OAK RIDGE National Laboratory

An Update on AARE V1.0 and CINDER2008

Igor Remec

for the CINDER development team

Oak Ridge National Laboratory,
Oak Ridge, TN, USA

5th International Workshop on Accelerator Radiation Induced Activation (ARIA19)

Daejeon, Korea,
September 23-25, 2019

AARE V1.0 and CINDER2008 development team

Development team includes staff from US national laboratories and laboratories abroad

- **Oak Ridge National Laboratory**
  - Franz Gallmeier, Erik Iverson, Wei Lu, Irina Popova, Igor Remec
- **Paul Scherrer Institute (Switzerland)**
  - Michael Wohlmuther, Ryan Bergmann, Daniela Kiselev
- **Argonne National Laboratory**
  - Brad Micklich
- **Los Alamos National Laboratory**
  - Bill Wilson, Shannon Holloway, Hannah Little, Charles Kelsey, Michal Mocko, Eric Pitcher
- **European Spallation Source**
  - Günter Muhrer, Thomas Miller
- **University of Tennessee, Knoxville**
  - Tucker McClanahan

Oak Ridge National Laboratory is supported by the US Department of Energy, Office of Science, Office of Basic Energy Sciences under contract number DE-AC05-00OR22725.
Argonne National Laboratory is supported by the US Department of Energy's Office of Science under contract number DE-AC02-06CH11357.

Outline

- **AARE V1.0 Code Package:**

  Activation in Accelerator Radiation Environments
  - **What is included in AARE**
  - **What functionality it provides**

- **An example: CINDER90 vs. CINDER2008**

- **Conclusions**

Activation in Accelerator Radiation Environments AARE V1.0

AARE V1.0 (RSICC Code Package CCC-846) includes:

- **CINDER2008 transmutation code** (as distributed directly by LANL, with very slight modifications to make compilation more robust)
  - **LIBRARY_MAKER code** to prepare CINDER 2008 data libraries
  - **CINDER2008 data libraries**
  - **POST code** for processing CINDER 2008 results
  - **Accident Analyses Tools**
- **Activation Script Version 2.0**
- **Gamma Source Script 2.0**

The predecessor of AARE V1.0 is the CINDER-1.05 package.

CINDER2008: Overview

CINDER2008 is a transmutation code: it calculates the inventory of nuclides in an irradiated material as a function of irradiation and/or decay time.

Temporal history consists of one or more "campaigns". During each campaign flux magnitude and nuclide production/destruction rates remain unchanged.

When multiple materials (cells) are analyzed, each cell requires separate CINDER2008 run. Nuclide inventories of different cells may be merged if desired.

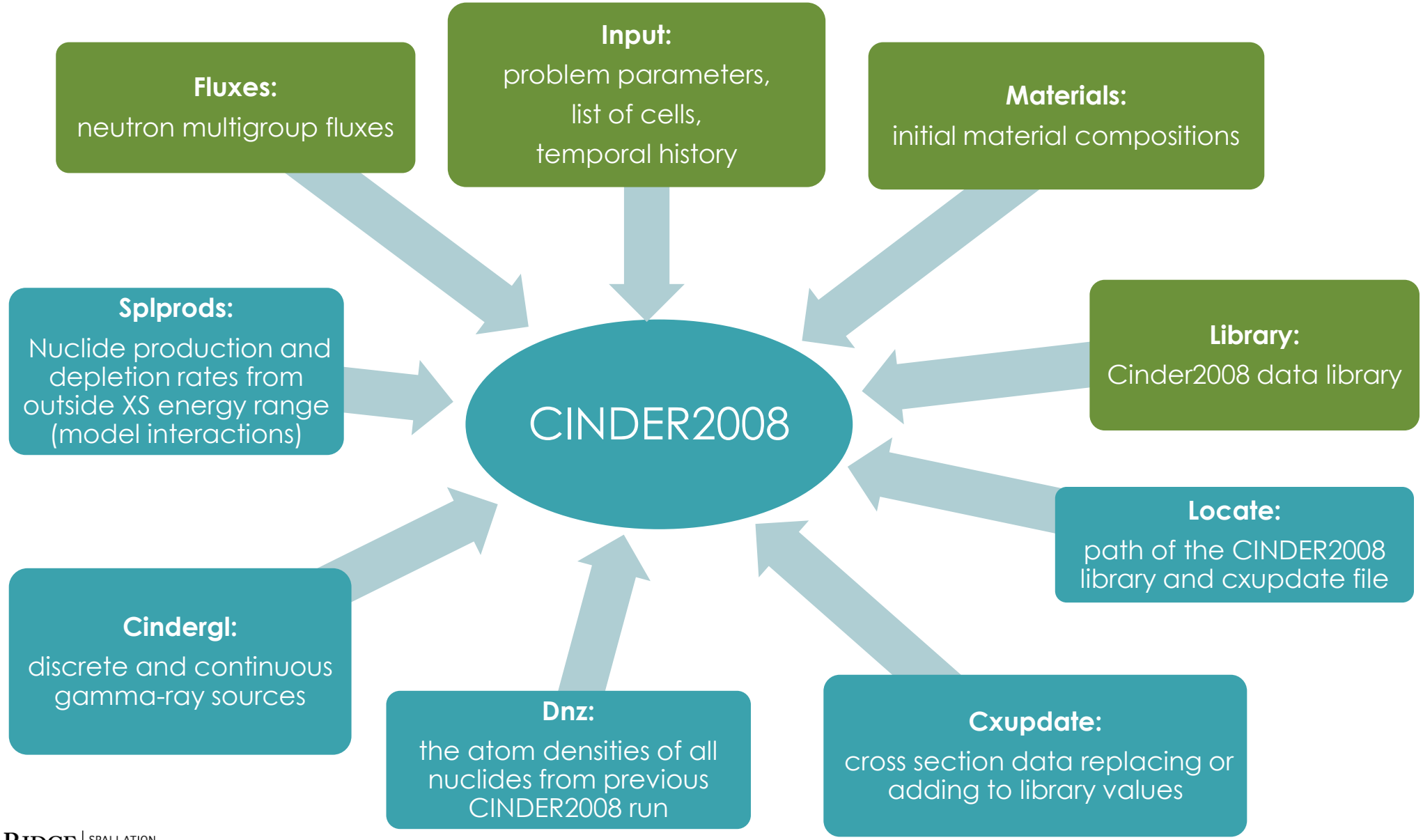
CINDER2008 (Cont.)

CINDER2008 is the latest release in the CINDER data and code development effort, built upon the original work of Tal England at Bettis Atomic Power Laboratory (BAPL) in the early 1960s.

CINDER2008 was developed at LANL by Shannon Holloway and is a significant upgrade in capability from CINDER90.

- **Improvements include**
  - Modern programming language (Fortran90)and methods
  - New algorithms to more accurately solve the underlying differential equations
  - Automatic post-processing capabilities
  - Namelist input option in addition to list-directed
  - Constant power approximation
  - High-fidelity β-delayed gamma spectra

CINDER2008 (Cont.): Inputs



CINDER2008 (Cont.): Outputs

Table Name
Atom Density (atoms/barn-cm)
Total Mass (kg)
Activity Density (Curies/cc)
Total Activity (Curies)
Decay Power Density (Watts/cc)
Total Decay Power (Watts)
Macroscopic Particle Absorption (/cm)
Radionuclide Hazard Air Dilution Factor
Radionuclide Hazard Water Dilution Factor
SF Density (#/cc-s)

Table Name
SF Power Density (Watts/cc)
SF Power (Watts)
(n,f) Density (#/cc)
(n,f) Power Density (Watts/cc)
(n,f) Power (Watts)
Total Fission Density (#/cc)
Total Fission Power Density (Watts/cc)
Total Fission Power (Watts)
Multi-group Gamma Spectra (#/bin-s-cc)
Accident Analysis - Dose Equivalent
Accident Analysis - Threshold Ratio

Tables can be ordered by nuclide, element (Z), mass (A), major contributor (> 0.1%), or group (E); multiple cells can be combined, and the content of the tables can be sorted…

