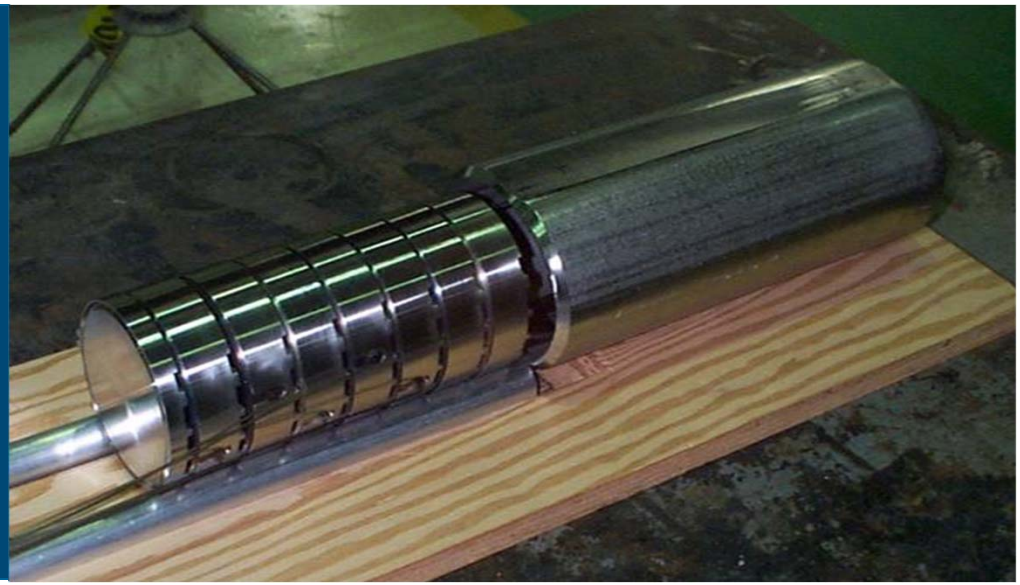
Recent Improvements to CINDER2008 and Activation Analysis Tools



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The CINDER Development Team

- CINDER development is due to a large team which includes staff from both US National Laboratories and laboratories abroad
- Argonne National Laboratory
  - Brad Micklich
- Oak Ridge National Laboratory
  - Franz Gallmeier, Erik Iverson, Wei Lu, Irina Popova, Igor Remec
- Paul Scherrer Institute (Switzerland)
  - Michael Wohlmuther, Ryan Bergmann, Daniela Kiselev
- Los Alamos National Laboratory
  - Bill Wilson, Shannon Holloway, Hannah Little, Charles Kelsey, Michal Mocko, Günter Muhrer, Eric Pitcher

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Outline of Presentation

- Introduction
- CINDER overview
- CINDER2008 and Activation (Perl) scripts – new features and developments
  - Correction of EAF-2010-derived reaction cross sections
  - cl_list data block
  - New USDOE HazCat-3 threshold values
  - CINDER accident analysis tools
- Examples
- Summary

The CINDER2008 Code Package

- CINDER has been developed since 1960, initially for reactor problems but more recently for accelerator problems
- The development team began in 2005 with the intent to package CINDER90 in a more user-friendly format
- The CINDER90 distribution from RSICC includes scripting tools in the Perl language to aid in preparing input for and running the code, and to construct an MCNP-compatible source deck for gamma-ray dose calculations

- We are attempting to clear up confusion over the names of codes/packages
  - The overall package name will be Activation in Accelerator Radiation Environments (AARE)
  - The names of Perl scripts in the AARE package are activation and gamma_source
  - CINDER2008 is the name of the transmutation code package (which can be obtained separately from LANL)
  - CINDER and POST are two codes within the CINDER2008 package
  - Although AARE supports the codes SP-FISPACT and ORIHET, these codes are not distributed as part of the AARE package

Running CINDER

- The CINDER code has four required input files …
  - *input* – identifies flux, material, temporal history, and other problem parameters
  - *fluxes* – multigroup fluxes for one or more homogenized regions
  - *material* – initial nuclide atom densities for one or more material regions
  - *library* – file with neutron reaction cross sections
- … and a number of optional input files
  - *splprods* – constant production/depletion rates of nuclides from reactions outside the particle/energy domain of the CINDER reaction library
  - *cxupdate* – multigroup cross section data that replaces or adds to the reactions in the data library
  - *locate* – gives paths to the CINDER library and *cxupdate* files
  - *dnz* – contains the results of a CINDER calculation for earlier times and a different irradiation history

