A nuclear libraries V&V Test Suite
         Release date: 25/05/2021

               MAIN MENU

       Powered by NIER, UNIBO, F4E
***********************************************
MAIN FUNCTIONS

* Open Quality check menu                (qual)
* Open Computational Benchmark menu      (comp)
* Open Experimental Benchmark menu        (exp)
* Open Post-Processing menu              (post)
-----------------------------------------------
UTILITIES

* Print available libraries          (printlib)
* Translate an MCNP input               (trans)
* Print materials info               (printmat)
* Generate material                  (generate)
* Switch fractions                     (switch)
-----------------------------------------------
* Test installation                      (test)

* Exit                                   (exit)
```

This menu allows users to interact with the tool directly from the command prompt via pre-defined commands. The following main option are available typing from the main menu:

- `qual` not currently supported;
- `comp` opens the *Computational Benchmark menu*;

- `exp` opens the *Experimental Benchmark menu*;
- `post` opens the *Post-processing menu*;
- `exit` exit the application.

Additionaly to these main options, a series of "utilities" can be also accessed from the main menu. These are a collection of side-tools initially developed for JADE that nevertheless can be useful also as stand-alone tools. A detailed description of these functionalities can be found in *Utilities*.

5.1 Quality check menu

Not implemented.

5.2 Computational Benchmark menu

```
***********************************************
             Welcome to JADE v1.1.0
     A nuclear libraries V&V Test Suite
         Release date: 25/05/2021

         COMPUTATIONAL BENCHMARK MENU

       Powered by NIER, UNIBO, F4E
***********************************************

* Print available libraries          (printlib)
* Assess library                       (assess)
* Continue assessment                (continue)
* Back to main menu                      (back)
* Exit                                   (exit)

Enter action:
```

The following options are available in the computational benchmark menu:

- `printlib` print to video all the available nuclear data libraries in the xsdir file selected during JADE configuration;
- `assess` start the assessment of a selected library on the computational benchmarks. The library is specified directly from the console when the selection is prompted to video. The library must be contained in the xsdir file (available libraries can be explored using `printlib`);
- `continue` continue a previously interrupted assessment for a selected library. **Currently, this option is implemented only for the Sphere Leakage benchmark.**
- `back` go back to the main menu;
- `exit` exit the application.

The selection of the libraries is done indicating their correspondent suffix specified in the xsdir file (e.g. `31c`).

Note: Whenever an assessment is requested, all the benchmarks selected in the main configuration file will be considered. In case the requested library was already assesed on one or more of the active benchmarks, the user will be asked for permission before overriding the results.

See also:

Configuration for additional details on the benchmark selection.

5.3 Experimental Benchmark menu

```
**********************************************
             Welcome to JADE v1.1.0
     A nuclear libraries V&V Test Suite
         Release date: 25/05/2021

         EXPERIMENTAL BENCHMARK MENU

       Powered by NIER, UNIBO, F4E
**********************************************

* Print available libraries          (printlib)
* Assess library                       (assess)
* Continue assessment                (continue)
* Back to main menu                      (back)
* Exit                                   (exit)

Enter action:
```

The following options are available in the experimental benchmark menu:

- `printlib` print to video all the available nuclear data libraries in the xsdir file selected during JADE configuration;
- `assess` start the assessment of a selected library on the experimental benchmarks. The library is specified directly from the console when the selection is prompted to video. The library must be contained in the xsdir file (available libraries can be explored using `printlib`);
- `continue` **[not implemented]**
- `back` go back to the main menu;
- `exit` exit the application.

The selection of the libraries is done indicating their correspondent suffix specified in the xsdir file (e.g. `31c`).

Note: Whenever an assessment is requested, all the benchmarks selected in the main configuration file will be considered. In case the requested library was already assesed on one or more of the active benchmarks, the user will be asked for permission before overriding the results.

See also:

Configuration for additional details on the benchmark selection.

5.4 Post-processing menu

```
***********************************************
             Welcome to JADE v1.1.0
     A nuclear libraries V&V Test Suite
         Release date: 25/05/2021

         POST PROCESSING MENU

       Powered by NIER, UNIBO, F4E
***********************************************

* Print tested libraries             (printlib)
* Post-Process library                     (pp)
* Compare libraries                   (compare)
* Compare Vs Experiments              (compexp)
* Back to main menu                      (back)
* Exit                                   (exit)

