McCARD Running for AGN-20K Analysis

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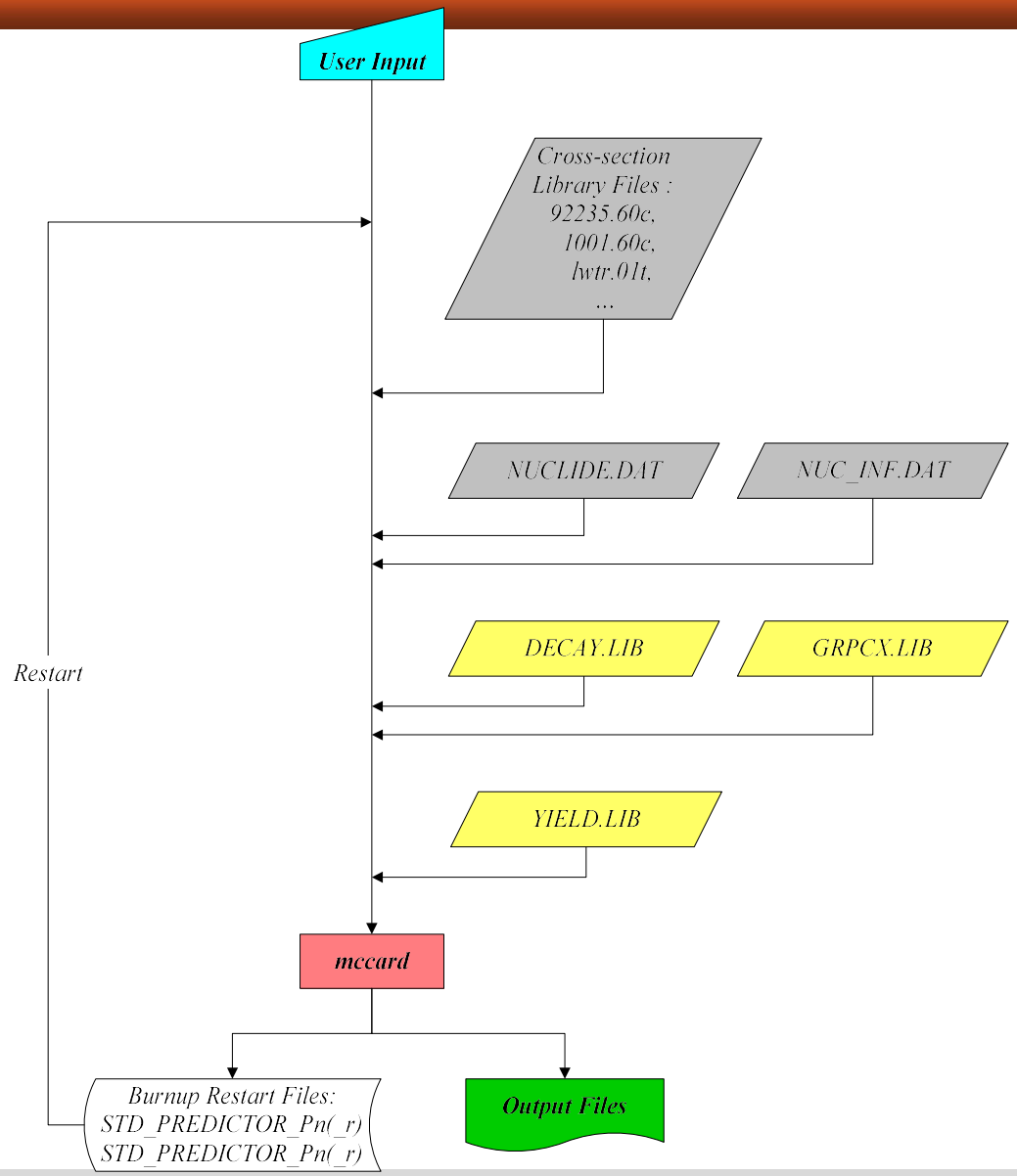
McCARD Running



File	Descriptions
user input	A user input file can be named arbitrarily. Default file name is *INPUT*.
NUCLIDE.DAT	It records cross-section library file names.
cross-section library files	Cross-section library files must exist in proper directories specified in the *NUCLIDE.DAT* file.
NUC_INF.DAT	Nuclide information file.
DECAY.LIB	Decay data file for burnup calculations.
GRPCX.LIB	One-group cross-section library file for burnup calculations.
YIELD.LIB	Fission yield data of fissionable nuclides.