Running CINDER

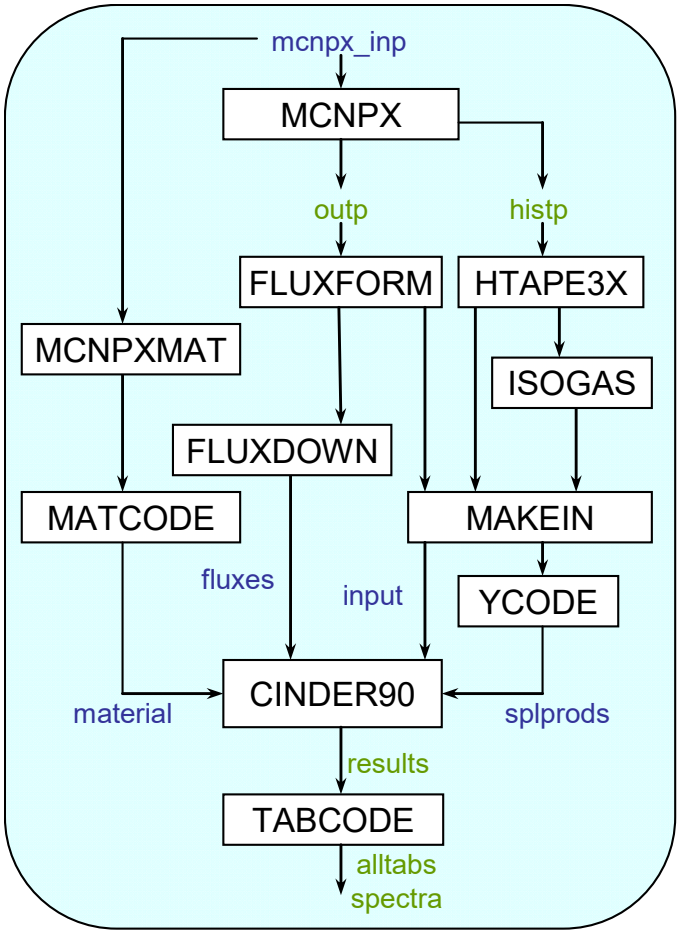
- CINDER produces a number of output files, including
  - *results* – the main output file provides initial nuclide inventories and, for each nuclide, the atom density, activity density, and delayed neutron production at the end of each time step; also decay rate, absorption rate, spontaneous fission rate and fission rate
  - *alldnz* – a binary file giving the atom densities of all nuclides present initially or produced during the calculation at each time step
  - *newshort* – a binary file containing the library data used with flux-integrated reaction data

- The code POST generates tables for a single region (or a group of regions), photon spectra, radionuclide hazards, power, dose equivalents, HazCat-3 fractions, etc.
- The tables produced by POST can be ranked at a specified time step, making it easier to determine which nuclides have the greatest contribution to a given quantity
- POST now checks that the time steps agree when combining results from several regions