Enter action:
```

The following options are available in the post-processing menu:

- `printlib` print all libraries that were tested and that are available for post-processing;
- `pp` post-process a single library;
- `compare` compare different libraries results on computational benchmarks;
- `compexp` compare different libraries results on experimental benchmarks;
- `back` go back to the main menu;
- `exit` exit the application.

For the `pp`, `compare` and `compexp` the selection of the libraries will be directly prompt to video. The selection of the libraries is done indicating their correspondent suffix specified in the xsdir file (e.g. `31c`). When comparing more than one library, the suffixes should be separated by a '-' (e.g. `31c-32c`). The first library that is indicated is always considered as the *reference library* for the post-processing. There may be a limitation on the number of libraries that can be compared at once depending on the post-processing settings.

Only one library at the time can be post-processed with the `pp` option. Nevertheless, when a comparison is requested that includes libraries that were not singularly post-processed, an automatic `pp` operation is conducted on them.

> **Warning:** Please note that `printlib` will simply show all libraries for which at least one benchmark has been run.

Warning: Please note that part of the single post-processing of the libraries is used in the comparisons. Also, JADE does not perform any checks on the consistency between the two. This responsability is left to the user. The following is an example of incorrect usage that can lead to erroneous results:

1. a first assessment is run;
2. single post-processing is completed;
3. some configuration settings are changed and the assessment is re-run;
4. a comparison is requested.

In this case, JADE cannot know that the first single post-processing was done on a different benchmark run wiith respect to the requested comparison. As a result, the outputs coming from different assessments will be mixed up.

Note: Whenever a post-processing is requested, all the benchmarks selected in the main configuration file will be considered. In case one or more of the requested libraries were already post-processed on one or more of the active benchmarks, the user will be asked for permission before overriding the post-processing results.

See also:

Configuration for additional details on the benchmark selection.

CHAPTER

SIX

DEFAULT BENCHMARKS

6.1 Computational Benchmarks

6.1.1 Sphere Leakage

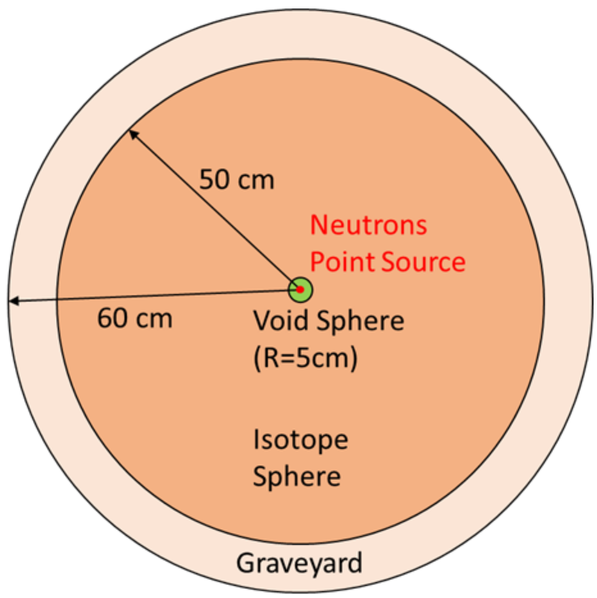


Fig. 1: Sphere Leakage geometrical model

The Sphere Leakage benchmark is arguably the most important benchmark included in the JADE suite. Indeed, it allows to test individually each single isotope of the nuclear data library under assessment plus some typically used material in the ITER project namely:

- Water;
- Ordinary Concrete;
- Boron Carbide;
- SS316L(N)-IG;
- Natural Silicon;
- Polyethylene (non-borated).

The Sphere Lekage geometry consists of actually three concentric spheres. The inner one is void and has a radius of 5 cm. Here is located the uniform probability 0-14 MeV neutron point source. The second sphere has a radius of 50 cm and it is composed entirely by a single isotope or a typical ITER material. Finally, the last 60 cm radius sphere acts as a graveyard where particles importance is set to zero and the boundary of the model is defined.

TBD: Describe tallies

See also:

Related papers and contributions:

- D. Laghi, M. Fabbri, L. Isolan, R. Pampin, M. Sumini, A. Portone and A. Trkov, 2020, "JADE, a new software tool for nuclear fusion data libraries verification & validation", *Fusion Engineering and Design*, **161** 112075

6.1.2 ITER 1D

See also:

Related papers and contributions:

- M. Sawan, 1994, "FENDL Neutronics Benchmark: Specifications for the calculational and shielding benchmark", (Vienna: INDC(NDS)-316)

6.1.3 Test Blanket Module

HCPB TBM in ITER 1D

WCLL TBM in ITER 1D

C-Model

This benchmark input cannot be distributed directly with JADE. The user must request to obtain it from ITER organization and insert it in the `<JADE root>\Benchmarks inputs` directory renaming it 'C_Model.i'.