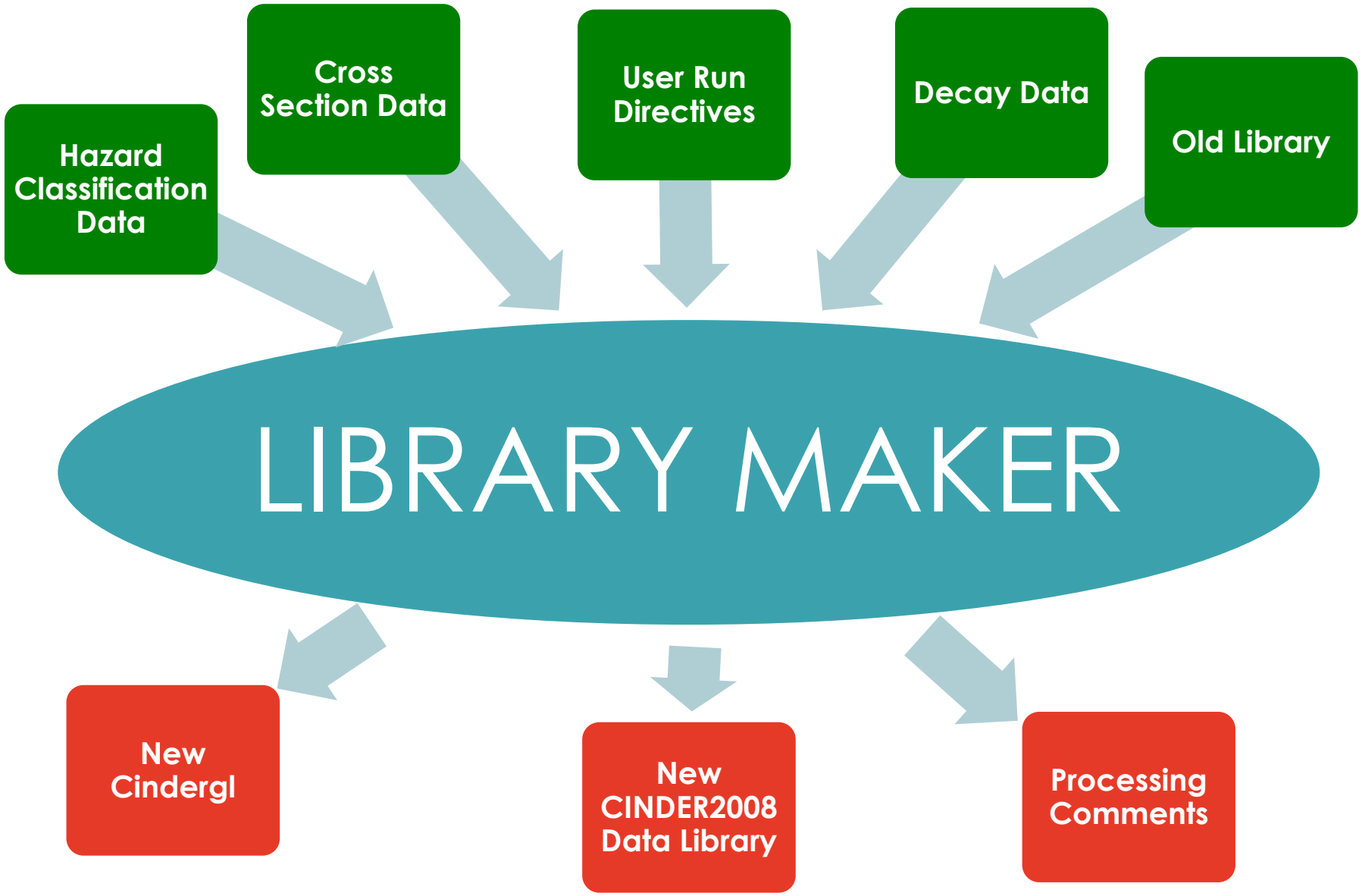
LIBRARY_MAKER

Was developed at LANL by Shannon Holloway together with the CINDER2008 code: both are written in FORTRAN90

LIBRARY MAKER:

- **Allows for flexible build and modifications of custom libraries for CINDER2008 applications (multi-component isotopic data sets)**
- **Is capable of combining consistent isotopic information from different data sources**
- **Makes choices picking nuclear data from multiple data library sources**
- **Was used to produce the standard CINDER2008 libraries**
- **Examples of library modifications are provided with the AARE V1.0 package**

LIBRARY MAKER (Cont.)



LIBRARY MAKER (Cont.)

- **Decay Data Files**
  - Decay source files have to be in ENDF-6 format
  - Contain: half lives, isotope characteristics (excitation energy, spin, parity, abundance, half-life, decay modes), decay products & energies
  - All isotopes from one source (ENDF/B, JEF, JENDL …) are contained in one file
  - As many as 10 sources can be considered
- **Activation Cross Sections**
  - Provided in groupwise ENDF format (GENDF)
  - Processed from ENDF formatted libraries by NJOY code with the GROUPR module
  - Organized in directories by the source (ENDF-B-VII.1, JEF3.3 …)
  - Provided in one file per isotope, identified by the ENDF MAT number
  - Can be from as much as 10 sources
- **Hazard Classification File:**
  - Provides air and water dilution factors and CAT3 hazard classification values for analyses of nuclear hazards according US-CFR (could be substituted by other country specific information)
- **The fission yield data are fixed for now and based on ENDF/B-VI**

LIBRARY MAKER (Cont.)

Data Selection:

- **Option of building complete library or supplementing/modifying library**
- **In case multiple decay sources are provided:**
  - Data for a specific isotope are picked from the first source of a ranked list of sources
  - Data for isotopes with beta decay are picked from the first source providing decay gamma information
- **In the case of multiple activation cross section sources:**
  - the source with the most complete reaction branches is picked
  - If multiple sources provide equally complete data, the ranking of the source listing is decisive
  - Combining the partial cross sections from different sources is possible

CINDER2008 Data Libraries

Neutron cross section libraries were completely reformulated for CINDER2008

- The **CINDER90 used one library** with 63 groups from 10^{-11} MeV to 25 MeV
  - Cross sections collapsed from pointwise ENDF using a hybrid fission-fusion weighting function
- **CINDER2008** has three data libraries with energies 10^{-11} MeV to 20 MeV or 25 MeV

Weighting Function	Number of Groups	Maximum Energy (MeV)
Fission	66	25
Fusion	175	19.64
Constant	321	25

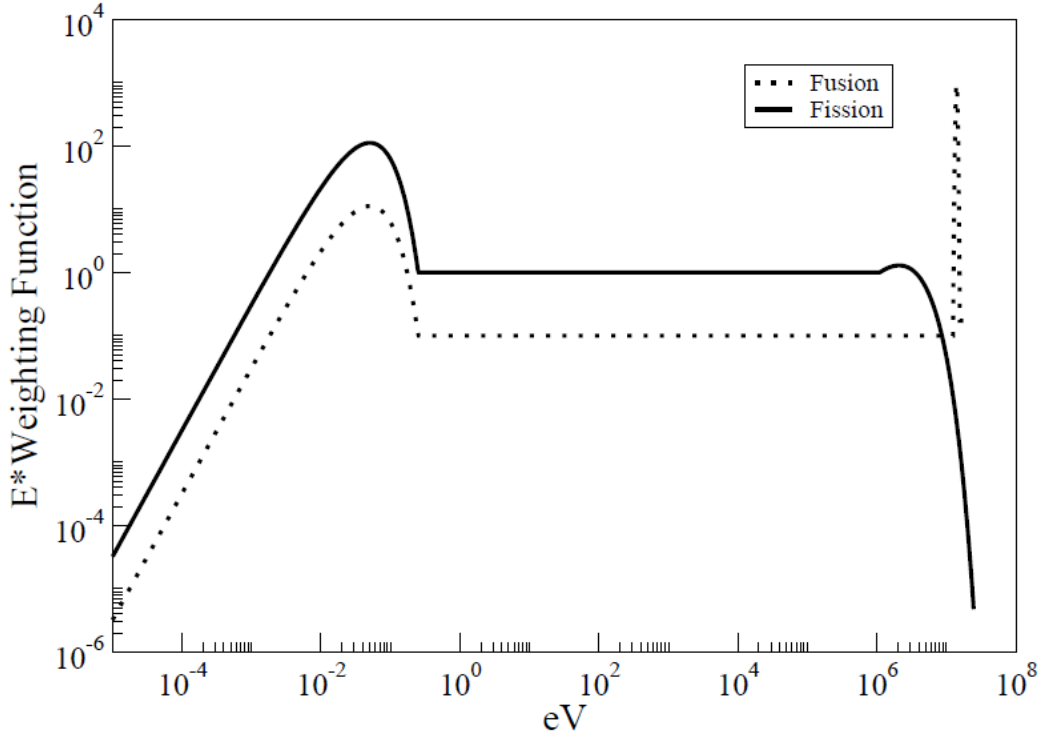
CINDER2008 Data Libraries (Cont.)