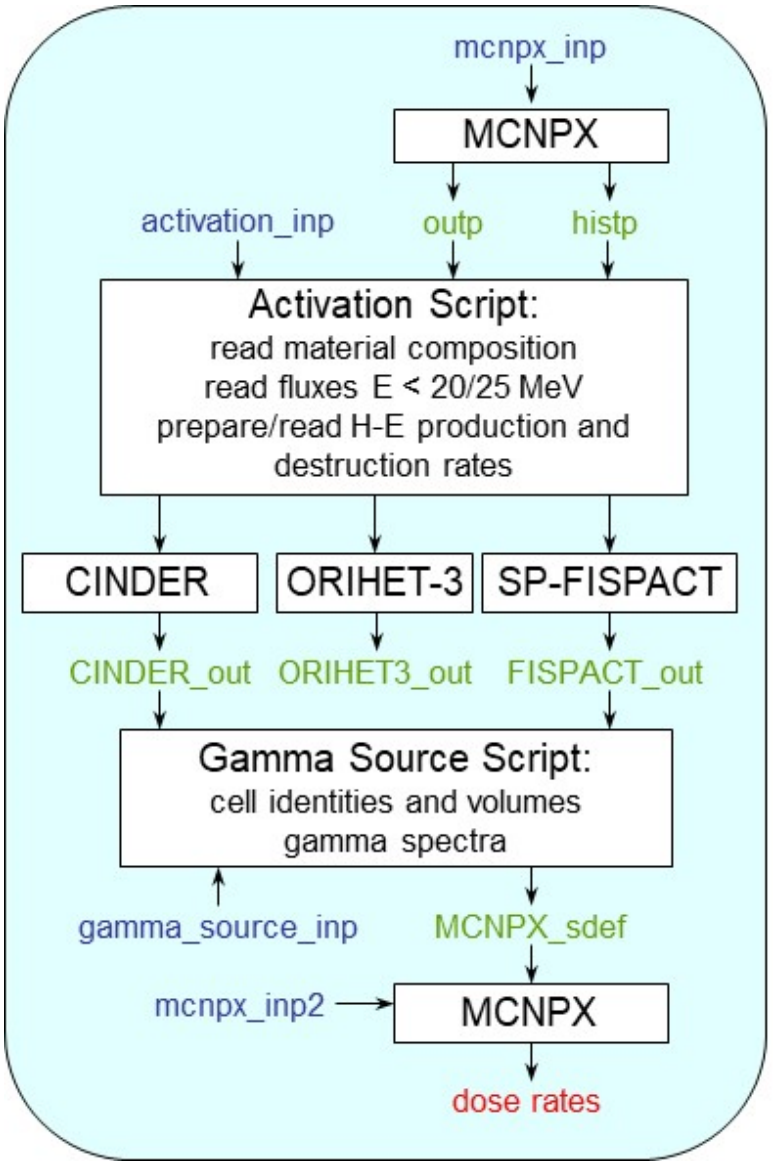
Activation Perl Script

- Scripting tools written in Perl facilitate preparing CINDER input and running the code

Original CINDER90



CINDER2008 with Perl script



Running CINDER Using the Activation Perl Script

- The script input file is used to specify the regions, irradiation history, etc. through a series of option blocks

```
title_lines
  radionuclide inventory of mini-MIPS experiment
  activity buildup during irradiation of uranyl nitrate solution
  20 kW of 35 MeV electrons on depleted uranium target

files
  mcnpx_outp du20o

normalization
  snorm    20

history
13 1.0
  0.5 h -1 h -2 h -3 h -4 h -6 h -8 h -10 h -12 h -14 h -16 h -20 h -24 h

cinder_options
  kchn     0
  klib     0
  nfe      1
  nosame   0
  fine     10000
  coarse   100000
  post     1
  itsord   13

post_options
  run  1
  postdir  UNsoln-buildup

run_options
  dname c08-soln
  dcounter 1

cell_list
 U02(SO4) solution
   15
```

MCNP output file to use

source normalization factor

irradiation history

post-processing requested; rank by values at time step 13

directory for post-processing results

directory for CINDER results (one per region)

list of cells/regions to process

CINDER Data Libraries

- The neutron cross section libraries were completely reformulated for CINDER2008
- The CINDER90 library used 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 reaction libraries covering energies 10^{-11} to 25 MeV (20 MeV)
  - 66-group fission-weighted library has the same group structure as the 63-group library, except the lowest group ($E_n < 10^{-9}$ MeV) has been broken into four groups
  - 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
  - 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 for each cross section is that from the respective reference data