Important: The NPS card needs to be removed from the input. It is recommended to also delete total bins from standard tallies for a clearer post-processing results.

See also:

Related papers and contributions:

- D. Leichtle, B. Colling, M. Fabbri, R. Juarez, M. Loughlin, R. Pampin, E. Polunovskiy, A. Serikov, A. Turner and L. Bertalot, 2018, "The ITER tokamak neutronics reference model C-Model", *Fusion Engineering and Design*, **136** 742-746

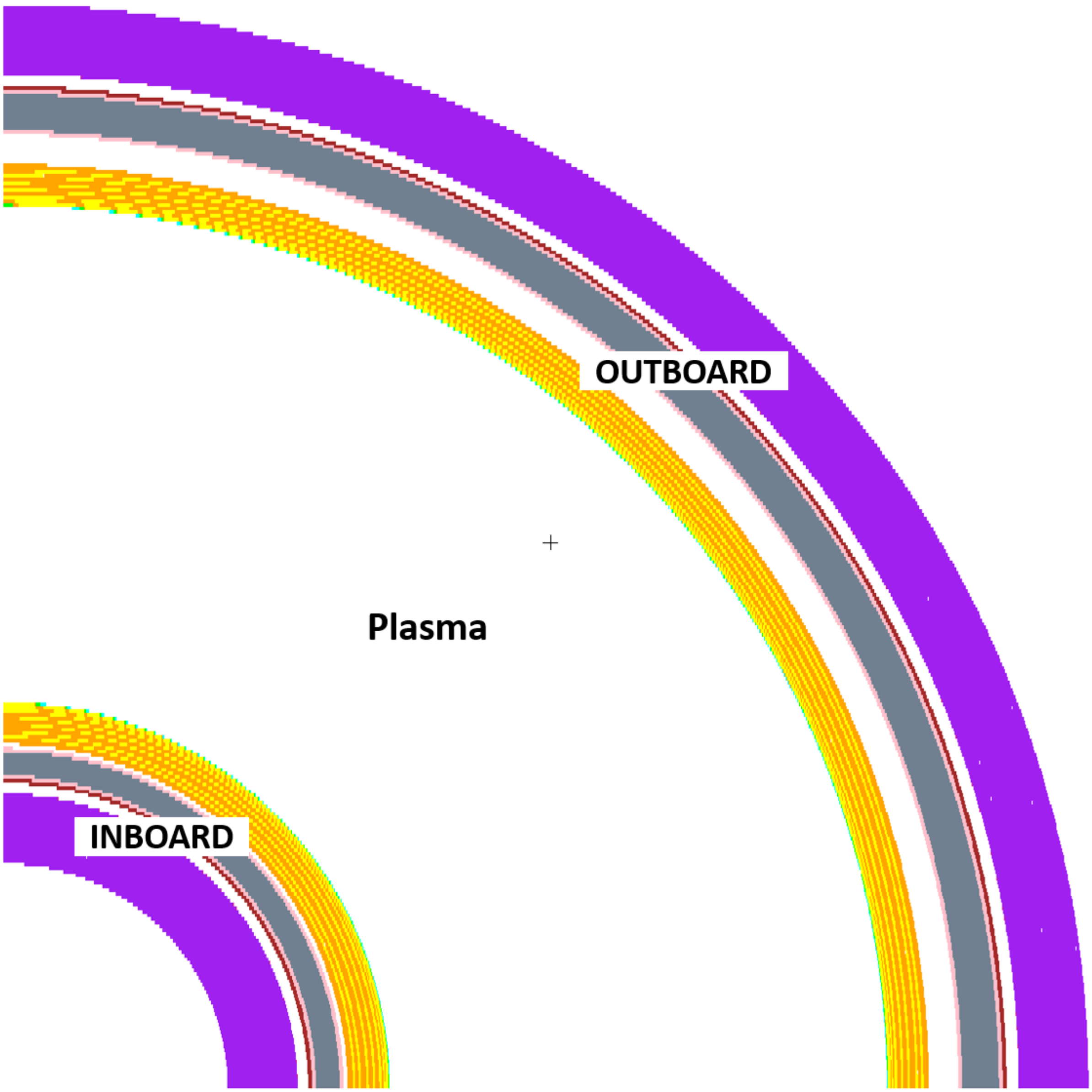


Fig. 2: ITER 1D MCNP geometry (quarter)

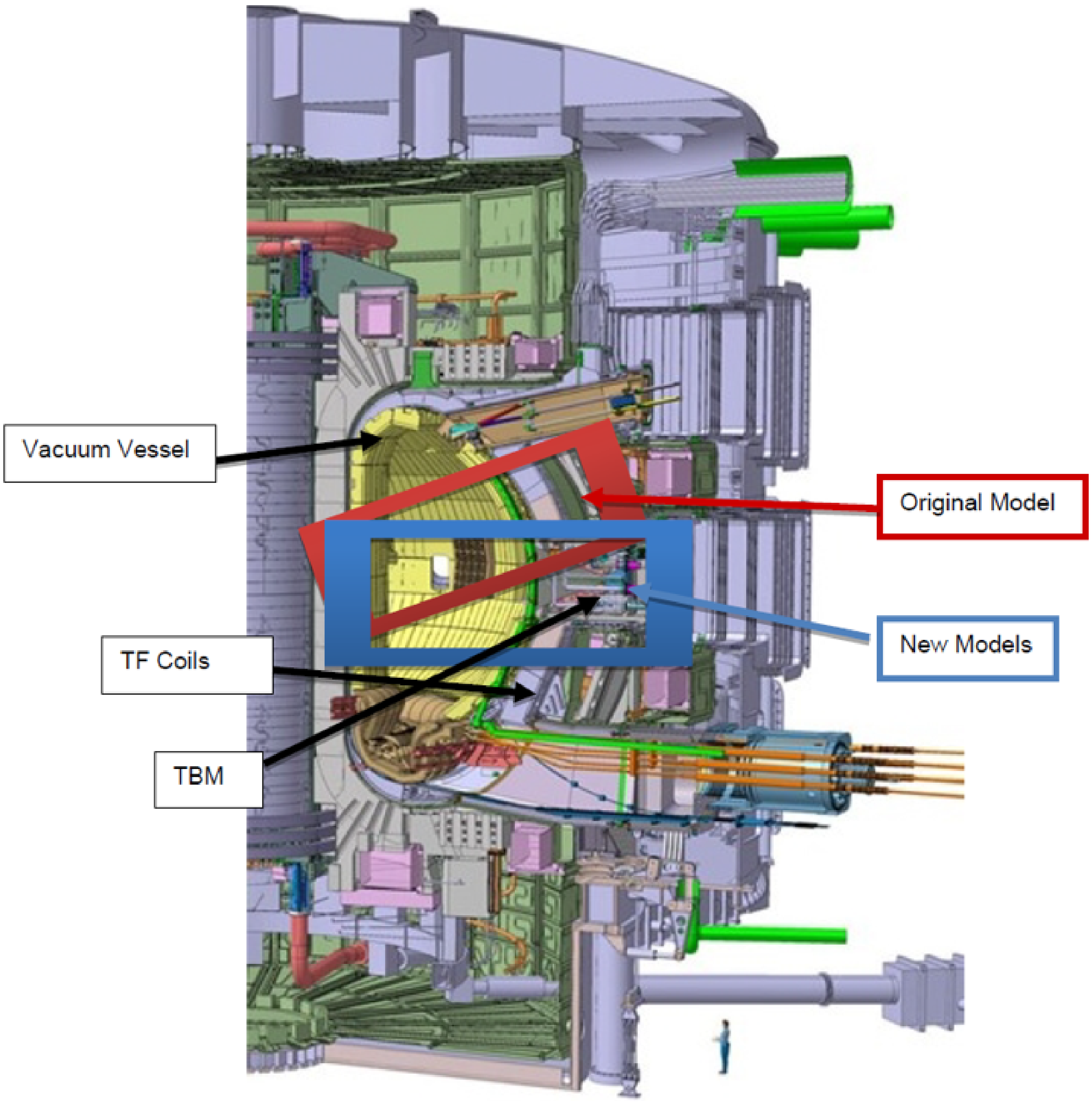


Fig. 3: Position of the MCNP model in the ITER tokamak

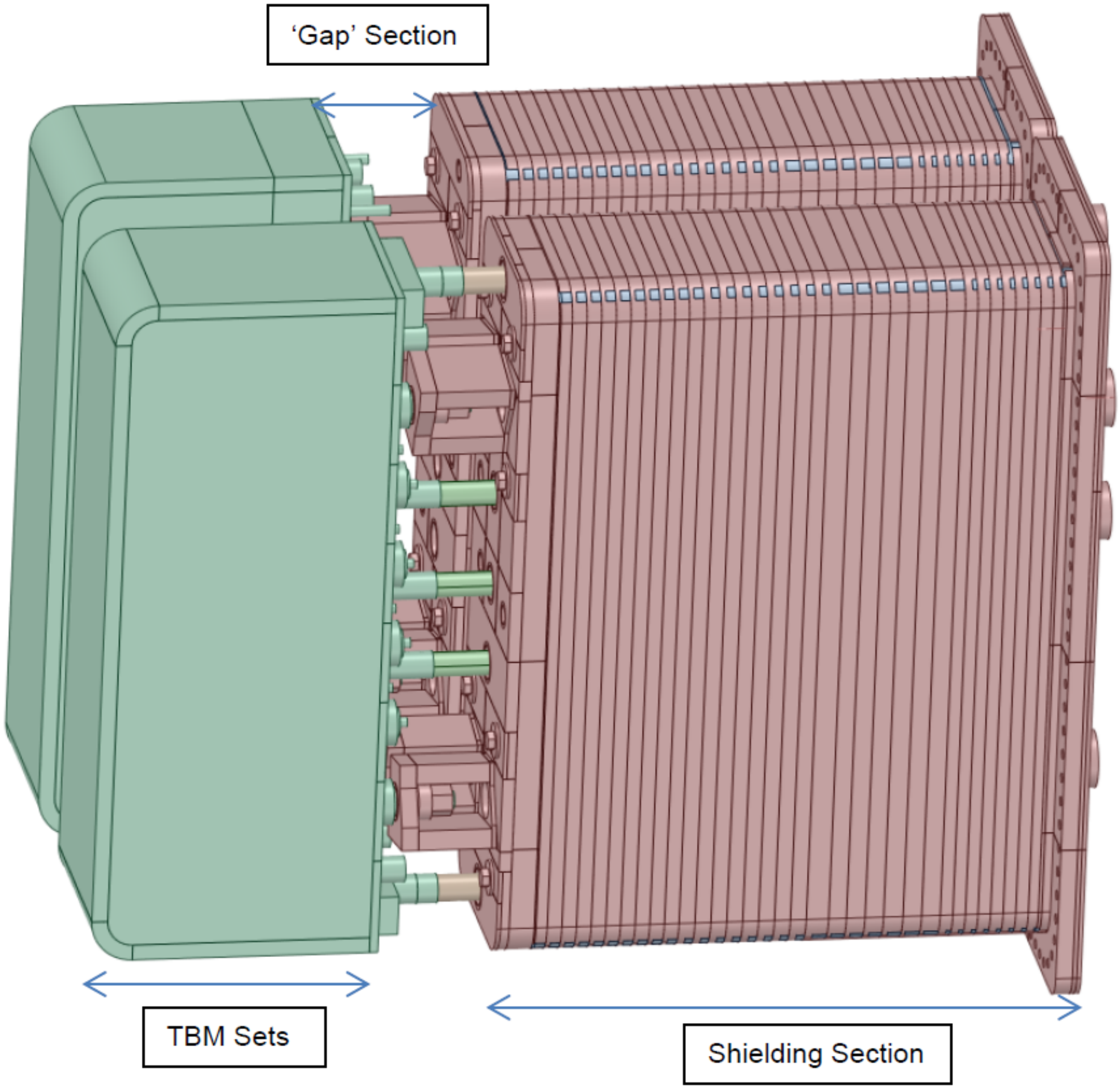


Fig. 4: CAD model of the TBM component

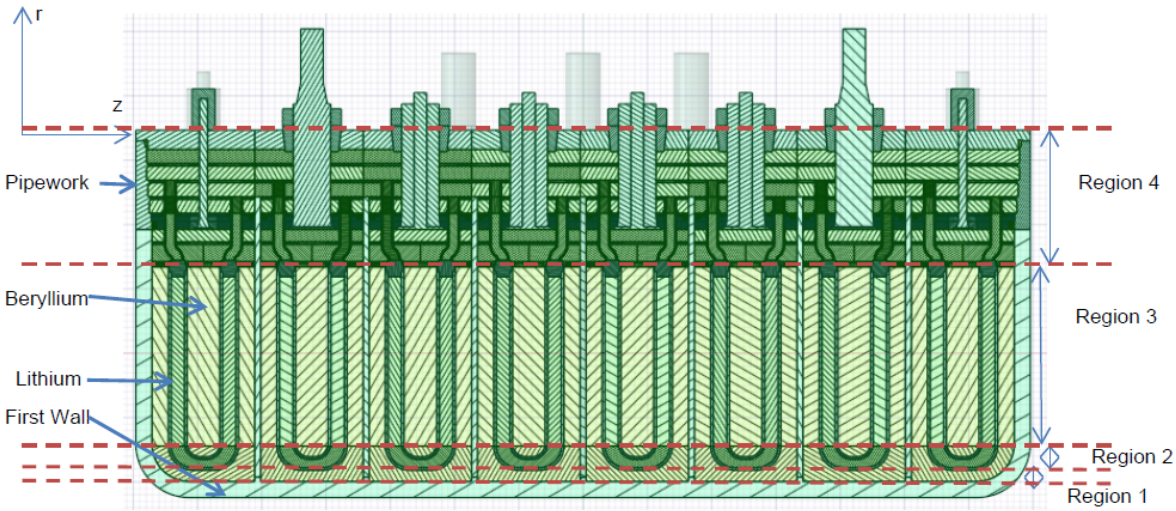


Fig. 5: Section of the CAD model of the HCPB TBM set

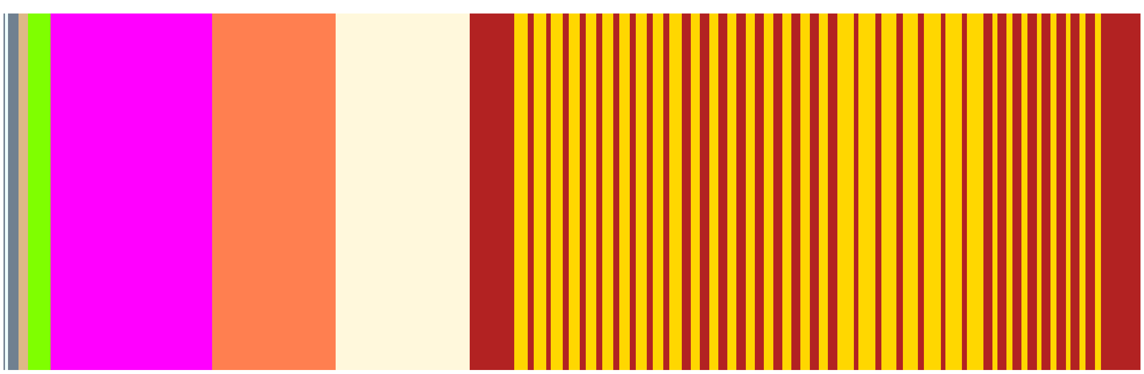


Fig. 6: Visualization of the TBM and and shielding section in the 1D MCNP geometry

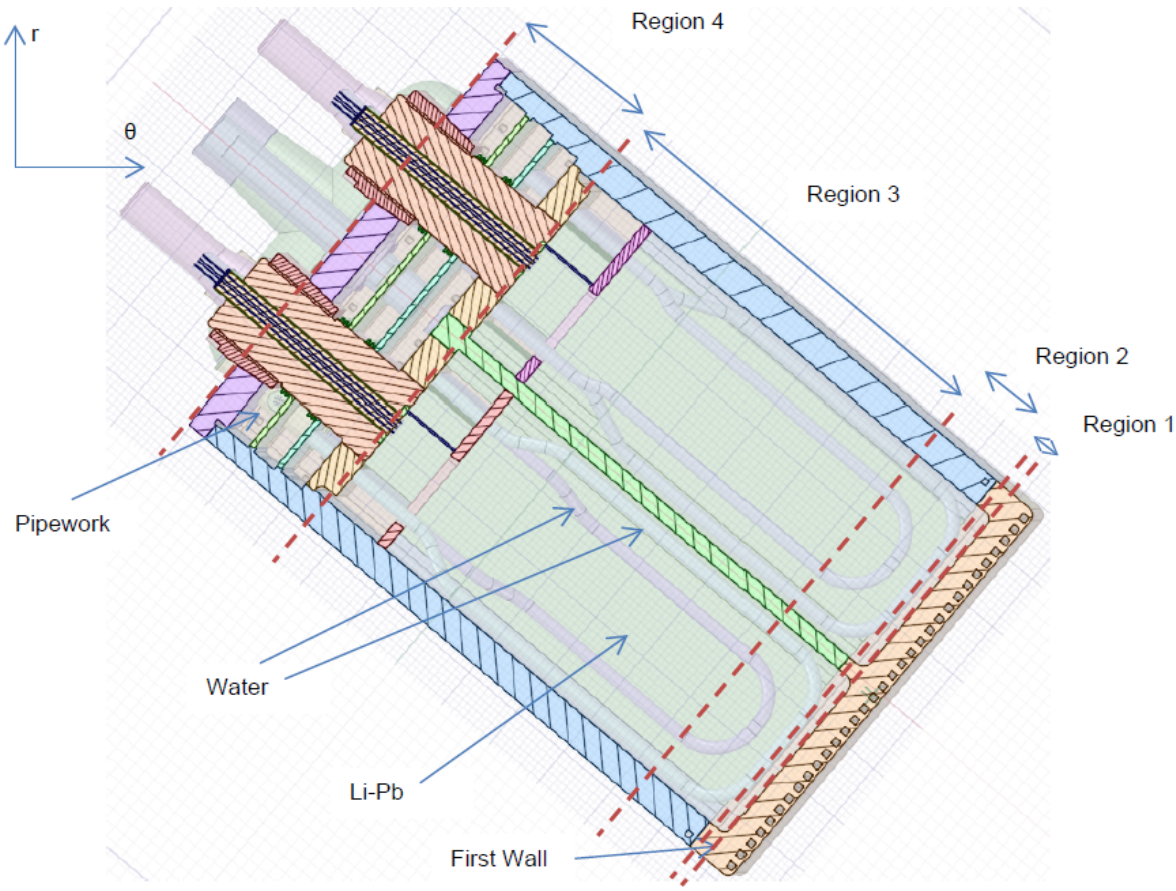


Fig. 7: Section of the CAD model of the WCLL TBM set

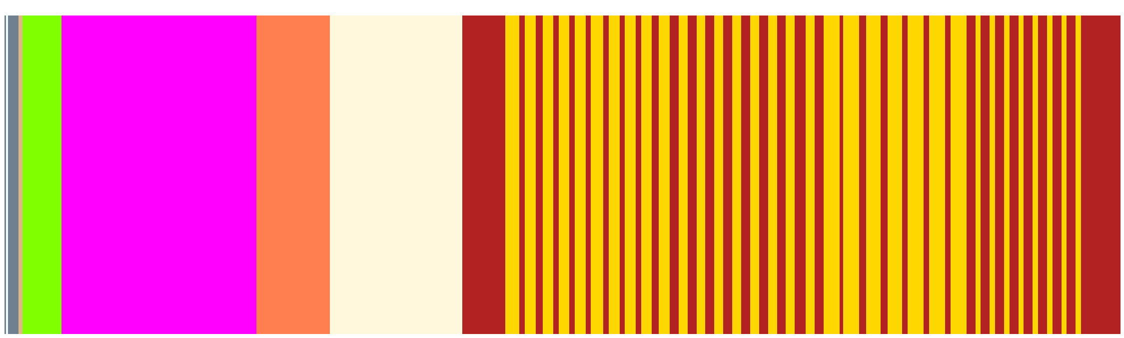


Fig. 8: Visualization of the TBM and shielding section in the 1D MCNP geometry

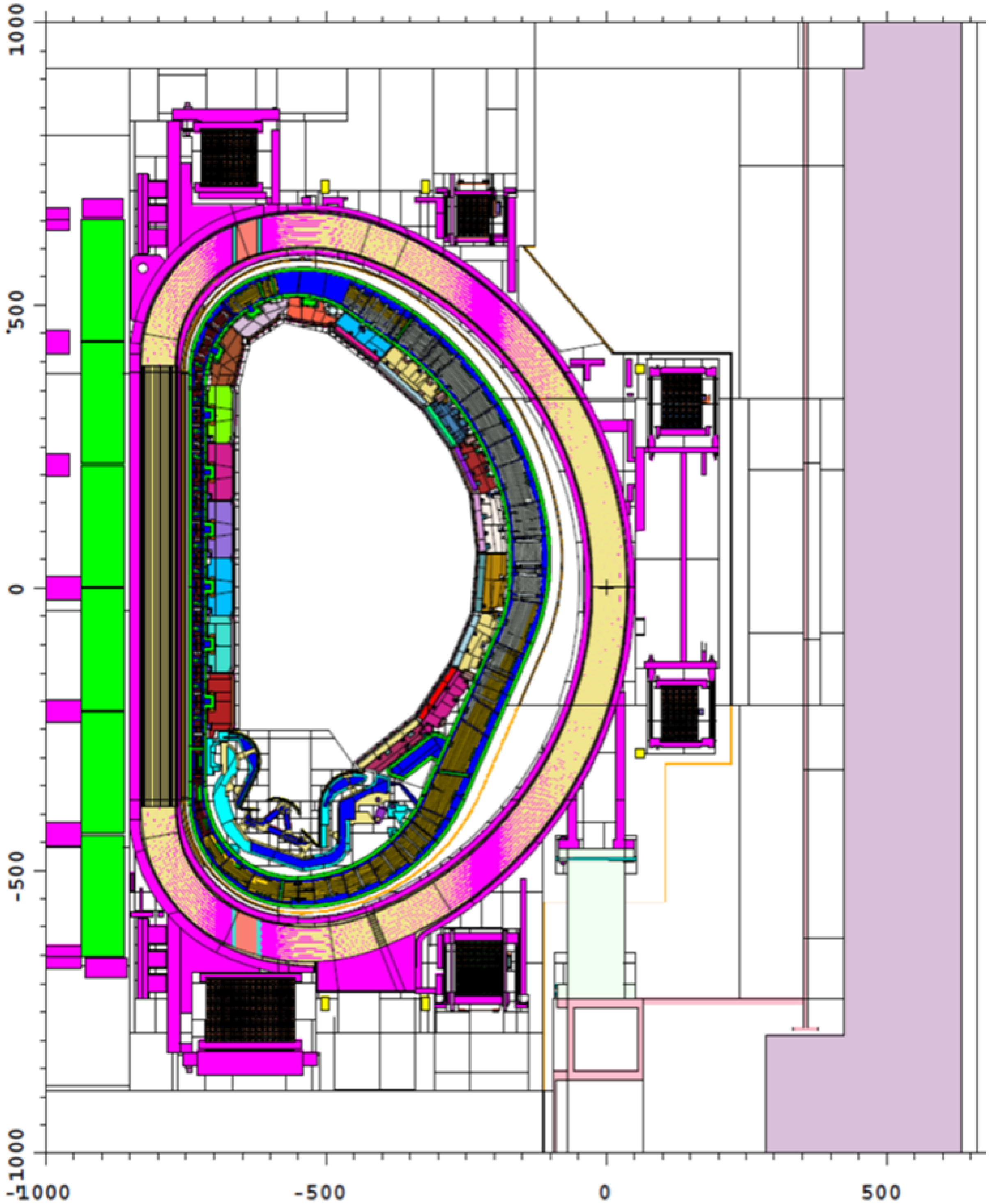


Fig. 9: C-model R181031. Origin (1050,200,0). Basis (0.982339, 0.187112, 0.000000) (0,0,1). Extent (1000,1000)

6.2 Experimental Benchmarks

6.2.1 Oktavian

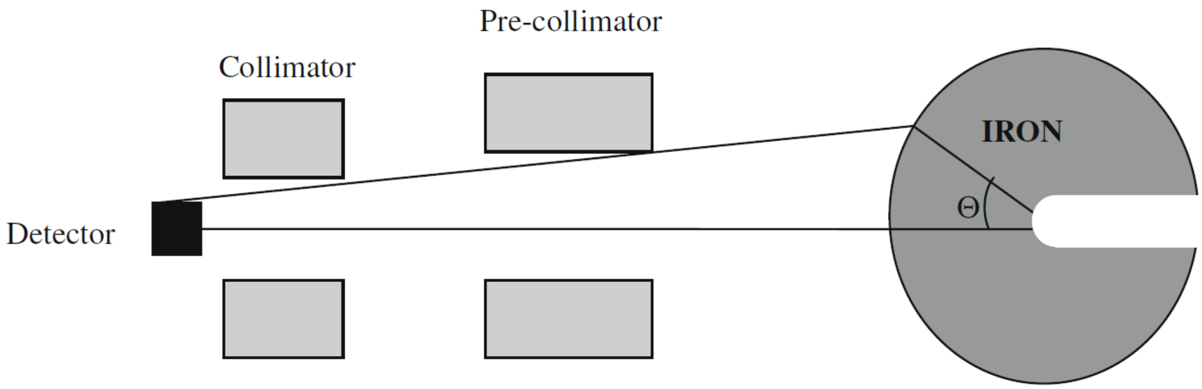


Fig. 10: Simplified layout of the OKTAVIAN Fe experimental setup (not on scale).

Experimental results derived from Oktavian experiments are publicly accessible at the CoNDERC database which is mantained by the IAEA Nuclear Data Section and built upon the database of shielding experiments (SINBAD), hosted by the RSICC and jointly mantained with the NEA data bank.

See also:

Related papers and contributions:

- A. Milocco, A. Trkov and I. A. Kodeli, 2010, "The OKTAVIAN TOF experiments in SINBAD: Evaluation of the experimental uncertainties", *Annals of Nuclear Energy*, **37** 443-449
- I.Kodeli, E. Sartori and B. Kirk, "SINBAD - Shielding Benchmark Experiments - Status and Planned Activities", *Proceedings of the ANS 14th Biennial Topical Meeting of Radiation Protection and Shielding Division*, Carlsbad, New Mexico (April 3-6, 2006)

CHAPTER

SEVEN

POST-PROCESSING GALLERY

7.1 Excel output

7.1.1 Benchmark specific

Sphere Leakage

SPHERE LEAKAGE TEST RESULTS RECAP: STATISTICAL CHECKS

ZAID		TALLY										
Zaid	Zaid Name	Neutron Flux at the external surface in Vitamin-J 175 energy groups [2]	Neutron heating with F4+FM multiplier [4]	Neutron heating F6 [6]	Neutron Flux at the external surface in course energy groups [12]	He ppm production [14]	T production [24]	DPA production [34]	Gamma flux at the external surface [22]	Gamma flux at the external surface [FINE@FISPACT MANUAL 24 Group Structure] [32]	Gamma heating with F4+FM multiplier [44]	Gamma heating F6 [46]
1001	H-1	Passed	Passed	Passed	Passed	All zeros	All zeros	Passed	Missed	Missed	Passed	Passed
1002	H-2	Missed	Passed	Passed	Missed	All zeros	Passed	Passed	Passed	Passed	Passed	Passed
1003	H-3	Passed	Passed	Passed	Passed	All zeros	All zeros	Passed	All zeros	All zeros	All zeros	All zeros
2003	He-3	Passed	Passed	Passed	Passed	Passed	Passed	Passed	Passed	Passed	Passed	Passed
2004	He-4	Passed	Passed	Passed	Passed	All zeros	All zeros	Passed	All zeros	All zeros	All zeros	All zeros

Fig. 1: 10 MCNP statistical checks for each zaid and tally

SPHERE LEAKAGE TEST RESULTS RECAP: ERRORS

ZAID		TALLY								
Zaid	Zaid Name	Neutron Flux at the external surface in Vitamin-J 175 energy groups	Neutron heating with F4+FM multiplier	Neutron heating F6	He ppm production	T production	DPA production	Gamma flux at the external surface [FINE@FISPACT MANUAL 24 Group Structure]	Gamma heating with F4+FM multiplier	Gamma heating F6
1001	H-1	9.66%	0.99%	0.99%	0.00%	0.00%	1.61%	2.78%	2.61%	2.61%
1002	H-2	2.48%	12.00%	0.95%	0.00%	1.64%	0.47%	2.46%	2.44%	51.00%
1003	H-3	0.84%	0.96%	0.96%	0.00%	0.00%	0.47%	0.00%	0.00%	0.00%
2003	He-3	3.34%	1.40%	1.40%	1.29%	9.73%	24.00%	6.09%	1.18%	1.18%
2004	He-4	0.78%	1.09%	1.09%	0.00%	0.00%	0.69%	0.00%	0.00%	0.00%

LEGEND
> 50%
20% ≤ 50 %
10% ≤ 20 %
< 10%

According to MCNP manual