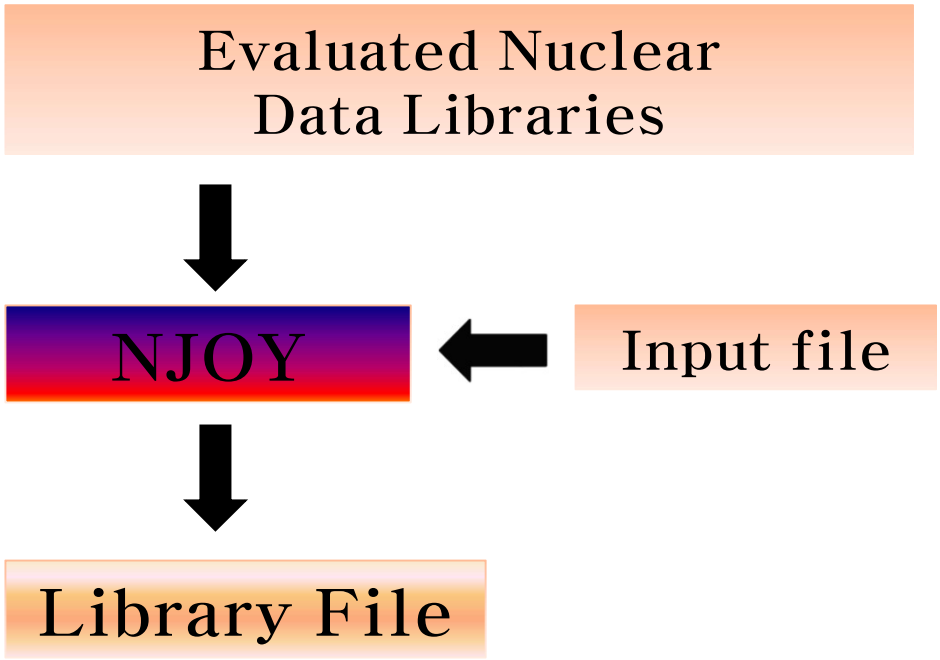
NUCLIDE.DAT

```
//-------------------------------------------------------------------------
//MCNAP RECOMMENDED CROSS SECTION LIBRARY FILE NAME (filename - temperature(K))
//-------------------------------------------------------------------------

//directory of continuous energy neutron libraries
DIR.C = "./cxlib7/"
//directory of continuous energy photon libraries
DIR.P = "./cxlib/"
//directory of multi-group neutron libraries
DIR.M = "./cxlib.m/"

//-------------------------------------------------
 H :   1001.70c_0300 -  300     1001.70c_0400 -  400
       1002.70c_0300 -  300     1002.70c_0400 -  400
       1003.70c_0300 -  300     1003.70c_0400 -  400
       1000.02p //photon lib.
-------------------------------------------------

...

-------------------------------------------------------------------------------
+h_h2o :  h_h2o.70c_0300 -  300   h_h2o.70c_0350 -  350   h_h2o.70c_0400 -  400
          h_h2o.70c_0450 -  450   h_h2o.70c_0500 -  500   h_h2o.70c_0550 -  550
          h_h2o.70c_0600 -  600   h_h2o.70c_0650 -  650   h_h2o.70c_0800 -  800
-------------------------------------------------------------------------------
```

ZAID_K = *ZZZAAA.nnX_KKKK*
ZZZ = 3 characters for Z,
AAA = 3 characters for A,
a decimal point,
nn = 2 characters for evaluation identification,
X=an identifier for the library type
(C = continuous energy neutron table,
T = thermal scattering table,
P = continuous energy photon table,
E = continuous energy electron table,
M = multigroup neutron table,
G = multigroup photon table,
D = discrete reaction table,
Y = dosimetry table)
KKKK = temperature [K]

Generation of Neutron XS Libraries

- Continuous energy or point-wise energy cross-section libraries for MCNP running are made using the ACER module of the NJOY code.
- ACE stands for "A Compact ENDF".