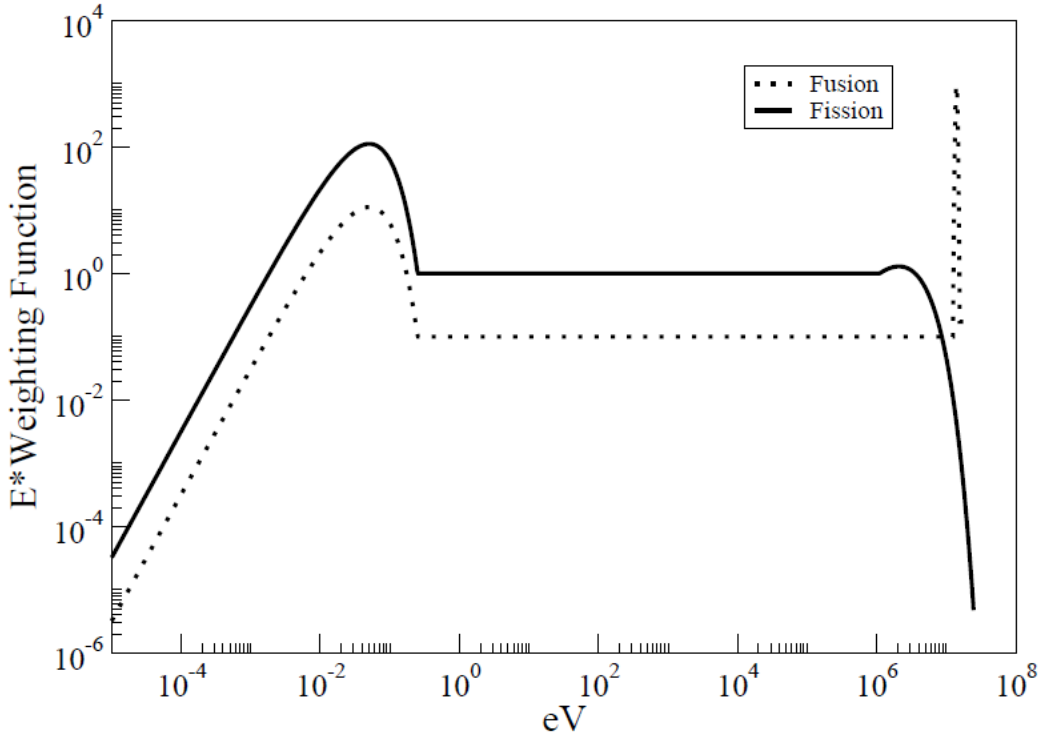
CINDER2008 Reaction Data Libraries

- The reaction 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 files (nuclide properties) are useful since CINDER can run a decay-only problem (e.g., calculating the decay products from a ^{252}Cf source)

Sources of CINDER data

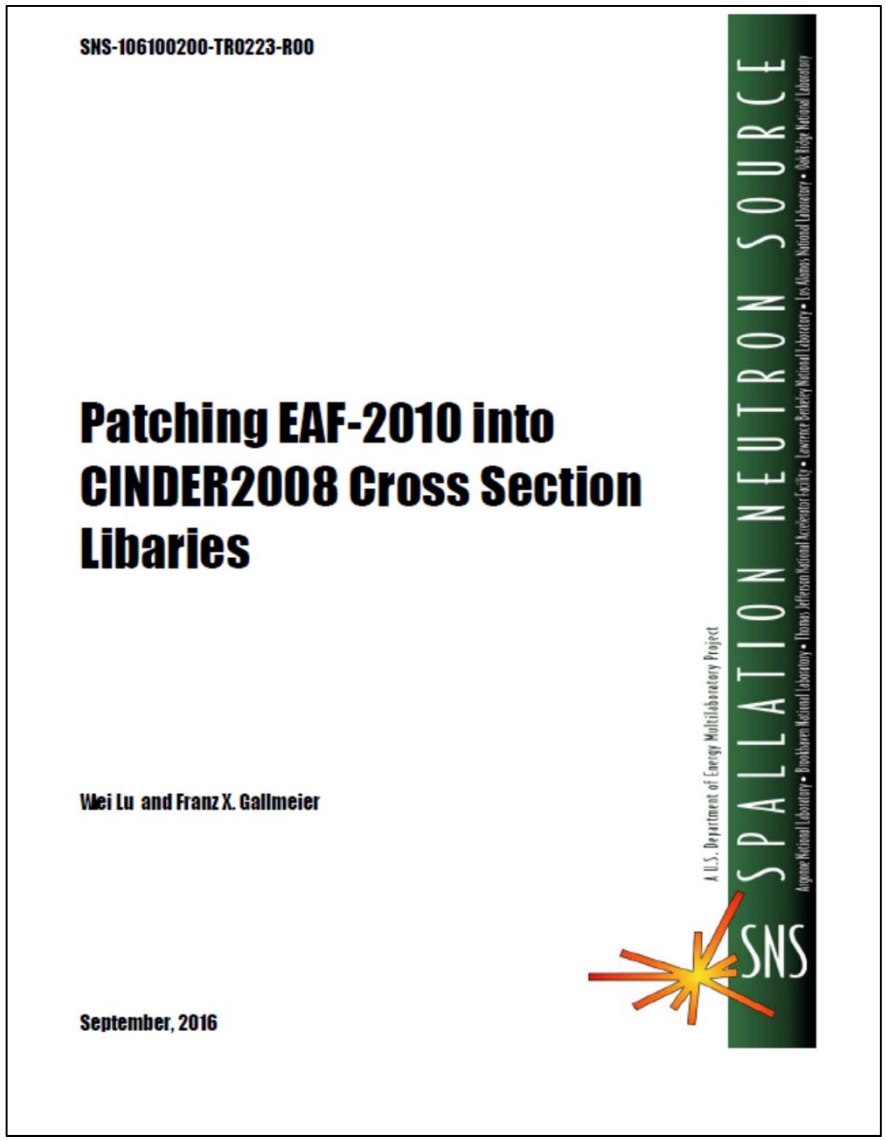
xsec library	number of nuclides
none (decay only)	3265
EAF-2010	386
ENDF VII	162
JENDL 4.0	138
mixed libraries	113
JENDL 3.1	20