Fig. 2: Statistical error associated with each tally for each zaid

SPHERE LEAKAGE TEST RESULTS RECAP: VALUES

ZAID		TALLY							
Zaid	Zaid Name	Neutron Flux at the external surface in Vitamin-J 175 energy groups	He ppm production	T production	DPA production	Gamma flux at the external surface [FINE@FISPACT MANUAL 24 Group Structure]	Neutron Heating comparison [F4 vs F6]	Gamma Heating comparison [F4 vs F6]	Notes
1001	H-1	Value > 0 for all bins	Value = 0 for all bins	Value = 0 for all bins	Value > 0 for all bins	Value > 0 for all bins	0.00%	1.00%	
1002	H-2	Value < 0	Value = 0 for all bins	Value > 0 for all bins	Value > 0 for all bins	Value > 0 for all bins	2.00%	0.00%	
1003	H-3	Value > 0 for all bins	Value = 0 for all bins	Value = 0 for all bins	Value > 0 for all bins	Value = 0 for all bins	0.00%	0.00%	
2003	He-3	Value > 0 for all bins	Value > 0 for all bins	Value > 0 for all bins	Value > 0 for all bins	Value > 0 for all bins	0.00%	6.00%	
2004	He-4	Value > 0 for all bins	Value = 0 for all bins	Value = 0 for all bins	Value > 0 for all bins	Value = 0 for all bins	0.00%	0.00%	

LEGEND
> |5| %
|3| % ≤ |5| %
|0.5| % ≤ |1| %
< |0.5| %

Fig. 3: Consistency checks on zaid tally results

SPHERE LEAKAGE COMPARISON RECAP

ZAID		Neutron Flux (Coarse energy bins) Tally n.12						Gamma Flux (Coarse energy bins) Tally n. 22										
		1e-06 [MeV]	0.1 [MeV]	1.0 [MeV]	10.0 [MeV]	20.0 [MeV]	Total	0.01 [MeV]	0.1 [MeV]	1.0 [MeV]	5.0 [MeV]	20.0 [MeV]	Total	T production	He ppm production	DPA production	Neutron heating F6	Gamma heating F6
1001	H-1	-0.01%	0.00%	0.00%	0.00%	Identical	0.00%	0.23%	-0.02%	-0.09%	-0.21%	Identical	-0.12%			-12.58%	-0.04%	-0.01%
1002	H-2	0.19%	Identical	0.00%	Identical	Identical			-0.01%	0.30%	-0.24%	-0.09%	-0.06%	0.12%		0.00%	4.97%	-0.13%
1003	H-3	0.00%	Identical	0.00%	Identical	Identical	0.00%									Identical	Identical	
2003	He-3		-0.26%	Identical	Identical	Identical	0.00%		0.00%	0.00%	Identical	-0.08%	-0.01%	0.00%	0.00%	0.00%	0.00%	0.00%
2004	He-4	31.42%	6.21%	0.08%	0.80%	-0.08%	5.44%		32.79%	13.87%	55.98%	-0.67%	26.67%	1.77%	-0.04%	4.13%	1.47%	12.55%

LEGEND
>|20|%
|10|% ≤ |20|%
|5|% ≤ |10|%
< |5|%

Fig. 4: Comparison of tally results for each zaid

Oktavian

"C/E (mean +/- σ)"			
Particle	**Energy Range [MeV]**	**FENDL 3.1d**	**FENDL 3.2 beta**
Neutron	**0.1 - 1**	1.01 +/- 0.44	1.03 +/- 0.44
	1.0 - 5	0.9 +/- 0.08	0.9 +/- 0.08
	10.0 - 20	3.38 +/- 9.97	3.38 +/- 9.95
	5.0 - 10	0.91 +/- 0.11	0.9 +/- 0.11
Photon	**0.1 - 1**	0.42 +/- 0.26	0.44 +/- 0.27
	1.0 - 5	2.21 +/- 1.06	2.21 +/- 1.05
	10.0 - 20	18.45 +/- nan	17.96 +/- nan
	5.0 - 10	7.87 +/- 4.76	7.75 +/- 4.74

Fig. 5: C/E table summarized per energy range

LIBRARY:		31c
10 MCNP Statistical Checks		
Tally Number	**Tally name**	**Result**
44	H in 316SS appm/FPY	Missed
54	T in 316SS appm/FPY	Missed
64	Cu dpa/FPY	Missed
74	He in CuBeNi appm/FPY	Missed
84	H in CuBeNi appm/FPY	Missed
94	T in CuBeNi appm/FPY	Missed
104	Ni dpa/FPY	Missed
114	He in Inconel appm/FPY	Missed
124	H in Inconel appm/FPY	Missed
134	T in Inconel appm/FPY	Missed
144	He in Be appm/FPY	Passed

Fig. 6: 10 MCNP statistical checks recap

LIBRARY: 32c

ITER_1D RESULTS RECAP: Errors

according to MCNP

LEGEND	
(red)	> 50%
(orange)	20% ≤ 50 %
(yellow)	10% ≤ 20 %
(green)	< 10%

Neutrons Flux (energy binned) [#/cm^2]	Energy [MeV]	Cell 22	24	25	26	27	28	29	30	31	33	34	35	36	37	38	39	40	41	42	43
Tally n.4	1.00E-07	0.9999	0.6455	0.2003	0.1262	0.1061	0.0888	0.0927	0.0844	0.1568	0.071	0.0623	0.0552	0.0532	0.0476	0.0448	0.0419	0.0406	0.0359	0.0343	0.0342
	4.14E-07	0.9999	0.6576	0.2709	0.1332	0.1108	0.0942	0.0904	0.0862	0.1556	0.0996	0.0634	0.0769	0.0523	0.0648	0.0446	0.058	0.0404	0.0552	0.0354	0.0553
	5.32E-07	0	0.7164	0.3838	0.1709	0.1424	0.1321	0.1199	0.1075	0.2255	0.164	0.0851	0.1663	0.0783	0.1344	0.0667	0.1208	0.0662	0.1274	0.063	0.1298
	6.83E-07										0										
	8.76E-07	0	0.7075	0.3926	0.172	0.1442	0.1144	0.129	0.1108	0.2389	0.1675	0.0897	0.1592	0.0771	0.1243	0.0701	0.1268	0.0623	0.1155	0.0655	0.134
	1.13E-06	0	0.9999	0.3266	0.1636	0.1452	0.1304	0.1302	0.1203	0.2367	0.1914	0.0903	0.1633	0.0773	0.1157	0.0689	0.1196	0.0624	0.1145	0.0662	0.154
	1.44E-06	0.9999	0.8442	0.3543	0.1742	0.1512	0.1324	0.1181	0.1058	0.2186	0.1739	0.0861	0.164	0.0787	0.1145	0.07	0.1209	0.0629	0.1033	0.0609	0.1631