- The cross-section data for the **CINDER2008** libraries were taken from **several evaluated data files**, including ENDF/B-VII, JENDL-4.0 and -3.1, and EAF-2010
- The decay-only data (nuclide properties) were also combined from different sources

Sources of CINDER data

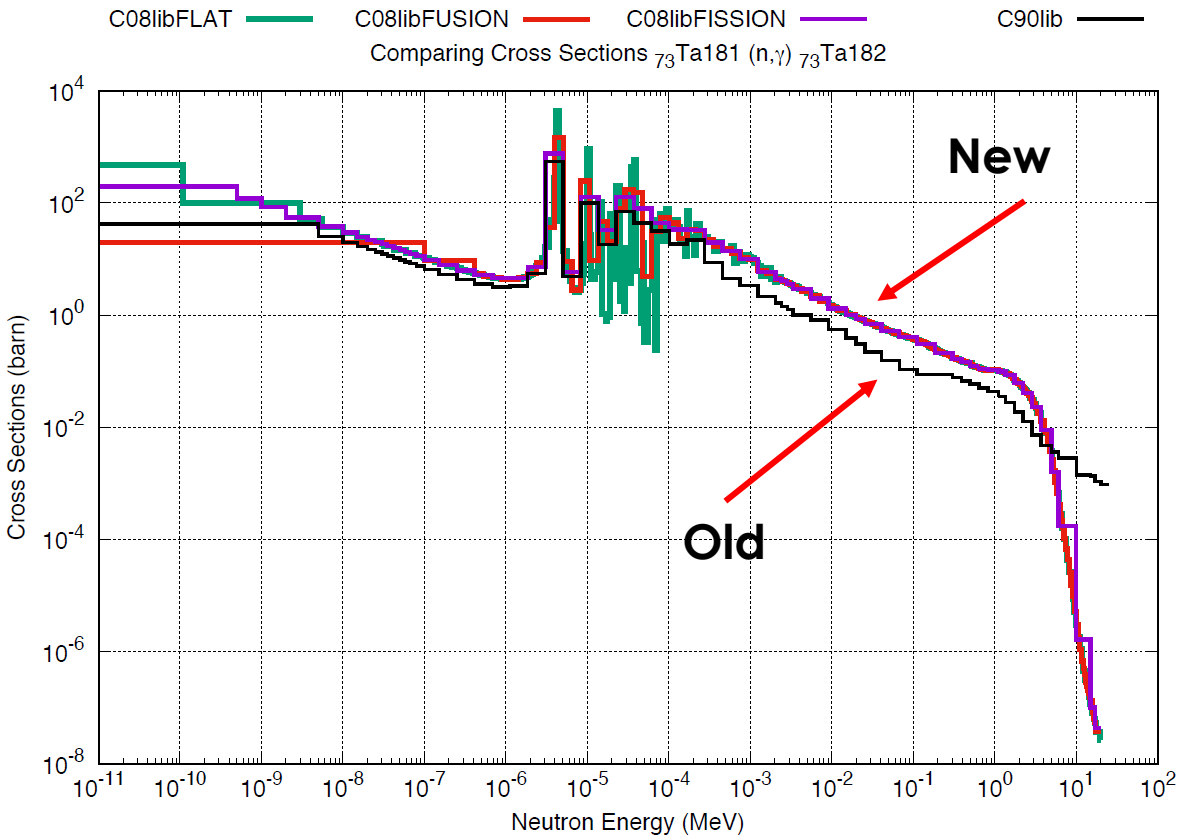
xsec library	number of nuclides
none (decay only)	3265
EAF-2010	386
ENDF VII	162
JENDL 4.0	138
mixed libraries	113
JENDL 3.1	20

Weighting spectra for CINDER2008 data libraries

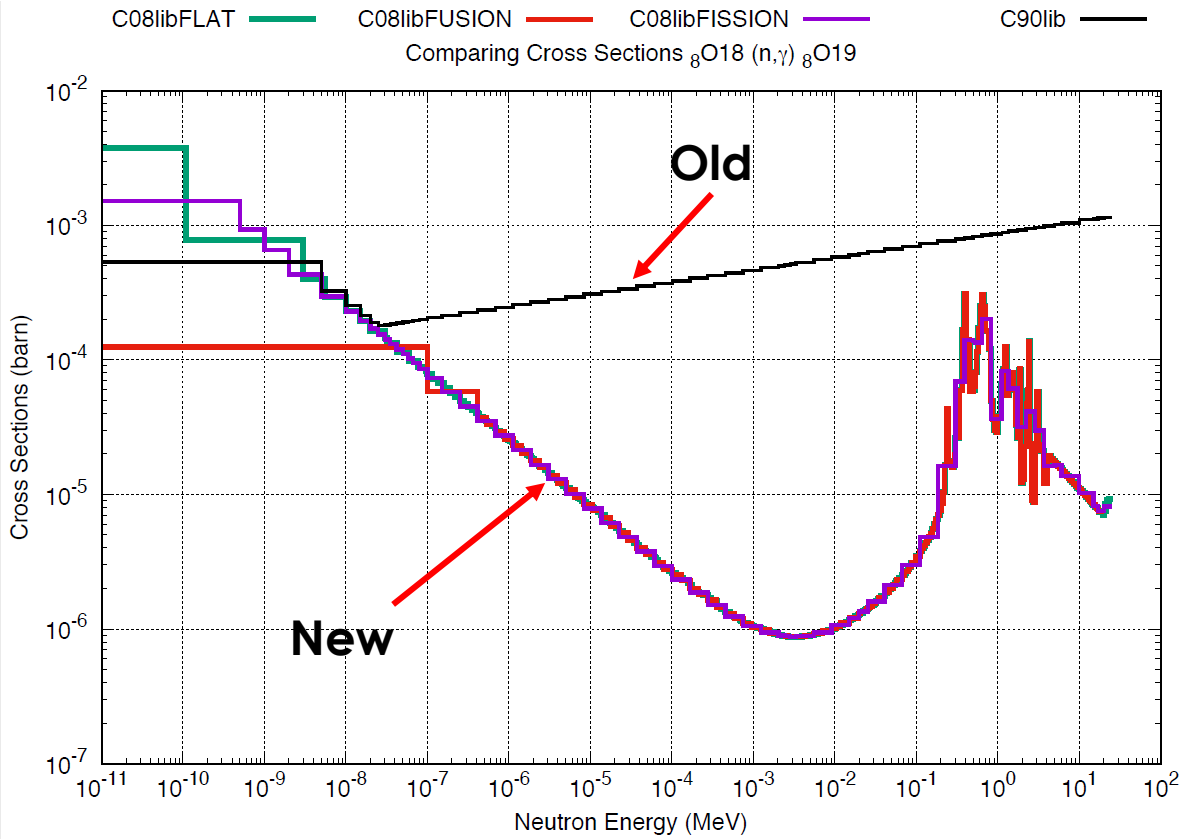


CINDER2008 Data Libraries (Cont.)

Ta-181 (n,g)



O-18 (n,g)



POST Code

In CINDER2008, post-processing can be done:

- **with POST code after CINDER2008 run(s)**
- **initiated directly from CINDER2008 input (new)**

The underlying routines of these two functionalities are the same, and the results are identical.

Both options allow processing multiple cells (regions) separately and merging results to obtain totals.

After the inventory of radioactive nuclides has been calculated, one of the frequent tasks is to determine the hazard category of the facility.

POST Code (Cont.): Hazard Category

In the US regulations the ***SOF*** is used to determine the hazard category of the facility.

$$\boldsymbol{SOF} = \sum_i \frac{A_i}{TV_i}$$, where $\boldsymbol{A_i}$ **is the activity of radionuclide *i*** and $\boldsymbol{TV_i}$ **is the threshold value of the isotope**, (for example for CAT-3) given in the DOE standard.

Using POST *SOF* are calculated with CAT-3 values that are contained in the reaction libraries; below is header for the Na-22 in CINDER2008 C08lib_fission:

```
# 114:  220110  Na 22     H-L=  8.2135E+07 DKref:E70 LEVEL_E: 0.0000E+00 SPIN:   3.0 PARITY:  1.0
 EL=  1.9524E-01, EEM= 2.1975E+00, EH=  0.0000E+00, SFBF=  0.0000E+00, ISFYSET= 0, PN=  0.0000E+00
      1 non-SF decay paths:
   1:   1.0000E+00 to # 113:  220100  EC
   AIR=   9.0000E-10   WATER=   6.0000E-06   REF: CRF          CAT3=   2.4000E+02
  25-group gamma spectra               average E = 2.1975E+00 eqv to  1.00 *EEM
  1.5978E-03  0.0000E+00  0.0000E+00  0.0000E+00  0.0000E+00  0.0000E+00  0.0000E+00  1.8076E+00  0.0000E+00  0.0000E+00
  9.9941E-01  0.0000E+00  0.0000E+00  0.0000E+00  0.0000E+00  0.0000E+00  0.0000E+00  0.0000E+00  0.0000E+00  0.0000E+00
  0.0000E+00  0.0000E+00  0.0000E+00  0.0000E+00  0.0000E+00
```

Recently updated CAT3 threshold values are included in AAREV1.0 in the **thcat3_lanl2014_zas.dat** file and can be applied by adding the instructions:

```
post_options
  run  1
  postdir  act08-31
  thcat3  ../data/thcat3_lanl2014_zas.dat
```

Threshold values relevant for a different country could be applied in the same way.

Accident Analysis Tools

The AAT combine user-supplied data with CINDER2008 inventory calculations to determine:

- **total effective dose equivalent** (TEDE), due to release of radioactive material
  - TEDE is the sum of “external” and “inhalation” dose (DDE and CEDE)
  - DDE deep-dose equivalent, DDE is whole-body dose from an external source of ionizing radiation at a tissue depth of 1 cm
  - and CEDE, the committed effective dose equivalent, CEDE is internal radiation dose (inhalation)

and/or

- **material inventory threshold ratios** for inventory control

If requested, tables of temporal CEDE, DDE, TEDE and/or the threshold ratios are produced for each region as well as the total of all regions

AAREV1.0 example problem #3 illustrates the use of the Accident Analysis Tool

Activation Script

Activation is a Perl script developed by Franz Gallmeier, Michael Wohlmuther and Ryan Bergmann

Activation script (version 2.0):

- processes MCNPX/6 output
- prepares CINDER2008 inputs
- runs CINDER2008
- runs POST to post-processes CINDER2008 results (if requested)
- runs Accident Analysis Tools

Requires very short input:

- suitable defaults appropriate for many cases are provided for most input parameters

Requires that MCNPX/6 run uses certain options and tallies.