Spectral weighting functions for CINDER data libraries



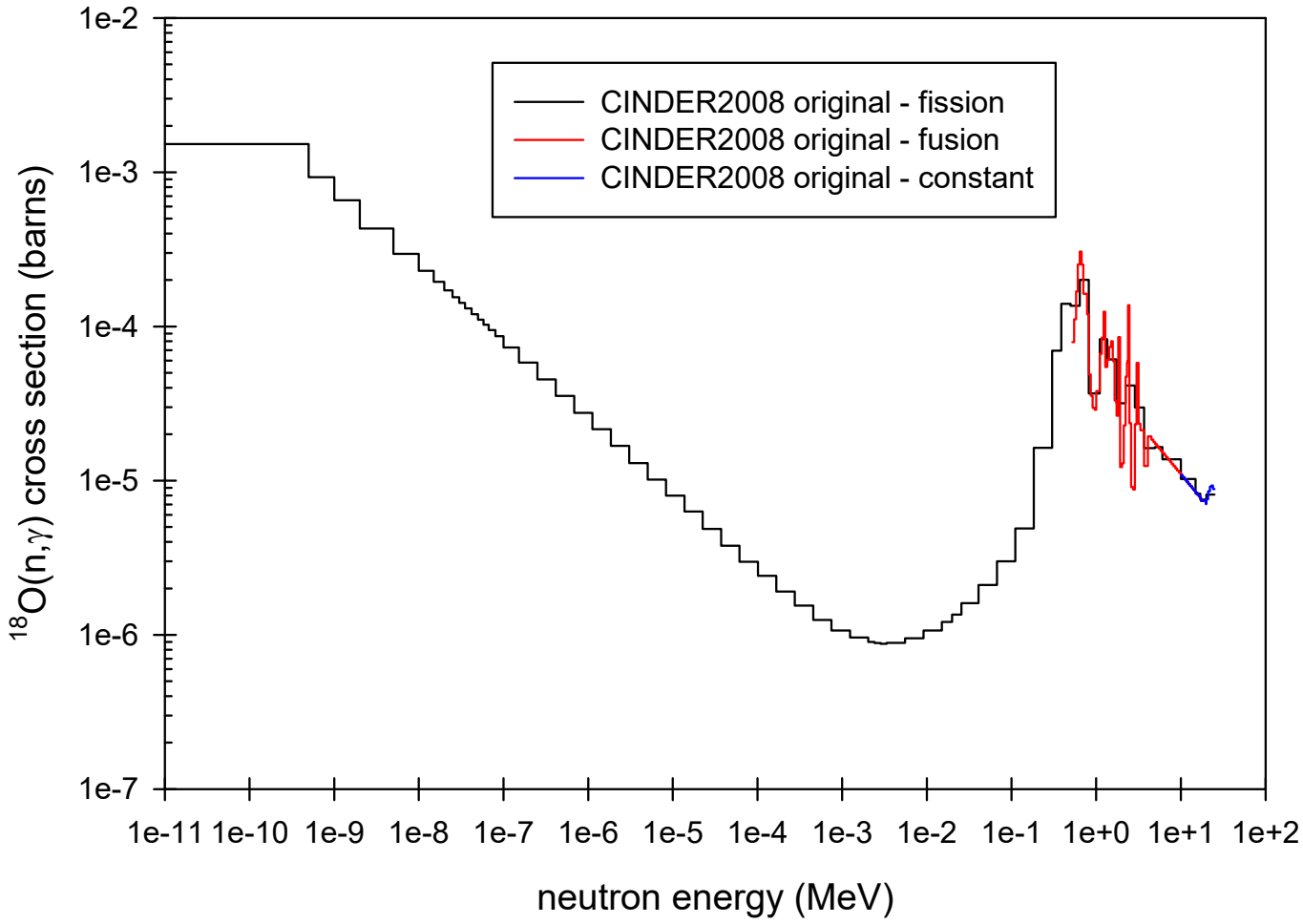
Sources of CINDER2008 Reaction Data

- Some of the reaction data written into the original CINDER2008 libraries were truncated (values were not included for the entire energy range) for the fusion-weighted and constant-weighted cross section sets
- This affected only the data that were taken from the EAF-2010 file
- The EAF-2010 file used for the original CINDER2008 libraries was a preliminary version
- These primarily impact radioactive nuclides, not stable ones (exceptions includes isotopes of C, Ne, Pt, Tl, and ^{18}O)