ENDF libraries like n-ENDF-VII0.endf.zip file can be downloaded from http://www.nea.fr.

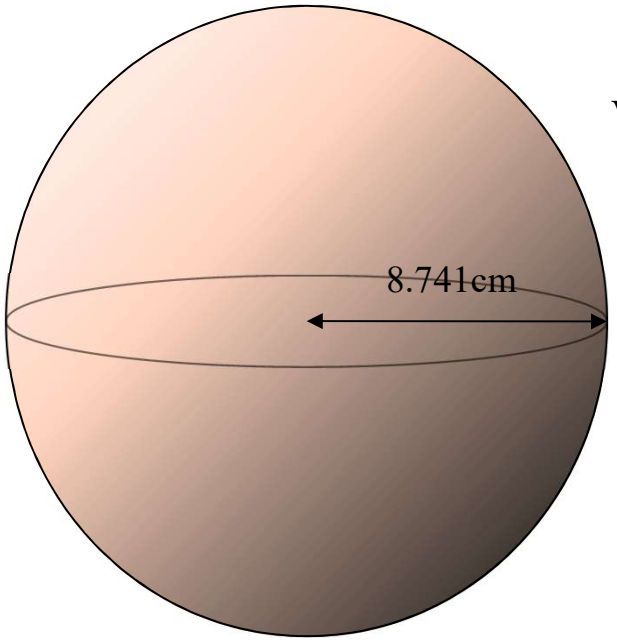
Make an NJOY input file.

Put the generated libraries in a directory described in NUCLIDE.DAT.

- 홍서기, 김강석, "Software Verification and Validation Report (ANJOYMC 1.0)," NCD-SVVR-012, 2007.11.30.

Lady Godiva

- The Godiva is a bare spherical uranium of a radius of 8.741 cm. The uranium density is 18.74 g/cm^3 and its composition is 94.73 wt% U^{235} and 5.27 wt% U^{238}.
- Calculate the effective multiplication factor (k_{eff}) of the Godiva critical assembly.



Vacuum Boundary Condition

Configuration of an Input File

- A user input is composed of divisions for a title, composition cell definitions, a structure definition, material data, source description, calculation options, burnup data, tally declarations and parallel options.
- Every division except the composition cell divisions should be made only once in a user input.

- Each division is composed of various input card commands.
- Each division starts with '(' and ends with ');'.

[*main-card*] (*main-card options*) (
    [*sub-card*] (*sub-card options*)
    [*sub-card*] (
        [*sub-card*] (*sub-card options*)
        …
    );
    …
);

Input Divisions and Corresponding Main-Cards

Division	Main-card	Descriptions
title	Title	It describes the analysis title.
composition cell	CCell	It defines a composition cell which could be used in other composition cells or the Structure division. The composition cells defined at each CCell card are not limited in number.
structure	Structure	It defines the system geometry.
material	Material	It defines the materials used in the composition cell or structure divisions
source	S_Source or C_Source	The S_Source card is used for the external neutron sources in the source-mode calculations. The C_Source card is used for the fission sources in the eigenvalue calculations.
calculation option	Data	The number of neutrons for the source-mode calculations and the cycle numbers for the eigenvalue calculations are inputted.
burnup	Burnup	The burnup step data are inputted for the depletion calculations.
tally	Tally	The user-defined tallies are declared.
parallel	Parallel	The options for the parallel computations are inputted.

Comments

- Two kinds of comments are allowed in the McCARD user inputs: C-style comments and C++-style comments.

Short C-style comment	/* This is a short C-style comment */
Short C++-style comment	// This is a short C++-style comment
Long C-style comment	/* This a long C-style comment /* that needs more than one line. /*/
Long C++-style comment	// This a long C++-style comment // that needs more than one line.