Bottom line: **Makes running activation calculations simple!**

- **greatly reduced user effort required for activation calculations**
- improved reliability due to automatic transfer of cell and material specifications from MCNPX/6 to CINDER2008

Supports not only CINDER2008, but also SP-FISPACT and ORIHET3 code version 1.12.

Activation Script (Cont.)

Activation script INPUT blocks:

- codes (defaults cinder, htape3x..)
- **title_lines**
- files (defaults assume outp, histp (if needed) and bigza in working directory)
- run_options
- cinder_options
- post_options
- aat_options
- fispact_options
- orihet_options
- **normalization**
- **history**
- **cell_list**

The blocks shown in bold represent minimum input and are always required.

Activation Script (Cont.)

Initial MCNPX/6 run must meet certain requirements:

- **An f4:n tally** provides cell-averaged neutron fluxes with "appropriate" energy binning
  - Matching energy binning to CINDER2008 data libraries is best but not required
  - No multiplier bins or FQ (print hierarchy) cards
- **Spallation products tally** (i.e., residual nuclei from model interactions) written to histp file or to MCNPX/6 output with "**rnucs**" tally
  - If you don't use one, you don't get those nuclei
- **Transition to model regime at 20 MeV or 25 MeV** (depending on XS library to be used with CINDER2008)
- **A "CSIZE" tally if GAMMA_SCRIPT is to be used** to obtain cell bounding dimensions (and patched MCNPX/6 is available)
- **No repeated structures or lattices**

Activation Script (Cont.)

ACTIVATION script INPUT example (minimal)

title_lines
one line is enough

assumes MCNPX files outp, histp (if needed), assumes bigza in working
directory (bigza gives natural abundance by isotope, is provided in AARE V1.0)
files

CINDER90 is used for the activation analyses: use all defaults
cinder_options

no defaults are given for the normalization
normalization
snorm 2.8e13

one time step
history
1 1.0E+00 1.0E+0 s

a one cell problem is started by giving the cell_list
cell_list
comment for cell 10
10

Gamma Source Script

Gamma Source is a Perl script which was developed by Franz Gallmeier and Michael Wohlmuther

GAMMA_SOURCE processes ACTIVATION / CINDER2008 output to produce source definition cards (SDEF) for MCNPX calculation of gamma-ray fields around activated structures

Required input data files are:

- Input for the script,
- cell_dir_vol_list file created by the Activation script,
- cell size file (optional) or cell size information provided by MCNPX/6 csize tally
- spectra/TAB4 files for the cells of interest (in the directories created by the Activation scrip

Typical gamma script input:

```
run_options
    time_step 6
    stype broad-high
files
    mcnpx_outp outp
    csize cell_size
```

AARE V1.0: Extensions for MCNPX/6

AARE V1.0 provides patches to include tallies RNUCS and CSIZE in MCNPX/6

- **Spallation products tally** "**RNUCS**" writes tallies of the residual nuclei from model interactions directly to MCNPX/6 output
  - The use of histp is not necessary
  - Works also with MCNP6 (in MCNP6 the spallation products are not written properly to the histp file)
- **The "CSIZE" tally** provides the information on the cell bounding dimensions in the form:
  - CELL NUMBER Xmax Xmin Ymax Ymin Zmax Zmin
  - This dimensions are then used in GAMMA SOURCE to prepare source definition for MCNPX/6. Sampling of gamma-ray staring point for the selected cell is restricted to the extent of volume bound by rectangle (Xmax Xmin Ymax Ymin Zmax Zmin) for that cell.

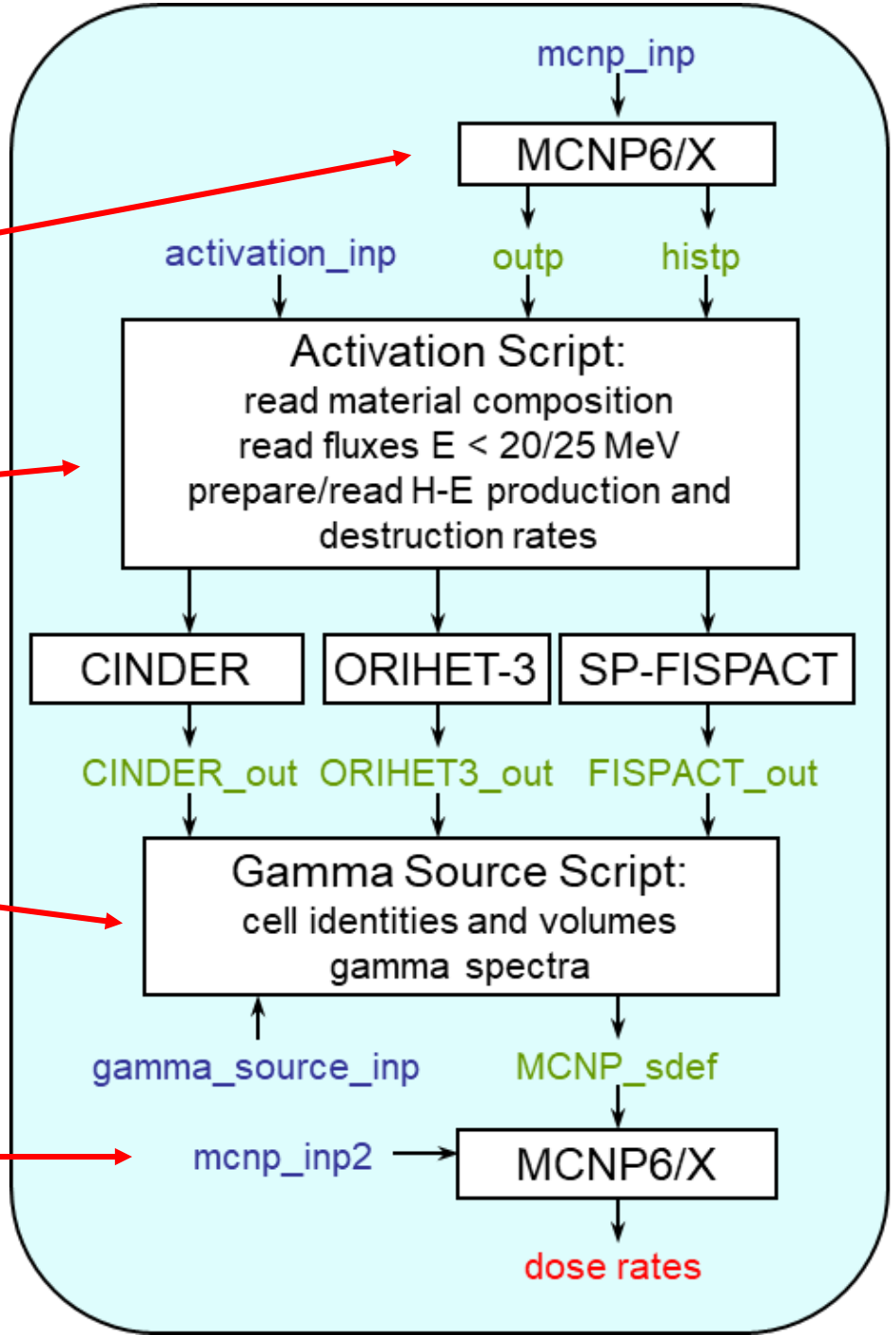
AARE V1.0: Run Sequence bringing it all together

First MCNPX/6 run calculates fluxes and nuclide production/destruction for the irradiated structure

Activation prepares and runs CINDER activation calculations for the specified irradiation history