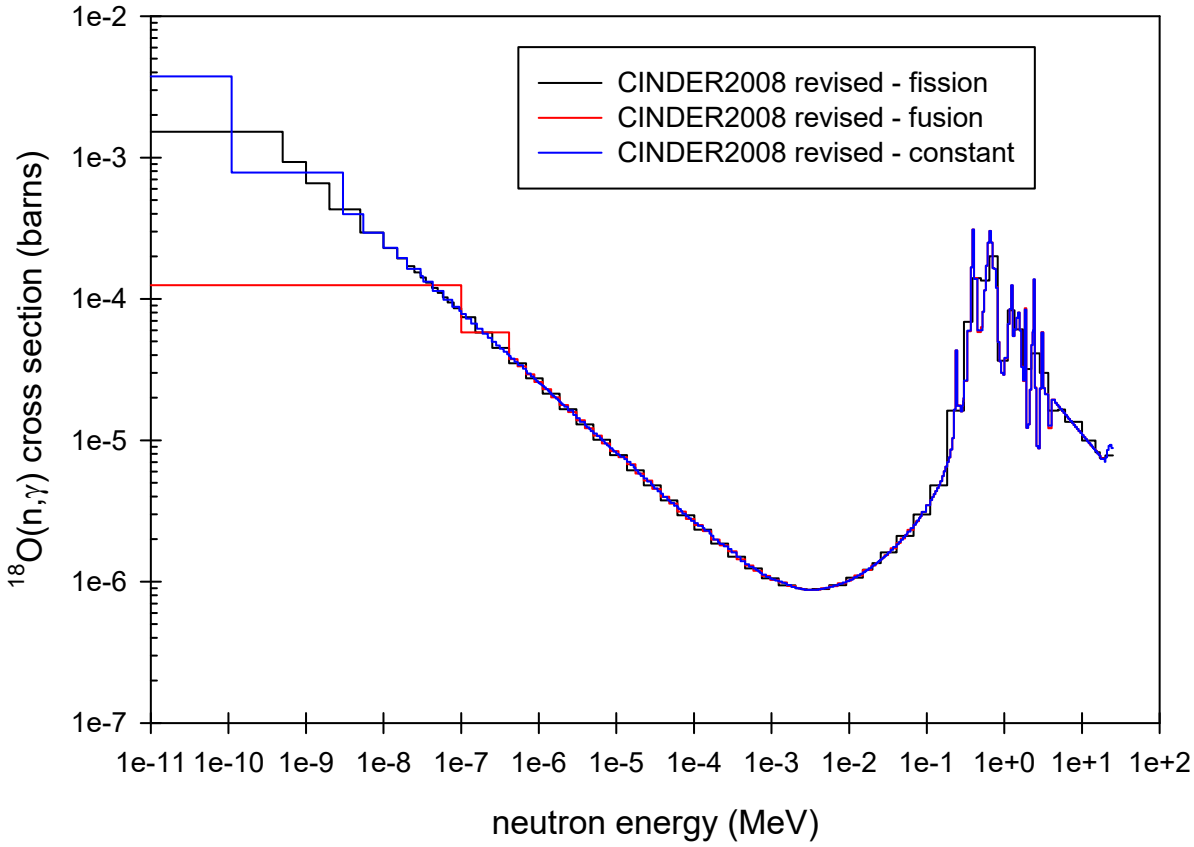
Sources of CINDER2008 Reaction Data

- Reaction data were present only for groups 101-175 for the fusion-weighted reaction library, and for groups 301-321 for the constant-weighted library



Revisions to CINDER2008 Reaction Data

- New versions of the EAF-2010 data files were downloaded from t2.lanl.gov
- The data were re-processed using the GROUPR module of NJOY99 and the three spectral weighting functions
- The new cross section libraries agree well and cover the entire energy range
- The revised fission-weighted libraries agree with the original fission-weighted libraries



cl_list Option

- If a large number of MCNP cells are being processed, it can be tedious to set up all the cell_list data blocks in the activation script input
- Using the new cl_list option block will automatically create the desired cell_list data blocks
- The only entry to this data block is the name of a file which contains the list of cells to be processed
- In the file containing the cell list, the number of the first cell should begin in column 1
- The remaining cells should be listed on a single line, separated by blanks

```
cl_file
  file  bma_cells
```