Title Card

- The Title card makes the title division. The text in the division will be printed in the user output file.

- **Format**

  Title ([*text*]);

  text text for the title

  The character or line number of *text* has no limit.

- **Example**

```
Title (
    16x16 PWR assembly with burnable poison rods
    D-type assembly of YGN3, 4
    100 active cycles, 20 inactive cycles
    on 10,000 sources/cycle
);
```

Structure Card

- The Structure card makes the structure division for the system geometry.

- **Format**

  Structure ([*cell div.*] [*surfacel div.*] (*agg. cell div.*));

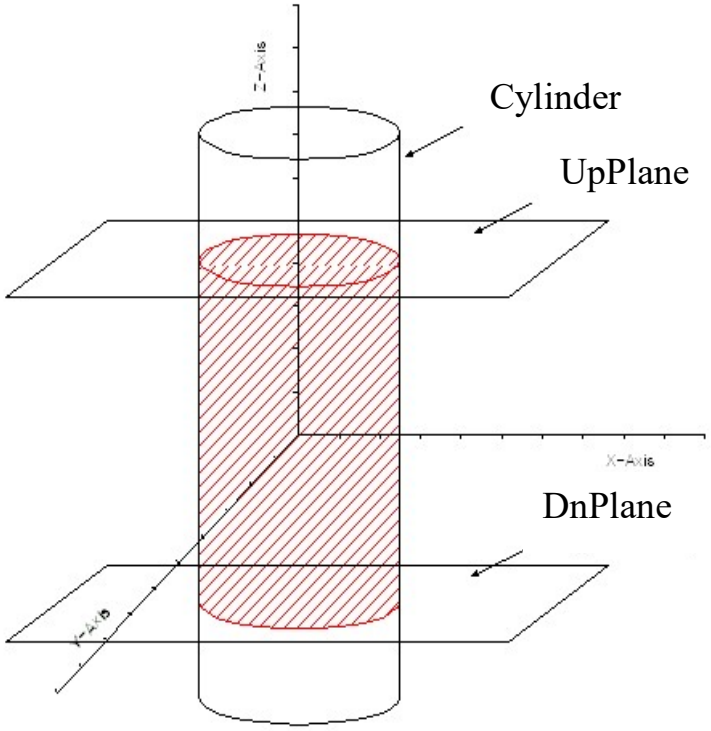
cell div.	a cell division
surfacel div.	a surface division
agg. cell div.	an aggregation cell division

- **Example**

```
Structure (
    Cells (
        ... // Cell definitions
    );
    Surfaces (
        ... // Surface definitions
    );
);
```

Defining a Cell Using Boundary Surfaces

- In McCARD, a system is defined as a sum of non-overlapping convex cells, where a cell is defined using logical operations on bounding surfaces.



-Cylinder AND –UpPlane AND +DnPlane

+ or -	= positive or negative region of the surface
AND	= intersection operator between surfaces,
OR	= union operator between surfaces.

Surfaces or Surface Card

- The Surfaces card makes a surface division in the structure or composition cell divisions. In the surface division, the normal surfaces, reflecting surfaces, and white boundary surfaces can be defined by SUR, RSUR, and WSUR, respectively.

- **Format**

  Surfaces ([*surface def's*]);

  surface def's surfaces defined by SUR, RSUR, and WSUR

- **Example**

```
Surfaces (
    SUR cylFuel CZ 0.4118
    SUR cylPin0 CZ 0.4759
    ... // Other surface definitions
);
```

SUR Card

- The SUR card defines a surface having continuous boundary condition.

- **Format**

  SUR [*name*] [*symbol*] [*parameters*]

name	name of this surface The maximum character length of the name is 255. The blank character (‘ ’) cannot be used in the name.
symbol	surface symbol like PG, PX, etc.
parameters	input parameters corresponding to *symbol* Each parameter is separated by the ‘ ’ character.