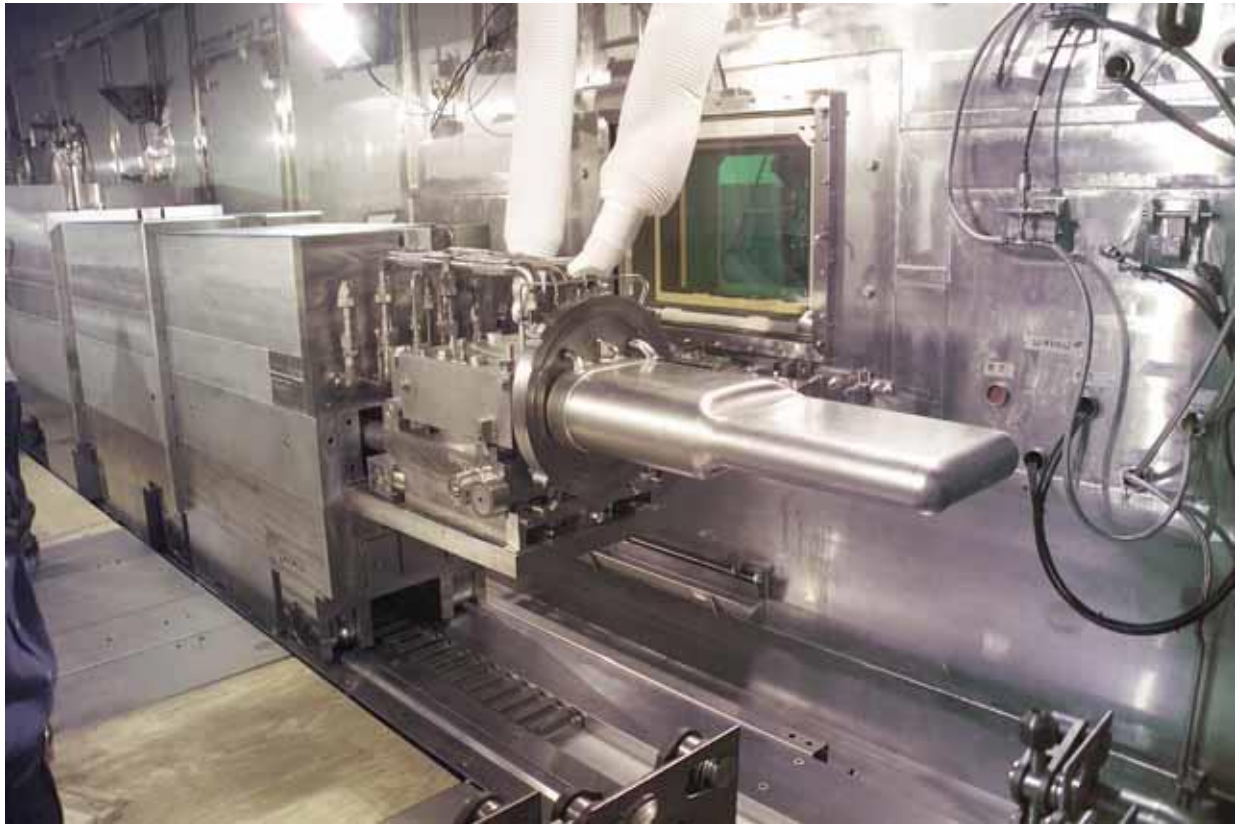
Gamma source scripts prepares gamma-ray sources

Second MCNPX/6 run calculates dose rates in/around irradiated structure.



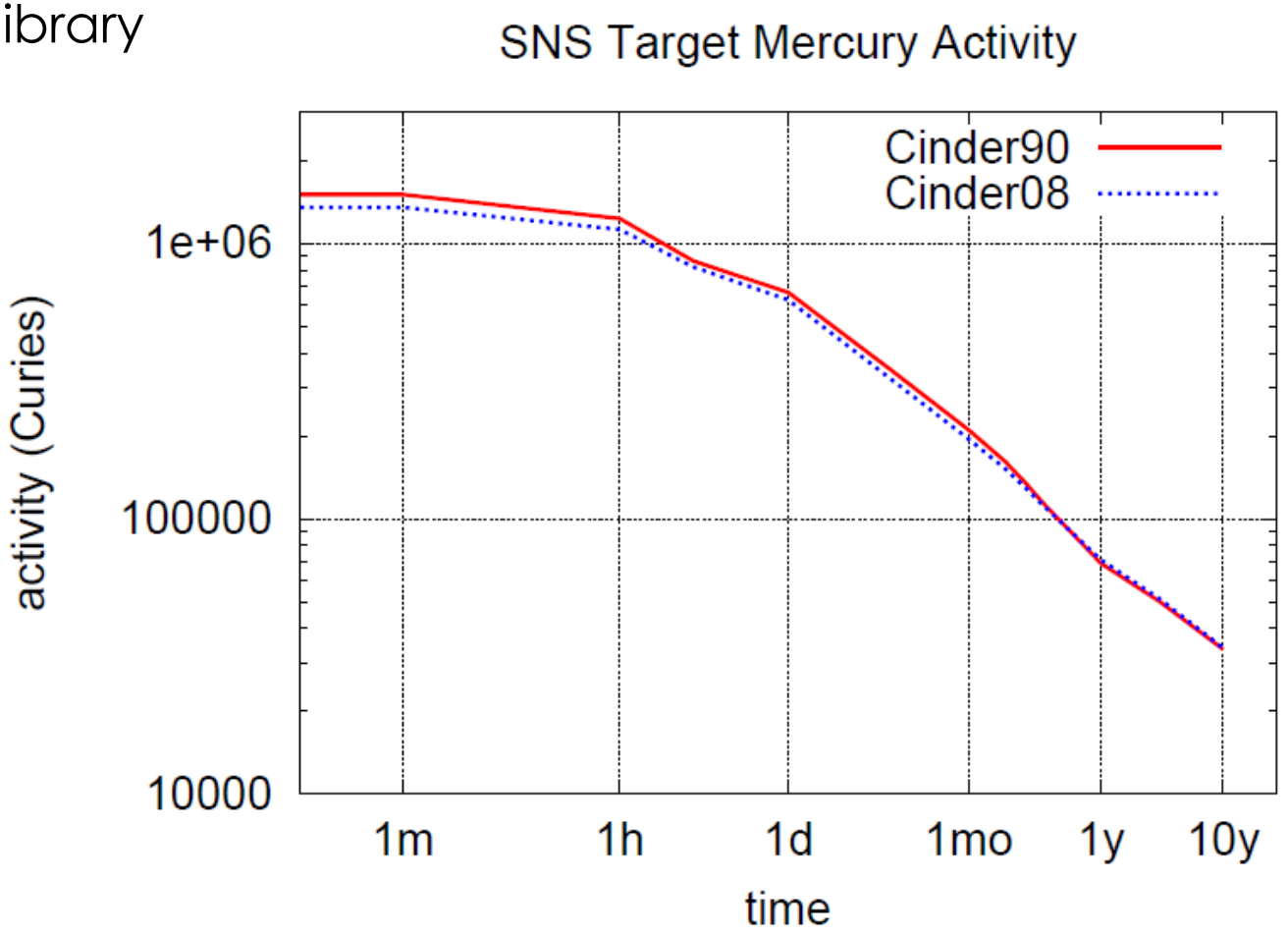
Comparison: CINDER90 vs CINDER2008 – SNS Mercury Target Activation

The ORNL Spallation Neutron Source uses a liquid mercury target (high Z, high density, liquid at room temperature) to generate neutrons for use in experiments in condensed matter and fundamental physics.



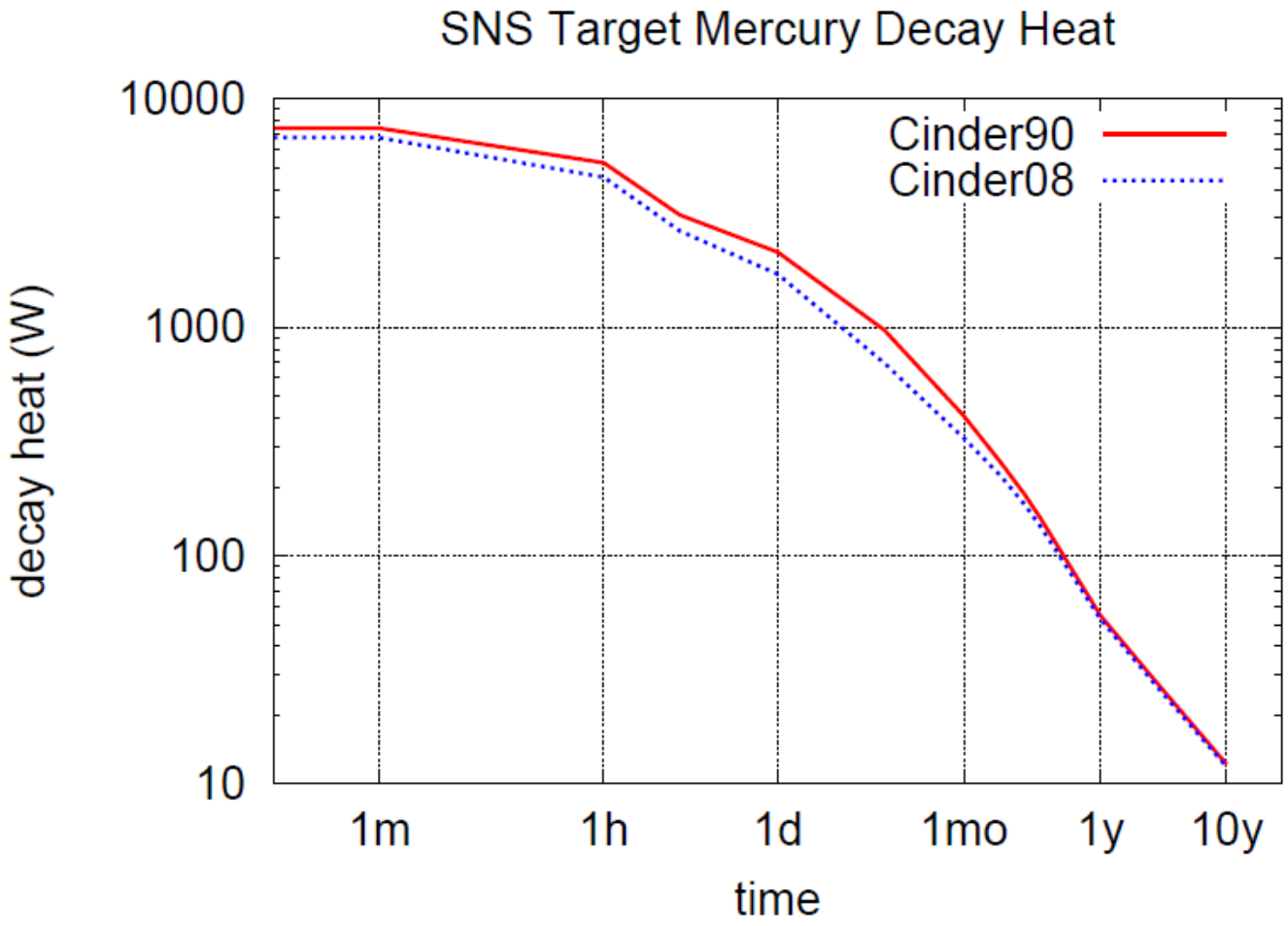
Comparison(Cont.):