- The file *bma_cells* contains

```
1 2 3 4 5 6 7 8 9 10 11 12 101
```

  which will create the cell_list blocks and process the cells for example problem #6
- A new script input file named *input_expanded_cell_list_file.inp* will be written and placed in the run directory

DOE HazCat-3 Thresholds

- One frequent use of CINDER is to calculate the Hazard Category - 3 sum-of-fractions for a radionuclide inventory $SOF = \sum_i ({}^{A_i}/_{TV_i})$
- This allows one to determine whether a facility should be considered a nuclear facility or a radiological facility
- In CINDER90 the HazCat-3 SOF was calculated in ALLCODE, using threshold values in a separate *thcat3* file
- In CINDER2008 HazCat-3 SOF are calculated in POST using threshold values that are contained in the reaction libraries – this was thought to be more convenient for users

header from Na-22 section of CINDER fission-weighted cross section data file

```
# 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
  NO (N,F) CROSS SECTION
  10 reaction products. If > 0, 66-group reaction cross sections follow:
```

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 below would 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

ZAS HC-3 threshold

```
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
```

Using Revised DOE HazCat Thresholds in CINDER

- If running CINDER2008 through the activation script, setting the thcat3 option in the script input (part of the post_options block) will cause the script to copy the specified file into the directory in which POST will run
- The filename can include the absolute path to the *thcat3* file, or the relative path from the directory in which the script is run
- Values from the data library are used for nuclides not contained in *thcat3*
- The simple *thcat3* file below would change the threshold values used from those in the reaction data library to those in the table for the specified nuclides

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

ZAS	HC-3 threshold
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

Accident Analysis Tools in CINDER2008

- 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

- Total Effective Dose Equivalent (TEDE)

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

where

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

Accident Analysis Tools in CINDER2008

- The CINDER2008 version of CINDER makes use of the normalized dispersion factor DF, which is the ratio of activity concentration X to release rate $\dot{Q}$
- The release is assumed to be constant in time so that $\dot{Q} = ST/T_R$ and then

$$X = DF \cdot \dot{Q} = DF \cdot (ST/T_R)$$

where

T_R	= release time
DCF_E	= external dose conversion factor (Sv/hr)/(Bq/m^3)
DCF_I	= internal dose conversion factor (Sv/Bq)
ST	= source term (Ci) = $MAR \cdot DR \cdot ARF \cdot LPF$
MAR	= material at risk (activity calculated by CINDER)
DR	= damage ratio
ARF	= airborne release fraction
LPF	= leakage path factor

Accident Analysis Tools in CINDER2008

- Putting all these together, we arrive at an equation for the total dose

$$TEDE = DF \cdot \underbrace{(MAR \cdot DR \cdot ARF \cdot LPF)}_{ST} \cdot \left(\frac{T_E}{T_R}\right) \cdot (DCF_E + DCF_I \cdot BR \cdot RF)$$

  where (T_E/ T_R) is called the time ratio (the user may specify a global value or nuclide-specific values)
- The release is constant and takes place over a time T_R
- The exposure occurs for a fraction of that time (T_E / T_R)
- The user provides an input file to CINDER called *dose_input.dat* which triggers running the Accident Analysis Tool
- The user can construct the *dose_input.dat* file if running CINDER in a stand-alone mode, or use the activation Perl script through the aat_options block

Accident Analysis Tools in CINDER2008

dose_input.dat file

```
&WARNING_ON_OR_OFF
WARNING=.TRUE.
/

&OTHER_INPUT
DF_DEFAULT= 5.90E-04
TIME_RATIO_DEFAULT= 1
DR_DEFAULT= 1
ARF_DEFAULT= 5E-03
LPF_DEFAULT= 1
RESP_FX_DEFAULT= 0.4
BR_DEFAULT= 3.47E-4
FILENAME='other.dat'
FORMAT1="(A2,1X,F4.1,1X,F4.1)"
SPEC="(SYM,ARF,RESP_FX)"
/

&DCF_INPUT
DCF_I_DEFAULT= 0.0
DCF_S_DEFAULT= 0.0
DOSE_UNIT="REM"
RANKED=.TRUE.
FILENAME="dcf.dat"
FORMAT1="(I8,E10.2,E10.2)"
SPEC="(AZS,DCF_I,DCF_S)"
/

&THRESHOLD_INPUT
THRESHOLD_DEFAULT= 0.0
RANKED=.TRUE.
FILENAME='threshold.dat'
FORMAT1="(I8,E10.2)"
SPEC="(AZS,THRESHOLD)"
/
```