	1.86E-06	0.9999	0.6581	0.3545	0.1634	0.157	0.1375	0.1254	0.1162	0.2288	0.1721	0.0855	0.1536	0.075	0.1143	0.0626	0.122	0.0652	0.1207	0.0642	0.1743
	2.38E-06	0.9999	0.5151	0.3185	0.1848	0.1548	0.1402	0.114	0.1146	0.2155	0.1716	0.0893	0.1553	0.0827	0.1217	0.068	0.1206	0.062	0.1178	0.0637	0.1683
	3.06E-06	0	0.7937	0.2756	0.1792	0.1554	0.1363	0.1177	0.1121	0.2405	0.1716	0.0919	0.1505	0.0803	0.1096	0.0689	0.1252	0.0638	0.1237	0.0651	0.1695
	3.93E-06	0	0.9999	0.3713	0.2005	0.149	0.142	0.1138	0.1095	0.2217	0.1645	0.0863	0.1654	0.084	0.1145	0.0667	0.115	0.0616	0.1256	0.0637	0.1479
	5.04E-06	0.9999	0.9999	0.3682	0.1769	0.1599	0.1377	0.1122	0.1107	0.1951	0.1528	0.0916	0.1566	0.0814	0.1035	0.0672	0.1169	0.0607	0.1256	0.07	0.1656
	6.48E-06	0.7096	0.853	0.3802	0.1927	0.1581	0.1287	0.1258	0.1129	0.1781	0.1623	0.0909	0.1451	0.0766	0.103	0.069	0.1116	0.0672	0.1241	0.0649	0.1641
	8.32E-06	0.9228	0.6615	0.3316	0.166	0.1598	0.1399	0.1171	0.1191	0.1775	0.1541	0.0878	0.1422	0.081	0.1143	0.0688	0.1226	0.0638	0.1244	0.064	0.1423
	1.07E-05	0	0.724	0.3292	0.1764	0.1669	0.1348	0.1135	0.1075	0.1658	0.1521	0.0927	0.1606	0.081	0.1141	0.0694	0.1163	0.0677	0.1148	0.0644	0.1487

Fig. 7: Statistical errors associated with the tally results

H in 316SS appm/FPY	Cells	Value
Tally n.44	21	-37.43%
	26	-24.62%
	27	-17.63%
	28	-7.39%
	29	-0.58%
	30	-22.90%
	33	-17.75%
	35	-3.39%
	37	-9.85%
	39	-6.89%
	41	-4.62%
	43	-4.75%
	45	-3.56%
	47	-5.62%
	55	-5.05%
	57	-4.42%
	59	-3.55%
	61	-2.28%
	63	-2.45%
	65	-5.27%
	67	-5.97%
	69	-2.21%
	72	0.51%
	73	-3.17%
	74	-5.71%
	75	-7.38%
	76	-8.82%
	77	0.33%
	78	3.28%
	79	0.68%
	80	-0.58%

Fig. 8: Print of a single binned tally

LIBRARY:	31c Vs 32c

ITER_1D RESULTS RECAP: Comparison

LEGEND	
red	>|20|%
orange	|10|% ≤ |20|%
yellow	|5|% ≤ |10|%
green	< |5|%

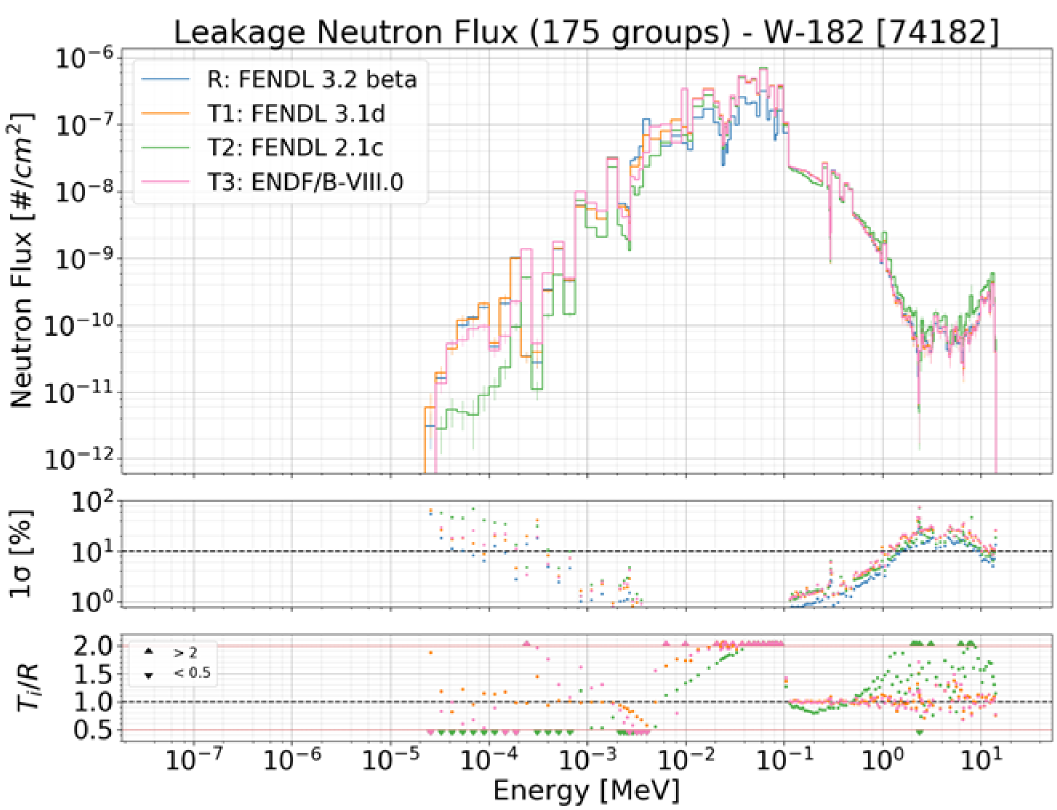
Neutrons Flux (energy binned) [#/cm^2]	Energy [MeV]	Cell 22	24	25	26	27	28	29	30	31	33	34	35	36	37	38	39	40	41	42	43
Tally n.4	1.00E-07	-57.14%	71.78%	2.86%	-6.56%	-14.24%	-2.35%	-5.40%	-3.85%	-0.02%	8.12%	3.21%	4.41%	1.72%	8.09%	-0.73%	3.79%	-2.73%	-0.47%	1.86%	7.74%
	4.14E-07	-251.51%	86.29%	-148.84%	-20.54%	-9.32%	-15.20%	-11.83%	-9.79%	-6.80%	3.64%	4.63%	15.42%	4.07%	-1.56%	3.77%	10.12%	1.44%	-4.31%	-0.48%	12.52%
	5.32E-07		-70.30%	-210.20%	-13.22%	-13.66%	-13.32%	-22.42%	-8.73%	2.53%	24.57%	-3.89%	2.24%	-10.15%	-29.96%	-8.43%	-23.72%	-1.20%	-22.96%	-2.60%	20.80%
	6.83E-07			-176.39%	-19.66%	-21.38%	-8.81%	-9.71%	-2.71%	-1.75%	19.55%	10.18%	-9.28%	9.97%	-12.34%	-16.47%	-58.00%	-9.61%	-20.99%	-5.30%	11.02%
	8.76E-07	6553500.00%	-141.27%	-46.27%	-44.20%	-14.98%	-18.99%	-37.25%	-3.13%	-42.82%	4.35%	6.51%	-27.08%	-6.03%	-10.03%	-1.69%	-17.43%	-6.25%	8.24%	-14.22%	2.84%
	1.13E-06	6553500.00%	-273.17%	-4.78%	-4.92%	0.77%	7.92%	0.09%	-12.71%	-1.66%	-48.45%	-11.19%	-19.74%	-0.89%	-17.65%	-9.54%	-0.80%	-9.52%	24.31%	-7.61%	25.49%
	1.44E-06	100.00%	88.48%	8.40%	-10.22%	-10.05%	-23.87%	-7.25%	13.85%	-24.80%	-8.22%	9.38%	0.92%	-23.27%	2.77%	15.37%	-3.56%	6.67%	15.31%	12.77%	-10.81%
	1.86E-06	23.28%	-38.43%	-9.15%	-26.62%	-52.32%	-19.16%	-21.59%	-0.75%	-36.70%	-32.11%	12.18%	7.86%	-3.19%	-3.47%	15.86%	-8.83%	-0.25%	-8.00%	-8.40%	-10.00%
	2.38E-06	100.00%	54.73%	-18.04%	5.69%	-23.70%	-6.98%	-10.72%	-7.56%	-32.19%	3.15%	12.14%	-7.61%	4.24%	11.83%	-2.14%	-30.30%	-0.02%	-0.52%	-10.54%	-30.08%
	3.06E-06		-297.74%	-55.29%	-4.07%	-8.11%	-11.39%	-30.67%	-3.71%	-64.06%	-1.97%	-7.79%	-6.21%	8.09%	-8.29%	-6.30%	-8.32%	-17.68%	-10.23%	-8.45%	-5.43%
	3.93E-06	6553500.00%	-287.14%	-80.96%	-42.79%	-11.58%	-6.96%	8.21%	-15.91%	-18.56%	-2.19%	1.13%	-7.44%	-1.29%	1.61%	-18.52%	-20.25%	-1.47%	22.85%	2.39%	5.47%
	5.04E-06	-21.70%	-2170.38%	-213.66%	-55.39%	-13.01%	11.94%	6.56%	-12.13%	-10.97%	-0.80%	8.03%	-9.38%	3.90%	0.35%	4.71%	-7.36%	2.60%	11.67%	-1.61%	10.72%
	6.48E-06	-61.42%	10.85%	-536.80%	-26.78%	-4.62%	3.16%	7.74%	-3.61%	21.09%	-31.10%	11.80%	-11.86%	2.55%	5.91%	-11.07%	-19.20%	-0.90%	3.32%	-1.22%	-7.48%
	8.32E-06	-115.41%	44.28%	-126.42%	-42.17%	-16.33%	30.19%	-12.32%	-3.84%	25.93%	-4.75%	3.76%	13.49%	-3.74%	-6.80%	-6.38%	6.32%	1.25%	-10.79%	5.29%	23.65%
	1.07E-05	6553500.00%	-4.80%	30.69%	-24.25%	-56.73%	-10.85%	-16.55%	-1.56%	5.28%	3.91%	11.17%	19.73%	9.25%	-1.84%	0.21%	-3.21%	-3.97%	-10.88%	-10.61%	14.21%