- **Example**

  When the surface equation is x-y+2z=3.5, the plane named S1 can be defined as below.

```
SUR S1 PG 1 -1 2 3.5
```

Surface Equations

Type	Symbol	Equation	Input parameters
Plane	PG	$Ax + By + Cz = D$	A, B, C, D
	PX	$x = D$	D
	PY	$y = D$	D
	PZ	$z = D$	D
Sphere	SG	$(x - x_0)^2 + (y - y_0)^2 + (z - z_0)^2 = R^2$	x_0, y_0, z_0, R
	SO	$x^2 + y^2 + z^2 = R^2$	R
	SX	$(x - x_0)^2 + y^2 + z^2 = R^2$	x_0, R
	SY	$x^2 + (y - y_0)^2 + z^2 = R^2$	y_0, R
	SZ	$x^2 + y^2 + (z - z_0)^2 = R^2$	z_0, R
Cylinder	CPX	$(y - y_0)^2 + (z - z_0)^2 = R^2$	y_0, z_0, R
	CPY	$(x - x_0)^2 + (z - z_0)^2 = R^2$	x_0, z_0, R
	CPZ	$(x - x_0)^2 + (y - y_0)^2 = R^2$	x_0, y_0, R
	CX	$y^2 + z^2 = R^2$	R
	CY	$x^2 + z^2 = R^2$	R
	CZ	$x^2 + y^2 = R^2$	R

Cells or Cell Card

- The Cells card makes a cell division in a structure or composition cell divisions. In the cell division, unit cells, translation cells, and fill cells can be defined by CEL, TCEL, and FCEL cards, respectively.

- **Format**

  Cells ([*cell def's*]);

  cell def's cells defined by CEL, TCEL, and FCEL

- **Example**

```
Cells (
    CEL Fuel UO2 { -cylF AND +pzB AND  -pzT }
    CEL Clad Zr  { +cylF AND  -cylP AND  +pzB AND  -pzT }
    ... // Other cell definitions
);
```

CEL Card

- The CEL card makes a unit cell composed of a single material. The region of the cell is defined as the logical combinations of the surrounding surfaces.
- **Format**

CEL [*name*] (*)[*mat_name*] { [*sign*][*surf_name*] [*operator*] … }
(*TMP option*) (*IMP option*) (*WWW option*) (*VOL option*)

name	name of this cell
	The maximum character length of the name is 255. The blank character (‘ ’) cannot be used in the name.
*	flag for the depletion cell declaration
	The depletion cell is declared by preceding its material name with the asterisk (*).
mat_name	name of the material filling this cell homogeneously.
	This material has to be defined in the material division.
	VOID is used for the outside cell.

CEL Card (Cont'd)

sign + or -

The plus and minus sign mean the region satisfying $f(x,y,z)>0$ and $f(x,y,z)<0$, respectively, where $f(x,y,z)$ is the equation of the following surface.

surf_name surface name defined in the surface division.

operator AND or OR.

The calculation order of AND and OR operators can be controlled by the parenthesis operator. It should be noted that a parenthesis operator cannot be used in another parenthesis pair.

TMP option cell temperature

TMP [*kT*] or *TMPK [K]*

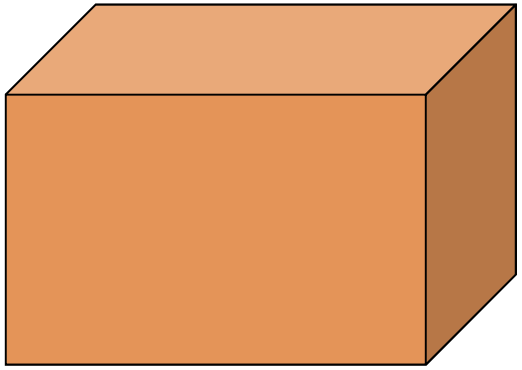
$$kT[\mathrm{MeV}] = \begin{cases} 8.617\times10^{-11}\,\mathrm{T[K]} \\ 8.617\times10^{-11}\left(\mathrm{T[^{\circ}C]}+273.15\right) \end{cases}$$

VOL option VOL [*V*]

cell volume in unit of [cm^3]

Making a Box

- Make a box made of a material named ‘Steel’.