- CINDER example problem #3 illustrates the use of the Accident Analysis Tool

other.dat file

```
He  1.0  1.0
Ne  1.0  1.0
Ar  1.0  1.0
Kr  1.0  1.0
Xe  1.0  1.0
Rn  1.0  1.0
```

dcf.dat file (excerpt)

```
 30010  6.40E+01  1.22E-06
 70040  3.21E+02  8.73E-03
100040  3.54E+05  4.14E-05
110060  1.22E+01  1.81E-01
130070  0.00E+00  1.81E-01
140060  2.09E+03  8.29E-07
150080  0.00E+00  1.82E-01
180090  8.36E+01  1.81E-01
190100  0.00E+00  1.82E-01
220110  7.66E+03  4.00E-01
240110  1.21E+03  8.07E-01
```

threshold.dat file (excerpt)

```
 30010  5.63E+04
 70040  1.04E+04
100040  1.02E+01
110060  6.75E+03
130070  6.89E+03
140060  1.73E+03
150080  6.88E+03
180090  5.94E+03
190100  6.87E+03
220110  4.09E+02
240110  1.02E+03
```

Accident Analysis Tools in CINDER2008

- Script example #2 shows how to use the aat_options block to construct *dose_input.dat*

```
aat_options
  run   1
  warning  .true.
  df_default   5.90e-4
  time_ratio_default   1.0
  dr_default           1.0
  arf_default   5.0e-3
  lpf_default   1.0
  resp_fx_default  0.4
  br_default    3.47e-4
  oi_filename  ../../examples/sample3/other.dat
  oi_format1   (A2,1X,F4.1,1X,F4.1)
  oi_spec  SYM,ARF,RESP_FX
  dcf_i_default   0.0
  dcf_s_default   0.0
  dose_unit       rem
  di_ranked   .true.
  di_filename  ../../examples/sample3/dcf.dat
  di_format1   (I8,E10.2,E10.2)
  di_spec   AZS,DCF_I,DCF_S
  threshold_default  0.0
  ti_ranked   .true.
  ti_filename  ../../data/thcat3_lanl2014_azs.dat
  ti_format1  (I8,E9.2)
  ti_spec AZS,THRESHOLD
```

activation Perl script input

resulting sample *dose_input.dat* file

```
&warning_on_or_off
  warning = .true.
/

&other_input
  df_default =  5.90000e-04
  dr_default =  1.00000e+00
  br_default =  3.47000e-04
  arf_default =  5.00000e-03
  lpf_default =  1.00000e+00
  time_ratio_default =  1.00000e+00
  resp_fx_default =  4.00000e-01
  filename = '../../examples/sample3/other.dat'
  format1 = '(A2,1X,F4.1,1X,F4.1)'
  spec = 'SYM,ARF,RESP_FX'
/

&dcf_input
  dcf_i_default =  0.00000e+00
  dcf_s_default =  0.00000e+00
  ranked = .true.
  filename = '../../examples/sample3/dcf.dat'
  format1 = '(I8,E10.2,E10.2)'
  spec = 'AZS,DCF_I,DCF_S'
/

&threshold_input
  threshold_default =  0.00000e+00
  ranked = .true.
  filename = '../../examples/sample3/threshold.dat'
  format1 = '(I8,E10.2)'
  spec = 'AZS,THRESHOLD'
/
```

MCNP6 Compatability

- The original production release of MCNP v6 did not include the ability to write the histp file
- A patch issued by Mike James of LANL enables writing of *histp*, but only for a single-processor version of MCNP
  - MCNP 6.2 will offer this same capability
- Versions of MCNPX can still write *histp* in parallel mode; a patched version of MCNPX writes the nuclide production and destruction rates directly into the MCNPX text output file
- A similar patch has been developed for MCNP v6.1

Summary

- CINDER2008 and scripting tools written in Perl can be used for problems in accelerator activation
- Truncated reaction data libraries taken from EAF-2010 evaluated libraries have been fixed
- cl_list and aat_options data blocks have been added to the activation script
- Users may supply updated HazCat-3 threshold values using a *thcat3.dat* file, which can also be triggered in the activation script input