	1.37E-05	41.81%	-86.81%	4.02%	3.31%	-11.05%	-2.59%	3.97%	-12.62%	-40.83%	8.60%	16.04%	16.98%	-19.25%	0.89%	3.88%	7.86%	4.36%	-18.10%	0.62%	30.52%
	1.76E-05	-190.37%	-783.30%	5.23%	14.23%	-19.00%	24.56%	-12.37%	-22.24%	-67.52%	1.81%	-1.03%	2.17%	-6.10%	-0.25%	6.53%	4.37%	4.74%	-6.07%	0.75%	1.20%
	2.26E-05	-180.76%	-204.85%	-32.95%	2.78%	-66.71%	9.82%	-7.02%	-19.26%	-19.87%	16.74%	12.23%	1.70%	2.49%	-6.84%	0.48%	16.47%	4.68%	4.66%	5.93%	2.53%
	2.90E-05	100.00%	-128.15%	-8.41%	-9.07%	-54.96%	-4.43%	-14.26%	-10.73%	-0.12%	30.80%	5.97%	32.16%	-8.93%	-38.71%	2.27%	-2.25%	-6.71%	8.14%	-10.94%	14.09%
	3.73E-05	6553500.00%		-222.82%	-24.85%	-39.82%	-7.04%	10.64%	-5.68%	2.32%	45.36%	16.32%	-3.27%	10.39%	-28.28%	-8.89%	-14.33%	1.78%	8.47%	8.95%	1.61%
	4.79E-05	6553500.00%	38.72%	-67.36%	-21.96%	-61.26%	-4.10%	8.05%	-17.26%	17.89%	8.48%	4.93%	-24.92%	-6.78%	-25.24%	-16.11%	-19.93%	1.33%	4.65%	2.32%	2.24%
	6.14E-05	-404.79%	-130.15%	-37.35%	-14.95%	-11.86%	-20.31%	-18.17%	-22.19%	16.30%	10.47%	-0.44%	1.96%	3.69%	-33.67%	-11.08%	-20.37%	-8.76%	3.49%	8.91%	-34.39%
	7.89E-05	6553500.00%	7.23%	18.89%	-44.61%	-5.85%	5.75%	3.70%	-24.24%	12.01%	-2.44%	-0.17%	20.61%	8.60%	-0.98%	3.83%	-8.90%	-13.89%	-37.05%	9.67%	-35.18%

Fig. 9: Print of a double binned tally

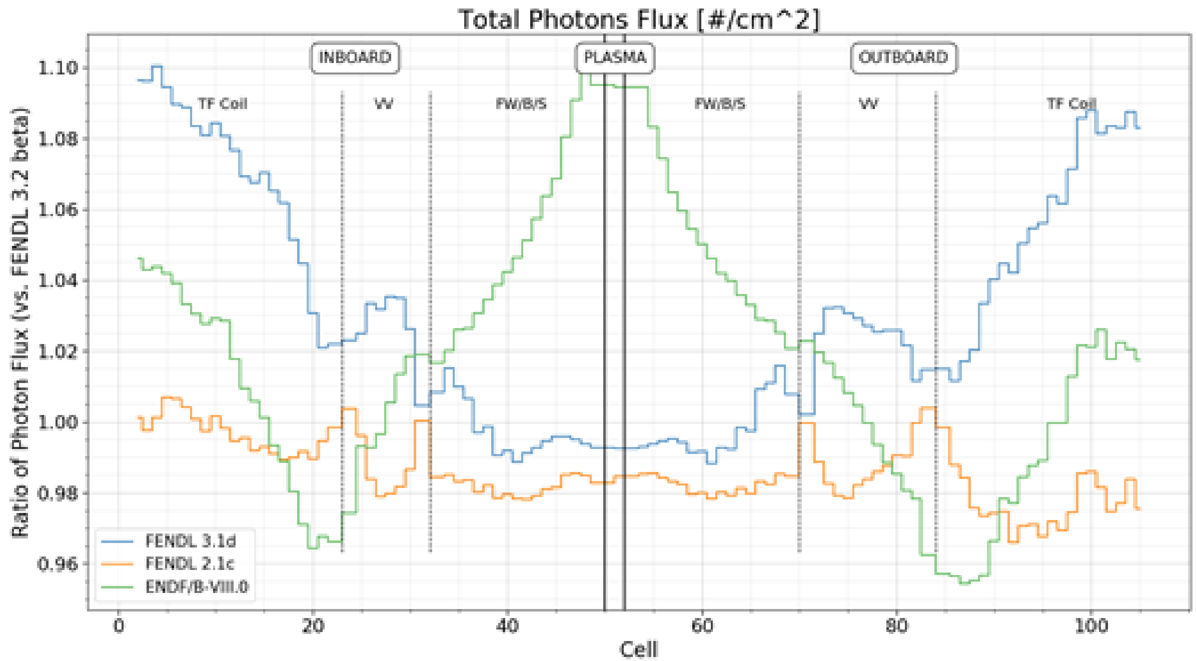
7.1.2 General output

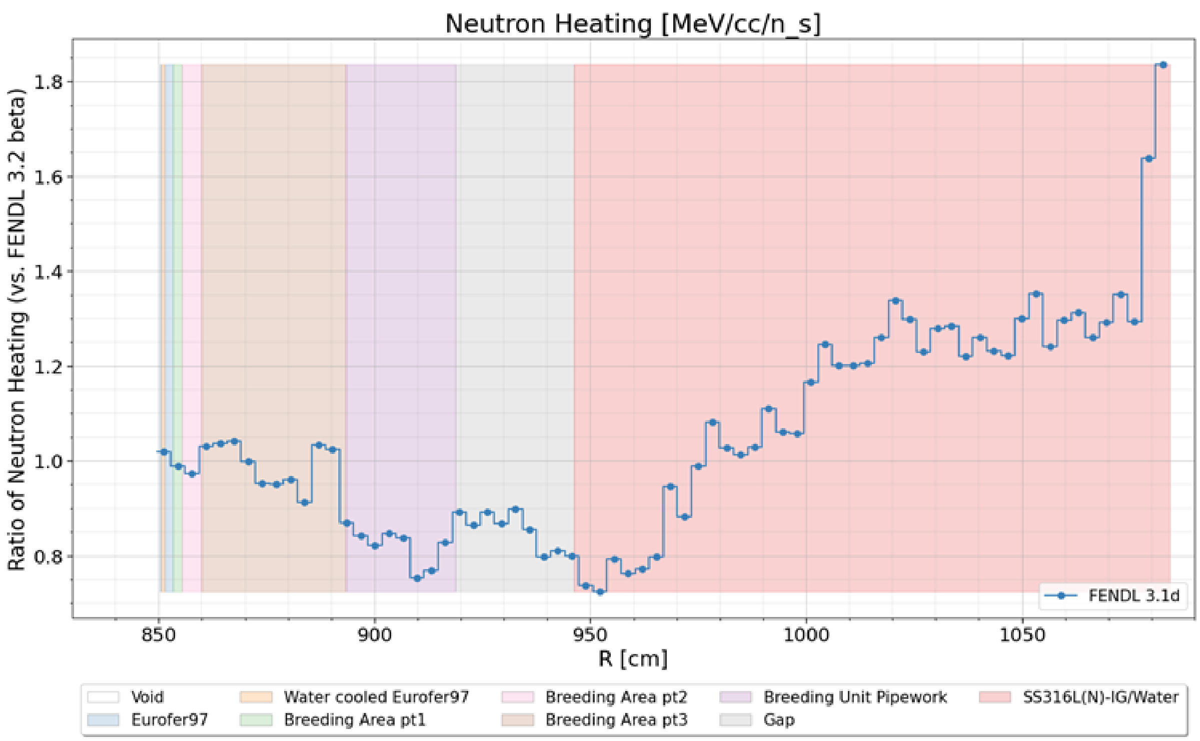
7.2 Plots Atlas

7.2.1 Binned graph

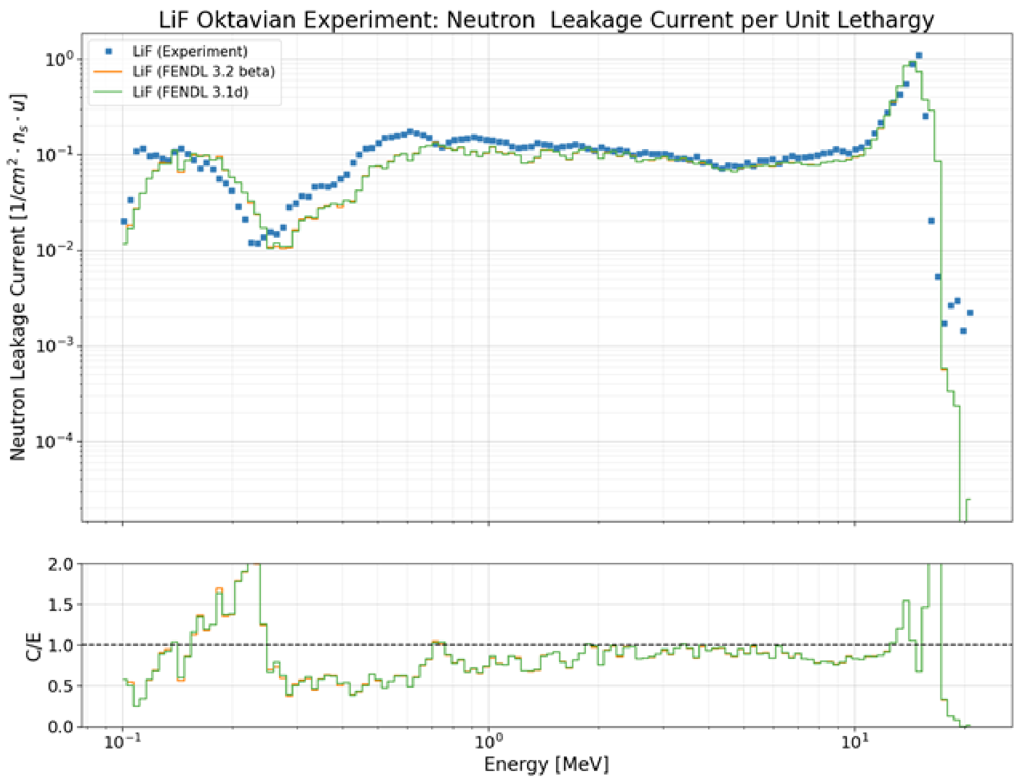


7.2.2 Ratio Graph

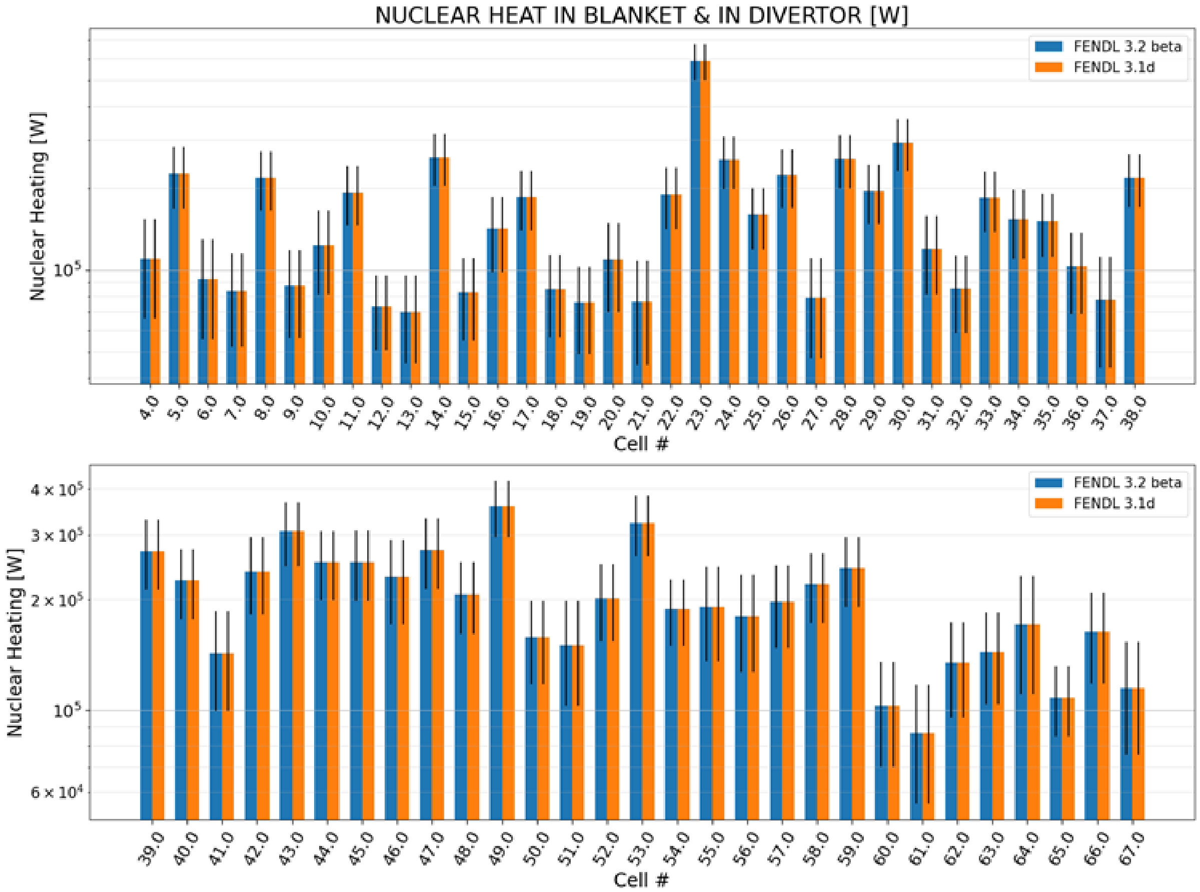




7.2.3 Experimental points



7.2.4 Grouped bars



CHAPTER

EIGHT

UTILITIES

During the development of JADE, many useful classes and methods were developed which could be used for small stand-alone tools, mostly operating on MCNP inputs.

A description of these *utilities*, accessible from the JADE main menu, is here provided.

The outputs (if generated) of these utilities can be found in specific subfolders of the `<JADE root>\Utilities` directory.

8.1 Print available libraries

`printlib`

This function allows to print to video all libraries (suffixes) that are available in xsdir file indicated in the main configuration file.

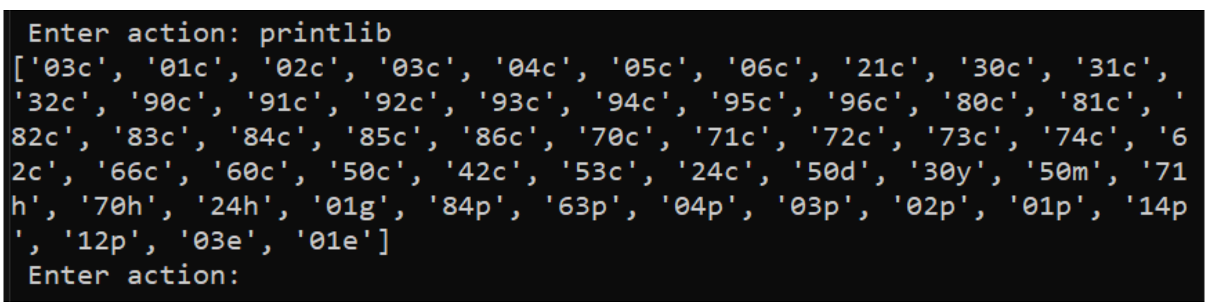


Fig. 1: Screenshot of the execution of the `printlib` command

8.2 Restore default configurations

`restore`

This function allows to restore the JADE configuration default settings. In other words, the content of the `<JADE root>\Configuration` directory is restored to "factory installation" and all user modifications to the configuration files are lost.

Note: When the the restoration is completed, the application will be terminated. The main configuration file ambient variable will need to be reconfigured before running another JADE instance.

See also:

Main Configuration

8.3 Translate an MCNP input

`trans`

This function allows to translate a material section of an MCNP input to a whatever nuclear data library available in the xsdir file.

The translation is carried out basically by the **convertZaid()** method of the **LibManager** class and by the **translate()** method of the **SubMaterial** class. The **convertZaid** method:

1. asks for a zaid (to translate) and for a library (to translate to);
2. checks if the library selected for the translation is available in the xsdir of the user;
3. **select the type of translation:**
    a. zaid not available in library: the default lib is used, no other changes applied;
    b. zaid available in library: the zaid is converted to the selected library, no other changes applied;
    c. the zaid is natural (i.e. it ends with 000).

For case c, at first, the selected library is checked for exact correspondence, i.e., it is checked if also in the selected library the zaid is expressed as natural. In this case, the behavior is identical to case b. If this is not true, the zaid needs to be expanded: all zaids of the same elements are returned with their atomic mass (m) and natural abundance (NA).

At this point, the **translate()** method completes the translation. No particular actions are required if there is no zaid expansion. In case of expansion, if the original natural zaid fraction is an atomic one (x_N^A), the new zaids deriving from the expansion will have as fraction their natural abundance (NA) multiplied for the original natural zaid fraction:

$$x_{zaid}^A = \text{NA}_{zaid} \cdot x_N^A$$

If, instead, the original natural zaid fraction is a mass one (x_N^M), the *equivalent mass* m_N of the natural zaid can be computed as:

$$m_N = \sum_{zaids} \text{NA}_{zaid} \cdot m_{zaid}$$

and then the mass fraction of each expanded new zaid (x_{zaid}^M) can be calculated as:

$$x_{\text{zaid}}^M = x_N^M \cdot (\text{NA}_{zaid} \cdot m_{zaid})/M_N$$

where $(\text{NA}_{zaid} \cdot m_{zaid})/M_N$ is basically the natural abundance in mass of the zaid.

The new input will be dumped in the `<JADE root>\Utilities\Translation` folder. The following scheme summarizes the JADE translation logic.

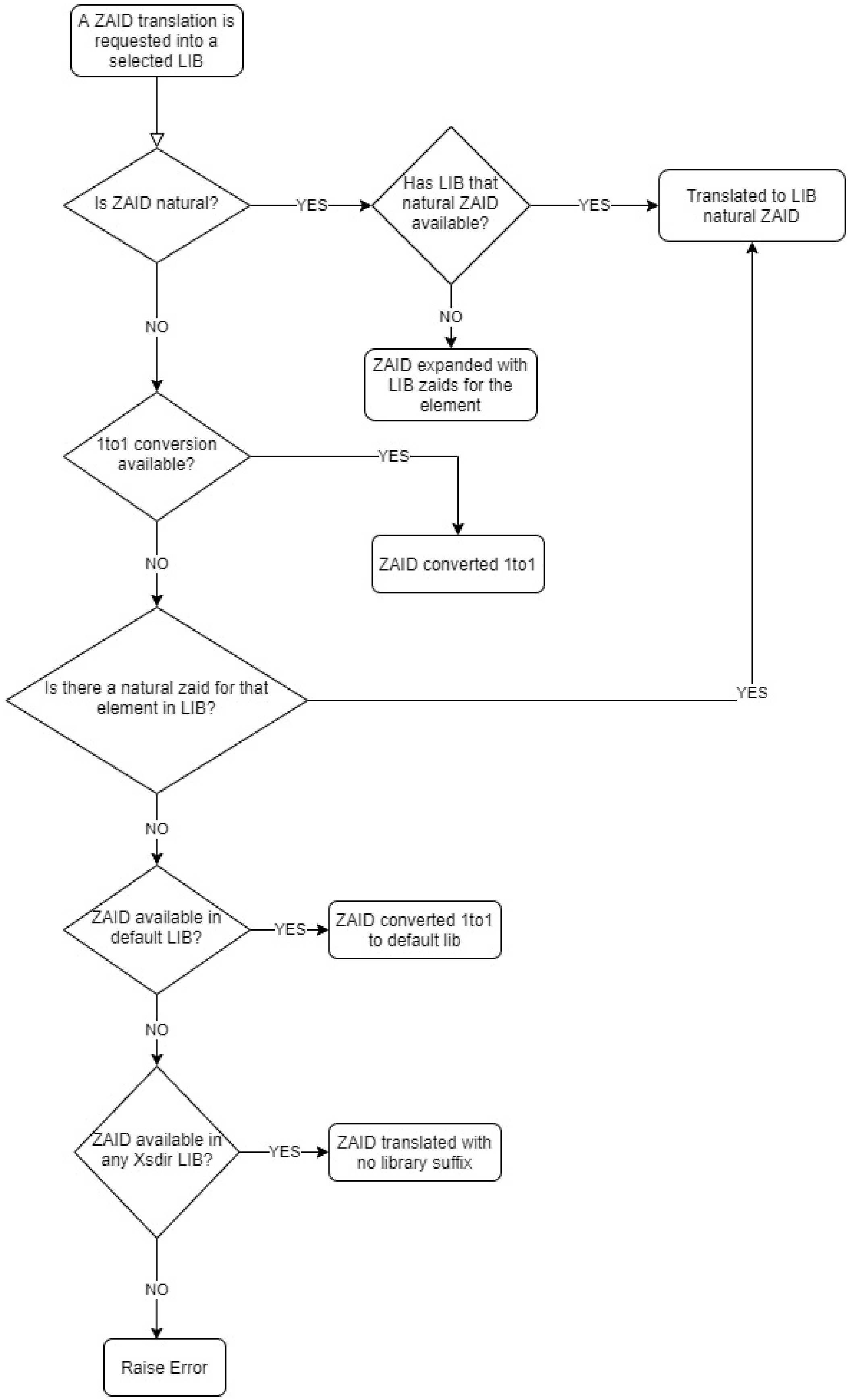


Fig. 2: Zaid translation logic

8.4 Print materials info

`printmat`

This function is used to print a summary of an MCNP input material section. The information is contained in two sheets of an Excel file dumped into the `<JADE root>\Utilities\Materials Infos` folder. The first sheet summarizes information at the single isotope level. Here both the atom and mass fraction for each zaid is reported divided by material and submaterial. It may happen that the original fraction appearing in the MCNP input is not normalized. JADE prints this fraction as it is and only the alternative fraction is normalized during its calculation.

Material	Submaterial	Element	Isotope	Atom Fraction	Mass Fraction
m1	1	H	H-1 [1001]	-1.90E-02	2.16E-02
			H-2 [1002]	-4.38E-06	2.49E-06
	2	C	C-12 [6012]	-1.96E-01	1.87E-02
			C-13 [6013]	-2.30E-03	2.02E-04
	3	N	N-14 [7014]	-2.51E-02	2.05E-03
			N-15 [7015]	-9.83E-05	7.50E-06
	4	O	O-16 [8016]	-3.77E-01	2.70E-02
			O-17 [8017]	-1.53E-04	1.03E-05
			O-18 [8018]	-8.72E-04	5.55E-05
	5	Mg	Mg-24 [12024]	-1.97E-02	9.40E-04
			Mg-25 [12025]	-2.60E-03	1.19E-04
			Mg-26 [12026]	-2.97E-03	1.31E-04
		Al	Al-27 [13027]	-9.26E-02	3.93E-03
		Si	Si-28 [14028]	-1.80E-01	7.38E-03
			Si-29 [14029]	-9.48E-03	3.75E-04
			Si-30 [14030]	-6.47E-03	2.47E-04
	6	S	S-32 [16032]	-1.35E-02	4.85E-04
			S-33 [16033]	-1.10E-04	3.83E-06
			S-34 [16034]	-6.37E-04	2.15E-05
			S-36 [16036]	-3.20E-06	1.02E-07
		Cu	Cu-63 [29063]	-3.46E-02	6.29E-04
			Cu-65 [29065]	-1.59E-02	2.81E-04
m2	1	Cu	Cu-63 [29063]	-6.85E-01	5.73E-02
			Cu-65 [29065]	-3.15E-01	2.56E-02
m3	1	Nb	Nb-93 [41093]	-7.01E-01	4.09E-02
	2	Sn	Sn-112 [50112]	-2.73E-03	1.32E-04
			Sn-114 [50114]	-1.89E-03	9.00E-05

Fig. 3: Extract of the isotope sheet. In the example, the material card was expressed in mass fraction and not normalized.

The second sheet summarizes information at the element level. Three fractions are here listed for each element: * the MCNP fraction of the element in the material; * the normalized fraction of the element in the submaterial; * the normalized fraction of the element in the material.

Depending on the orginal MCNP input, these three fraction need to be interpreted as either *mass* or *atom* fraction.

Material	Submaterial	Element	Fraction	Sub-Material Fraction	Material Fraction
m1	1	H	2.16E-02	1.00E+00	2.57E-01
	2	C	1.89E-02	1.00E+00	2.25E-01
	3	N	2.06E-03	1.00E+00	2.45E-02
	4	O	2.71E-02	1.00E+00	3.21E-01
	5	Al	3.93E-03	3.00E-01	4.67E-02
		Mg	1.19E-03	9.07E-02	1.41E-02
		Si	8.00E-03	6.10E-01	9.50E-02
	6	Cu	9.10E-04	6.41E-01	1.08E-02
		S	5.10E-04	3.59E-01	6.06E-03
m10	1	Cu	7.67E-02	1.00E+00	9.56E-01
	2	Sn	3.57E-03	1.00E+00	4.45E-02
m11	1	B	4.38E-06	1.00E+00	5.13E-05
	2	C	7.09E-05	1.00E+00	8.31E-04
	3	N	2.36E-04	1.00E+00	2.77E-03
	4	Al	5.26E-04	3.91E-01	6.17E-03
		O	5.90E-06	4.38E-03	6.92E-05

Fig. 4: Extract of the element sheet. In the example, the material card was expressed in mass fraction and not normalized.

8.5 Generate material mixture

`generate`

This function is used to generate a material mixture starting from two or more materials contained in a single MCNP input. The user will be asked for:

- absolute path to the MCNP input;
- if the zaids need to have a mass or atom fraction;
- material names (e.g. m1) to be used in the mixture;
- percentages to be used in the mixture for each material;
- nuclear data library to use for the new material mixture.