- All CINDER calculations use the same MCNPX output
- CINDER90 used CINDER90 library
- CINDER2008 used CINDER08_fission library
- SNS liquid mercury target activation is for 5000 h/y operation for 40 years at 2 MW proton beam power



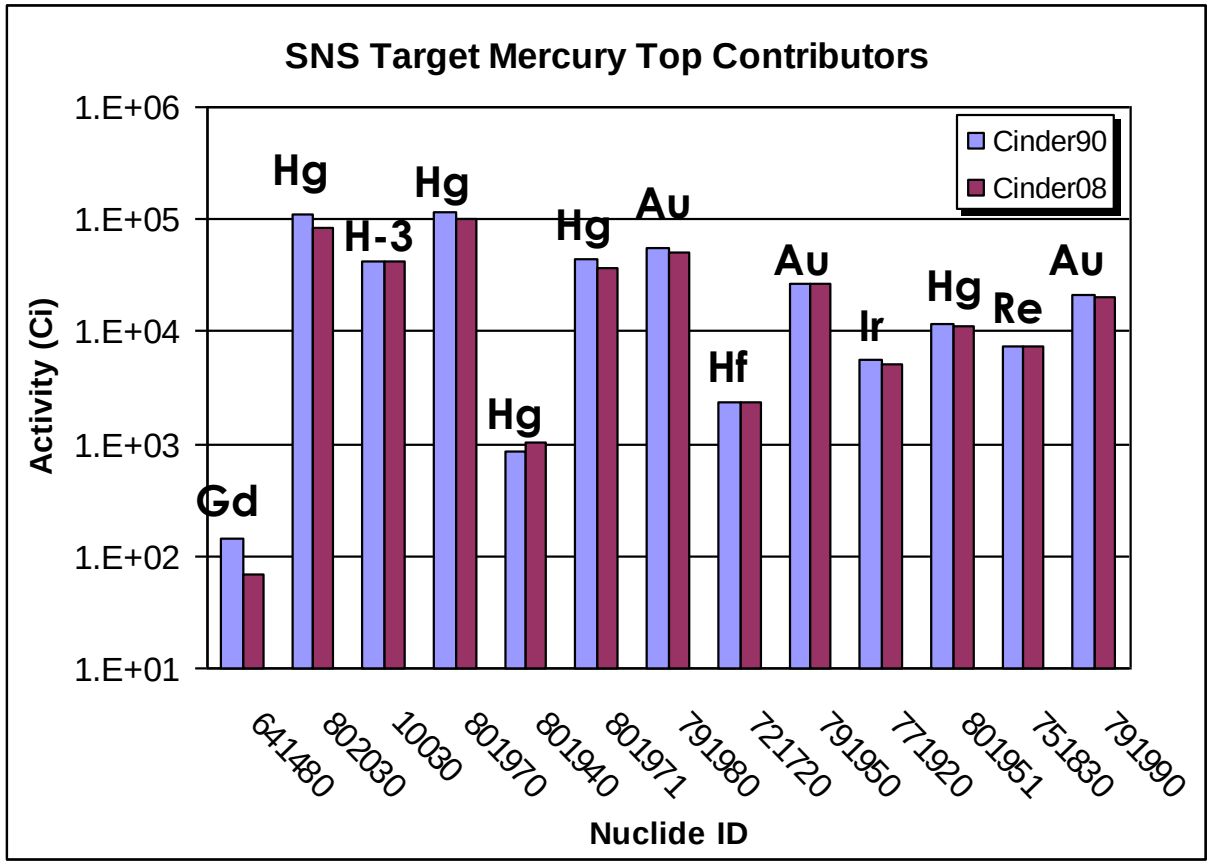
Comparison(Cont.):

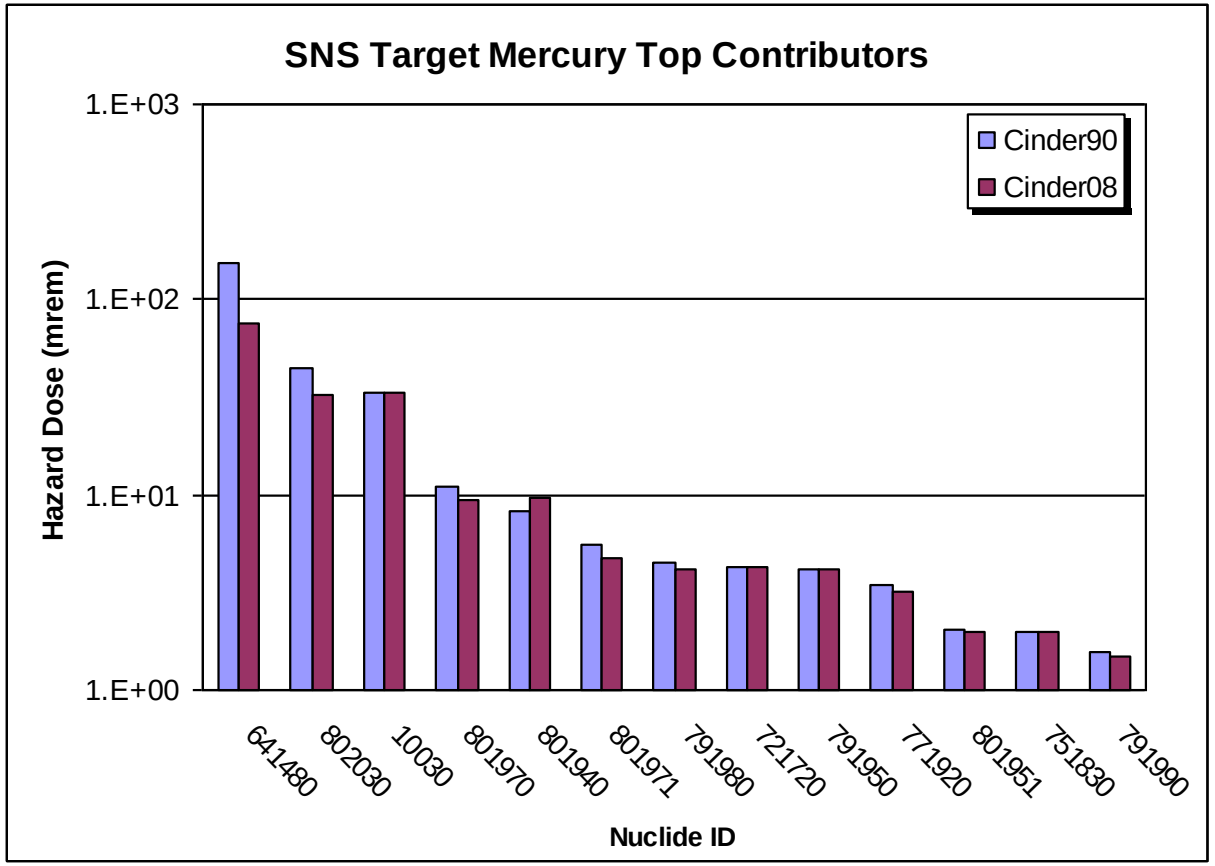
- SNS liquid mercury target decay heat for 5000 h/year operation for 40 years at 2 MW proton beam power



Comparison(Cont.):

- Radioactivity release due to loss of heat sink
- Hazard comparison based on dose calculated with the same release fractions, inhalation dose conversion factors, dispersion and breathing factors, and 30 minutes decay time following release.





Conclusion

AARE V1.0 is available from RSICC as Code Package CCC-846

- Contains CINDER2008 with LIBRARY_MAKER, three data libraries, POST code, and Accident Analyses Tools
- Activation Script Version 2.0
- Gamma Source

AARE V1.0 provides a versatile collection of tools which allows for faster and more reliable activation and dose rate calculations.