Height = 10cm
Width = 20cm
Depth = 15cm

```
Structure (
   Cells(
      CEL Box Steel { +left   AND -right AND
                      -front  AND +back  AND
                      +bottom AND -top } TMPK 300
      ...
   );
   Surface (
      SUR left PX -10          SUR front PY 7.5          SUR bottom PZ -5
      SUR right PX 10          SUR back  PY -7.5         SUR top    PZ 5
      ...
   );
);
```

Current Input for Godiva Analysis

```
Title (
    Godiva Keff Calculation
);

Structure (
    Cells (
        CEL USphere Uranium   { -sphere }
        CEL Outside VOID      { +sphere AND  -out }
    );
    Surfaces (
        SUR sphere   SO 8.741
        SUR out      SO 100.0
    );
);
```

Geometry ➡ Material

Material Card

- The Material card makes the material division by defining the materials used in the cell divisions.

- **Format**

  Material ([*material def's*]);

  material def's material definitions

- **Example**

```
Material (
    MAT UO2 6.7678856e-2
        1 92234 9.08573e-6 92234.60c
        1 92235 1.13067e-3 TEMPDEPT
        1 92238 2.14280e-2 TEMPDEPT
        0 08016 4.51111e-2 TEMPDEPT
    Zr  -6.55
        -1 40000  -1.0 TEMPDEPT
    ... // Other material definitions
);
```

MAT Card

- The MAT card defines a material to be used in the cell divisions. The 'MAT' keyword is optional because the MAT card is the only card available in the material division.
- **Format**

(MAT) [*name*] [*density*]

{ [*seg_idx*] [*NID*] [*density_frac*] [*lib_filename*] (+ [*thermal_filename*]) } …

name	material name The maximum character length of the name is 255. The blank character (' ') cannot be used in the name.
density	gram density in g/cm^3 or number density in #/barn/cm A negative value means the gram density and a positive value is the number density.
seg_idx	nuclide segmentation index for the depletion calculations -1 = a natural nuclide 0 = an activation product 1 = an actinide 2 = a fission product *seg_idx* must be -1 for the nuclide's NID of $Z\times1000$. The actinides are nuclides with atomic numbers from 89 to 103 . They include all the elements lying between actinium and lawrencium in the periodic table. A nuclide used for the structural material has *seg_idx* of 0.

MAT Card (Cont'd)

NID	nuclide identifier It is $Z\times1000+A$ for a nuclide in the ground state, $Z\times1000+A+500$ for a nuclide in the excited state and $Z\times1000$ for a natural nuclide.
density_frac	gram density or number density fraction of the *NID* nuclide Negative values mean the gram density fractions and positive values are the number density fractions.
lib_filename	continuous-energy library file name with the form of *ZZZAAA.nnX_KKKK* When the keyword of TEMPDEPT is written in the place of *lib_filename*, the nuclide's library file is automatically determined from the cross-section library lists of the *NUCLIDE.DAT* file by the cell temperature.
thermal_file	library file name of the S(a,b) scattering library When the library file name without its extension is written, the library file is automatically determined from the cross-section library lists of the *NUCLIDE.DAT* file by the cell temperature.

- **Example**

  light water with the density of 0.0747518 atoms/barn/cm:

```
Water 7.47518e-2
   0 1001 4.98334e-2 TEMPDEPT + lwtr
   0 8016 2.49184e-2 TEMPDEPT
```

Current Input for Godiva Analysis

```
Title (
    Godiva Keff Calculation
);

Structure (
     Cells (
          CEL USphere Uranium   { -sphere }
          CEL Outside VOID      { +sphere AND  -out }
     );
     Surfaces (
          SUR sphere   SO 8.741
          SUR out      SO 100.0
     );
);

Material (
     Uranium  -18.74
          1 92235  -0.9473 92235.60c
          1 92238  -0.0527 92238.60c
);
```

Geometry & Material

Calculation Option

Data Card

- The Data card makes a calculation option division by specifying the source neutron number, the cycle numbers, etc. The NSrc, Criticality, RNG and WeightWindow cards can be used in the calculation option division.