Each material will be transformed in a submaterial of the newly generated mixture retaining its header if present. The new material will be dumped in the `<JADE root>\Utilities\Generated Materials` folder.

8.6 Switch material fractions

`switch`

This function can be used to switch an MCNP input from having atom fractions to mass fractions and viceversa. The new input will be dumped in the `<JADE root>\Utilities\Fraction switch` folder.

CHAPTER

NINE

TIPS & TRICKS

This section reunites a series of tips and tricks that can be used to *unlock* JADE additional capabilities.

9.1 External Run of a benchmark

It may be useful for particularly computational-intensive benchmark to be run on a separate hardware (e.g. a server) with respect to the one used for JADE. This can be achieved quite easily with the following steps:

1. set the `OnlyInput` option in the `<JADE root>\Configuration\Conf.xlsx` file to `True` for the benchmark that needs to be run externally. This will generate the MCNP input file of the benchmark that can be found in `<JADE root>\Tests\MCNP simulation\<lib suffix>\<Benchmark name>` without running it;
2. copy the generated input file into the hardware selected for the run and start the MCNP simulation. The only requirement is to use the MCNP keyword `name=` when launching the simulation in order to obtain consistently named outputs;
3. once the simulation is completed, copy all MCNP outputs to the same `<JADE root>\Tests\MCNP simulation\<lib suffix>\<Benchmark name>` folder;
4. normally run the post-processing.

CHAPTER

TEN

JADE TESTING

TBD

CHAPTER

ELEVEN

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    available for as long as needed to satisfy these requirements.

    e) Convey the object code using peer-to-peer transmission, provided
    you inform other peers where the object code and Corresponding
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  A separable portion of the object code, whose source code is excluded
from the Corresponding Source as a System Library, need not be
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and execute modified versions of a covered work in that User Product from
a modified version of its Corresponding Source.  The information must
suffice to ensure that the continued functioning of the modified object
code is in no case prevented or interfered with solely because
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CHAPTER

TWELVE

CONTRIBUTORS

JADE is the results of a joint effort between NIER ingegneria, Università di Bologna (UNIBO) and Fusion For Energy (F4E).

Key People:

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Marco Sumini	Expert	UNIBO	marco.sumini@unibo.it

CHAPTER

THIRTEEN

LIST OF PUBLICATIONS AND CONTRIBUTIONS

13.1 Publications featuring JADE

- D. Laghi, M. Fabbri, L. Isolan, R. Pampin, M. Sumini, A. Portone and A. Trkov, 2020, "JADE, a new software tool for nuclear fusion data libraries verification & validation", *Fusion Engineering and Design*, **161** 112075, doi: https://doi.org/10.1016/j.fusengdes.2020.112075
- D. Laghi, M. Fabbri, L. Isolan, M. Sumini, G. Shnabel and A. Trkov, 2021, "Application Of JADE V&V Capabilities To The New FENDL v3.2 Beta Release", *Nuclear Fusion*, [Under minor review]

13.2 Benchmarks Related Publications

- A. Milocco, A. Trkov and I. A. Kodeli, 2010, "The OKTAVIAN TOF experiments in SINBAD: Evaluation of the experimental uncertainties", *Annals of Nuclear Energy*, **37** 443-449
- I.Kodeli, E. Sartori and B. Kirk, "SINBAD - Shielding Benchmark Experiments - Status and Planned Activities", *Proceedings of the ANS 14th Biennial Topical Meeting of Radiation Protection and Shielding Division*, Carlsbad, New Mexico (April 3-6, 2006)
- D. Leichtle, B. Colling, M. Fabbri, R. Juarez, M. Loughlin, R. Pampin, E. Polunovskiy, A. Serikov, A. Turner and L. Bertalot, 2018, "The ITER tokamak neutronics reference model C-Model", *Fusion Engineering and Design*, **136** 742-746
- M. Sawan, 1994, "FENDL Neutronics Benchmark: Specifications for the calculational and shielding benchmark", (Vienna: INDC(NDS)-316)

13.3 Miscellaneous

CHAPTER

FOURTEEN

INTRODUCTION

TBD

CHAPTER

FIFTEEN

INDICES AND TABLES

- genindex
- modindex
- search