Thank You for Your Attention

Additional Slides

CINDER2008 (Cont.): List-directed input option

```
Sample H-liq/He-liq/Li-Solid geometry: 1h@10mA X-MeV Protons; cool 90 days
1.25664e+002,1.00000e+001,,,,,,,,,,2,,,,0,1,'H ',,,/
Liquid Hydrogen Region
of a 3-Reg 10-cm long annular Cyl:0 < H-liq < 2cm < He-liq < 4cm < Li-sol < 6cm
Calculated with CINDER2008
H Region
H -liq
4 1.E1
     1.0D0 's'   -1.0E0 'm'   -1.0E1 'm'   -1.0E1 'h'
6 0.E0
     1.0E0 's'   -1.0E1 'm'   -3.0E0 'h'   -1.0E0 'd'
    -1.0E0 'w'   -9.0E1 'd'
START
```

File: input_H

from AAREV1.0, Examples,sample1

CINDER2008 (Cont.): NAMELIST input option

```
&INPUTS
CALCULATION = ' Sample H-liq/He-liq/Li-Solid geometry: 1h@10mA X-MeV Protons; cool 90 days',
VOLCC = 3.76991e+002
DESCRIPTION(1) = 'Liquid Helium Region',
DESCRIPTION(2) = 'of a 3-Reg 10-cm long annular Cyl:0 < H-liq < 2cm < He-liq < 4cm < Li-sol < 6cm',
DESCRIPTION(3) = 'Calculated with CINDER',
FLUXNAME = 'HeRegion',
MATNAME = 'He-liq',
FLXMLT = 1.00000e+001,
NTS = 10,
VOLS_INFO = 'CONTINUE',
SUFFIX = 'He',
GASOPT = 0,
/

&TSINFO
FACTOR(1:4) = 4*1.e1,
DELTAT(1:4) = 1.e0, -1e0, -1e1, -1e1,
IUBT(1:4) = 'S' 'M' 'M' 'H',
FACTOR(5:10) = 6*0.E0,
DELTAT(5:10) = 1.E0 -1.E1 -3.E0 -1.E0 -1.E0 -9.E1,
IUBT(5:10) = 'S', 'M', 'H', 'D', 'W', 'D'
/
```

File: input_He

from AAREV1.0, Examples,sample1

CINDER2008 (Cont.): Automatic post-processing capabilities

In CINDER2008, post-processing calculations can be:

- performed after completed CINDER2008 run utilizing the software package POST (traditional)
- **initiated directly from CINDER2008 input (new)**

The underlying routines of these two functionalities are the same, and the results are identical.

Both options allow processing multiple regions separately and merging results to obtain totals for the group of regions.

CINDER2008 (Cont.): constant power approximation

Allows the user to specify the total (*n,f*) neutron-induced fission power desired for each campaign.

- "turned on" by providing negative the flux multiplier, flxmlt
- the user must provide the desired constant power density (Watts/cc) and the acceptable deviation from the given power density (in percent difference) for each campaign
- if the desired constant power density is given as ≤ 0, the power density of the first non-zero flux time-step will be maintained
- For each non-zero flux time-step, CINDER2008 completes the time-step, calculates the power density and verifies that it is within the acceptable range. If it is not, the flux is renormalized and the time-step is recalculated. The final flux magnitude in each time-step is given in the output file *results*.

CINDER2008 (Cont.): high-fidelity β-delayed gamma spectra

Spectra of gamma ray emitted after particle decays are maintained in the CINDER2008 data library in a 25-group energy structure.

For some applications finer energy grid is preferred. CINDER2008 includes a separate data library, ***cindergl.dat*** which contains the available **discrete** and **continuous source** data used to obtain the 25-group library.

CINDER2008 can process the discrete and continuous data to provide delayed gamma spectra on a user-defined energy grid.

CINDER2008 could provide high-fidelity spectra for β-delayed neutrons. However, the underlying data library required for this feature, ***cinderdn.dat***, is not yet included.

POST Code (Cont.)

In the US regulations the SOF is used to determine the hazard category of the facility.

$SOF = \sum_i \frac{A_i}{TV_i}$, where A_i is the activity of radionuclide *i* and TV_i is the threshold value of the isotope given in ithe standard

Hazard Category - 3 sum-of-fractions for a radionuclide inventory

- DOE STANDARD HAZARD CATEGORIZATION AND ACCIDENT ANALYSIS TECHNIQUES FOR COMPLIANCE WITH DOE ORDER 5480.23, NUCLEAR SAFETY ANALYSIS REPORTS DOE-STD-1027-92December 1992CHANGE NOTICE NO.1September 1997
- DOE STANDARD HAZARD CATEGORIZATION OF DOE NUCLEAR FACILITIES, DOE-STD-1027-2018, November 2018

DOE HazCat-3 Thresholds

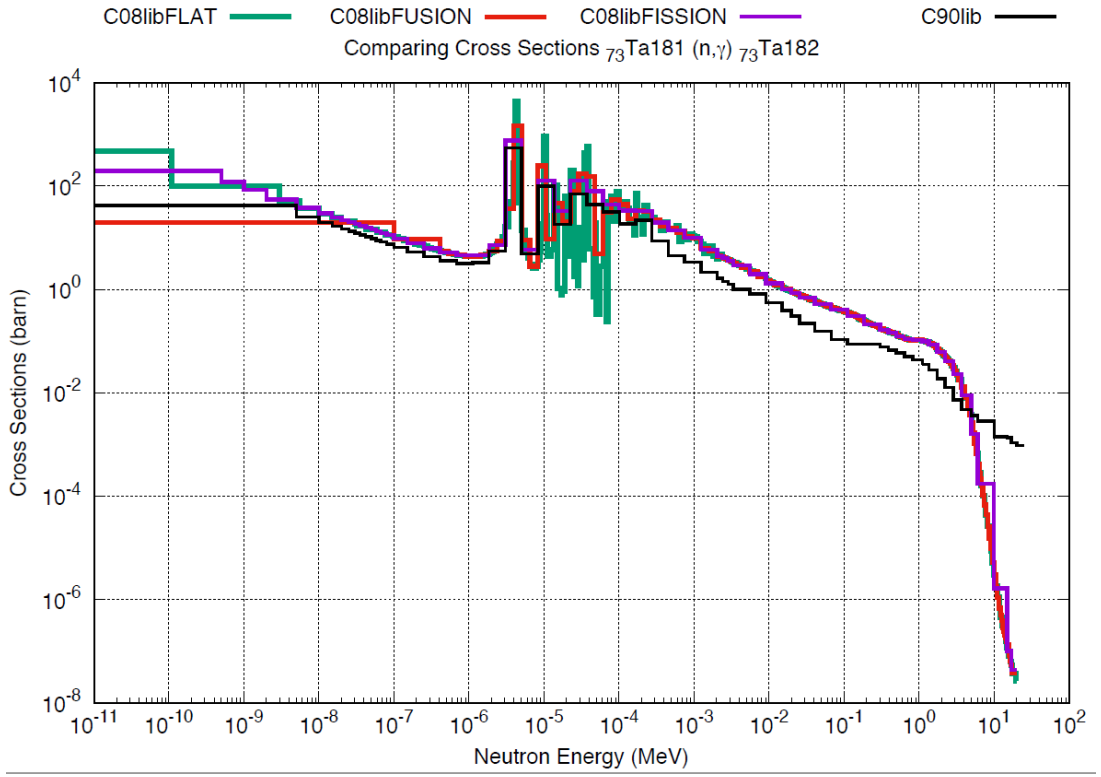
- USDOE (and the national laboratories) have adopted revised threshold values
- Some threshold quantities increased; others decreased
- Threshold values other than those given in the reaction libraries can be used by making a file *thcat3* available in the directory in which POST is run
- Note that while the CINDER2008 data libraries have nuclides organized according to AZS, the *thcat3* file still uses ZAS designators (as with CINDER90)
- The simple *thcat3* file can change the threshold values used for these nuclides from the ones in the reaction data library to those in the table

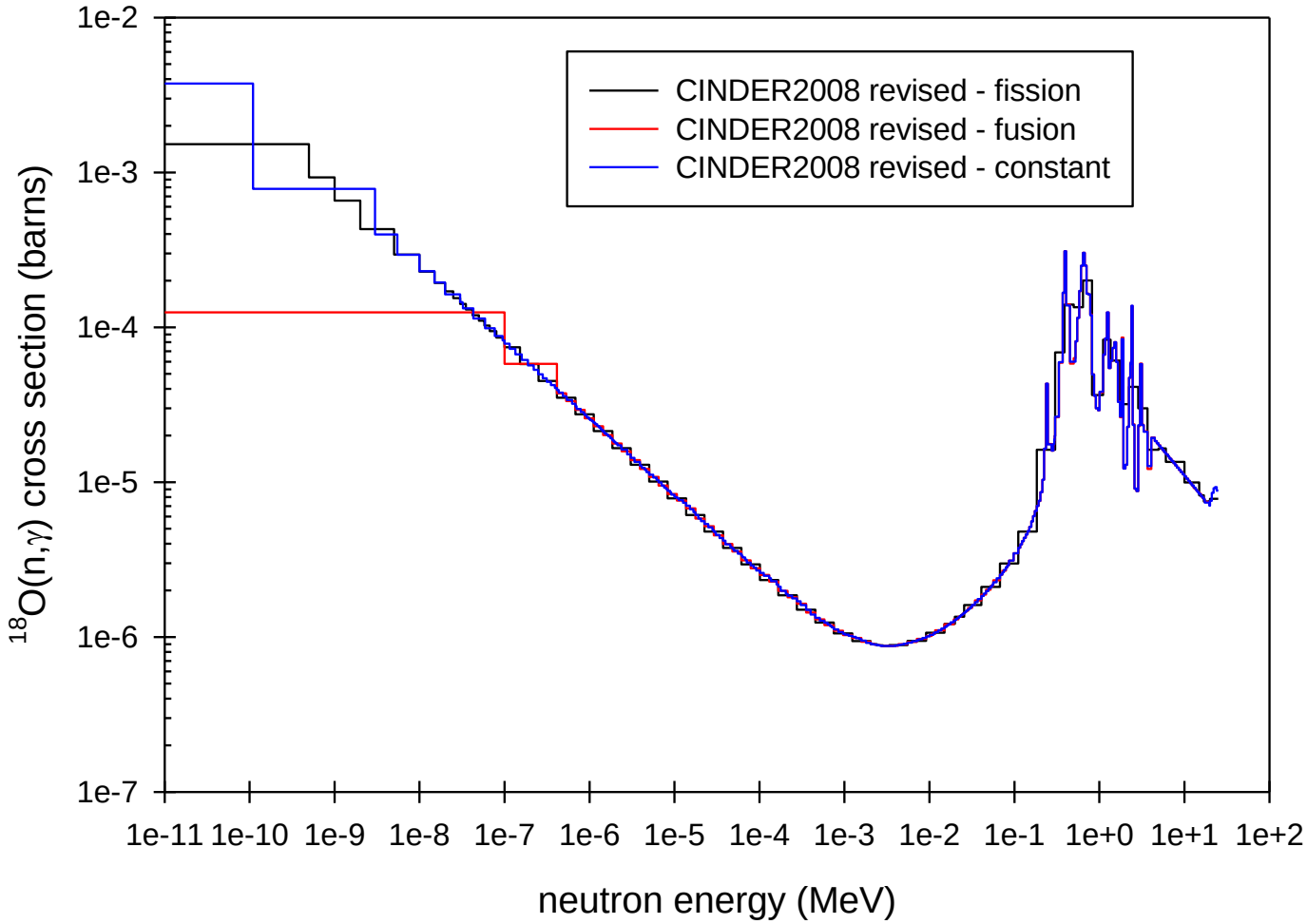
nuclide	original value		revised value	
	Ci	g	Ci	g
Na-22	2.4e+2	3.8e-2	2.54e+2	4.0e-2
Ti-44	6.2e+1	3.6e-1	9.31e+1	6.9e-1
Co-60	2.8e+2	2.5e-1	2.90e+2	2.6e-1
Zn-65	2.4e+2	2.9e-2	2.06e+2	2.4e-2
Mo-99	3.4e+3	7.1e-3	3.85e+3	8.8e-3
Cs-137	6.0e+1	6.9e-1	6.19e+1	7.0e-1
Hg-203	3.6e+2	2.6e-2	5.18e+2	1.3e-1

thcat3 file

```
110220 2.54E+02
220440 9.31E+01
270600 2.90E+02
300650 2.06E+02
420990 3.85E+03
551370 6.19E+01
802030 5.18E+02
```

CINDER2008 Cross Section Libraries (Cont.)

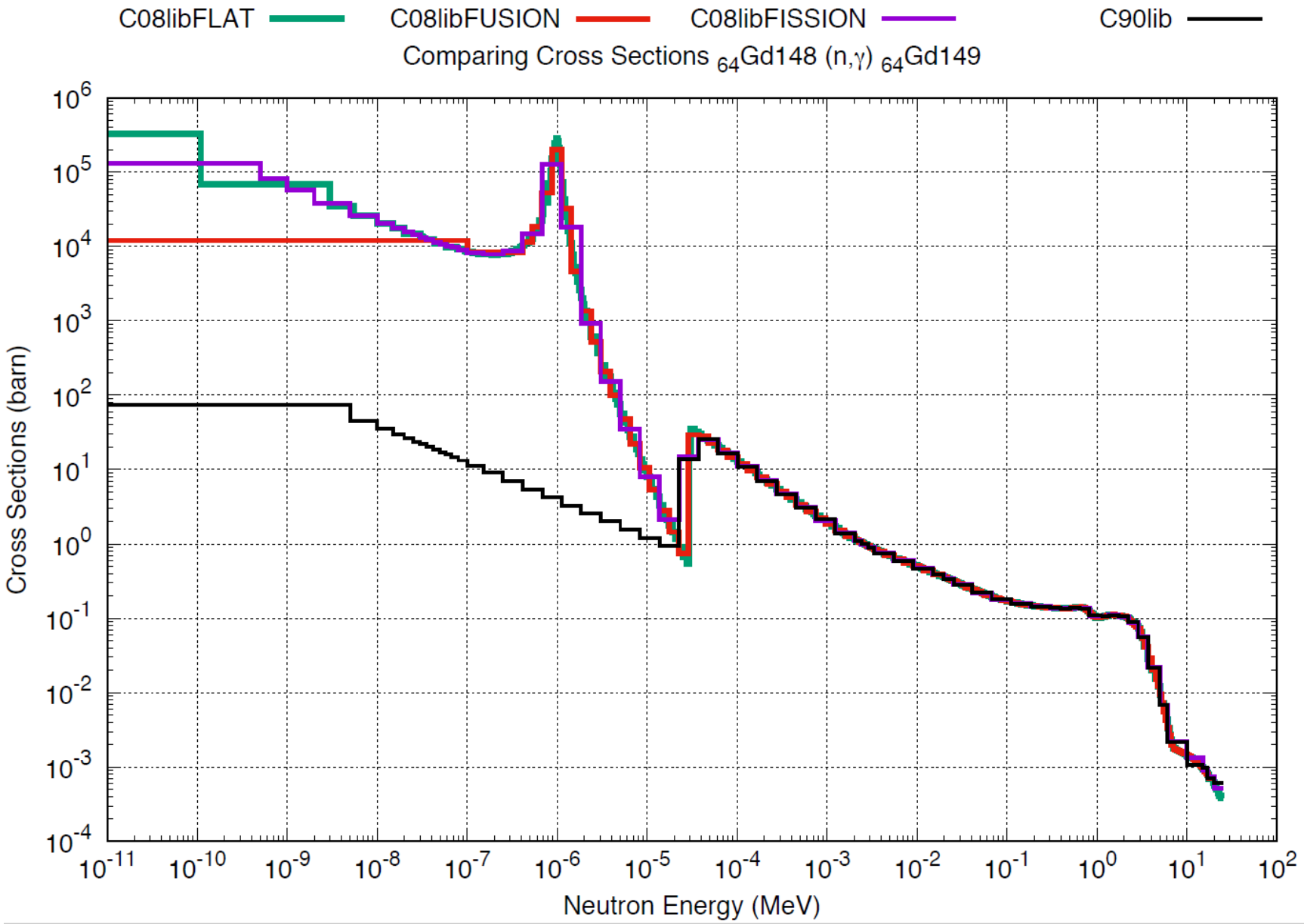




CINDER2008 Cross Section Libraries (Cont.)

Differences in Gd184 between Cinder90 and Cinder2008 shown on slide #29 are due to the differences in cross-sections shown here.

So they are caused by the differences in the Gd-148 destruction rates.



Accident Analysis Tool

- A new feature in CINDER2008 is an Accident Analysis Tool, which provides an estimate of the dose due to release of radioactive material
- The calculation takes into account both submersion (external) and inhalation (internal) dose
- The user may input nuclide-specific values for many quantities, or specify global values to be used for all nuclides
- CINDER does not perform an atmospheric dispersion calculation, but uses a user-specified dispersion factor, and thus has no explicit time dependence

$$TEDE = T_E \cdot X \cdot [DCF_E + DCF_I \cdot BR \cdot RF]$$

- Total Effective Dose Equivalent (TEDE), where:

T_E = exposure time
X = radionuclide concentration (Bq/m^3)
DCF_E = external dose conversion factor (Sv/h)/(Bq/m^3)
DCF_I = internal dose conversion factor (Sv/Bq)
BR = breathing rate (m^3/h)
RF = respirable fraction

CINDER2008 Data Libraries

Neutron cross section libraries were completely reformulated for CINDER2008

- The **CINDER90 used one library** with 63 groups from 10^{-11} MeV to 25 MeV
  - Cross sections collapsed from pointwise ENDF using a hybrid fission-fusion weighting function
- **CINDER2008** has three cross-section libraries with energies 10^{-11} MeV to 20 MeV or 25 MeV
  - **66-group fission-weighted library** has the same group structure as the 63-group library, except the lowest group ($E < 10^{-9}$ MeV) has been broken into four groups (Maximum energy 25 MeV)
  - **175-group fusion-weighted library**, in the VITAMIN-J group structure; this library doesn't have many groups at low energy and is probably best reserved for special problems for which the fusion spectrum serves as a good approximation to the actual neutron flux in the system (Maximum energy 19.64 meV)
  - **321-group flat-weighted library**, based on 315-group TRIPOLI group structure; this library is expected to provide the best results overall due to higher fidelity (Maximum energy 25 MeV)