- **Format**

  Data ([*cal. options*]);

  cal. options calculation parameters specified by NSrc, Criticality, RNG and WeightWindow

- **Examples**

```
Data ( // Eigenvalue calculation
     //1000 sources/cycle, 20 inactive and 100 active cycles
     Criticality 1.0 1000x120 20
);

Data ( // Source-mode calculation
    NSrc 10000
);
```

Criticality or Critical Card

- The Criticality card specifies the numbers of cycles and fission sources per cycle for the eigenvalue calculation. When this card is used in the calculation option division, the eigenvalue calculation is performed.

- **Format**

  Criticality [*k_init*] [*NFS*]x[*NCYC_TOTAL*] [*NCYC_INACT*]

k_init	assumed eigenvalue for the first cycle
NFS	number of fission sources per cycle
NCYC_TOTAL	number of cycles including the inactive and active cycles
NCYC_INACT	number of inactive cycles

- **Notes**

  The Criticality card should be accompanied by the C_Source card for the fission source input.

Calculation Mode by Source Type

Mode	Fixed Source Calculation	Criticality Calculation or Eigenvalue Calculation
Source	Predefined Fixed Source	Fission Neutron
Data Card	NSrc 10000	Criticality 1.0 1000x120 20
Source Card	S_Source	C_Source

C_Source and S_Source Card

- The C_Source and S_Source cards make the source divisions for the eigenvalue calculations and the source-mode calculations, respectively.
- **Format**

  C_Source ([*parameters*]);

  S_Source ([*parameters*]);

  parameters source parameters specified by Cell, Shape, Energy, and Direction

- **Examples**

```
C_Source ( //Sources for eigenvalue calculation
     Cell       Pin0
     Shape      PNT (0,0,0)
     Energy     WATT 0.965 2.29
     Direction ISO
);
S_Source ( //Sources for source-mode calculation
Cell       Src
Shape      CYL (0,0,0) RAD (0,2) EXT (20)
Energy     HIST 3  ENG  4.540e-4 5.531e-3 6.738e-2 8.209e-1 2.000e1
                   PROB 0.01     0.03     0.06     0.2      0.7
);
```

Input for Godiva Analysis

```
Title (
    Godiva Keff Calculation
);

Structure (
   Cells (
     CEL USphere Uranium   { -sphere }
     CEL Outside VOID      { +sphere AND -out }
   );
   Surfaces (
      SUR sphere  SO 8.741
      SUR out     SO 100.0
   );
);

Material (
     Uranium  -18.74
          1 92235  -0.9473 92235.60c
          1 92238  -0.0527 92238.60c
);
```

```
Data (
   Criticality 1.0 1000x120 20
);

C_Source (
   Cell        USphere
   Shape       PNT (0,0,0)
   Energy      WATT 0.988 2.249
   Direction ISO
);
```

Running

- The McCARD execution line has the following form:

  Form: McCARD (-i [*input file*]) (-o [*output file*])

input file	The default file name is *INPUT*.
output file	The default file name is *OUTPUT*.

Tally Card

Type	One-Group
Flux	Flux, GrpFlux, PhotonFlux, GrpPhotonFlux, SurfaceFlux
Power by Heating Number	Power PhotonPower
Power by kappa	FisPower
Reaction Rate	GrpRRate
Multi-group XS	GrpXS, NucGrpXS
Current	Current SurfaceCurrent

Running to Estimate a Flux

```
Title (
    Godiva Keff Calculation
);

Structure (
   Cells (
     CEL USphere Uranium  { -sphere }
     CEL Outside VOID     { +sphere AND -out }
   );
   Surfaces (
      SUR sphere  SO 8.741
      SUR out     SO 100.0
   );
);

Material (
     Uranium  -18.74
          1 92235  -0.9473 92235.60c
          1 92238  -0.0527 92238.60c
);
```

```
Data (
   Criticality 1.0 1000x120 20
);

C_Source (
   Cell        USphere
   Shape       PNT (0,0,0)
   Energy      WATT 0.988 2.249
   Direction ISO
);

Tally (
   Flux USphere
   Power USphere
);
```

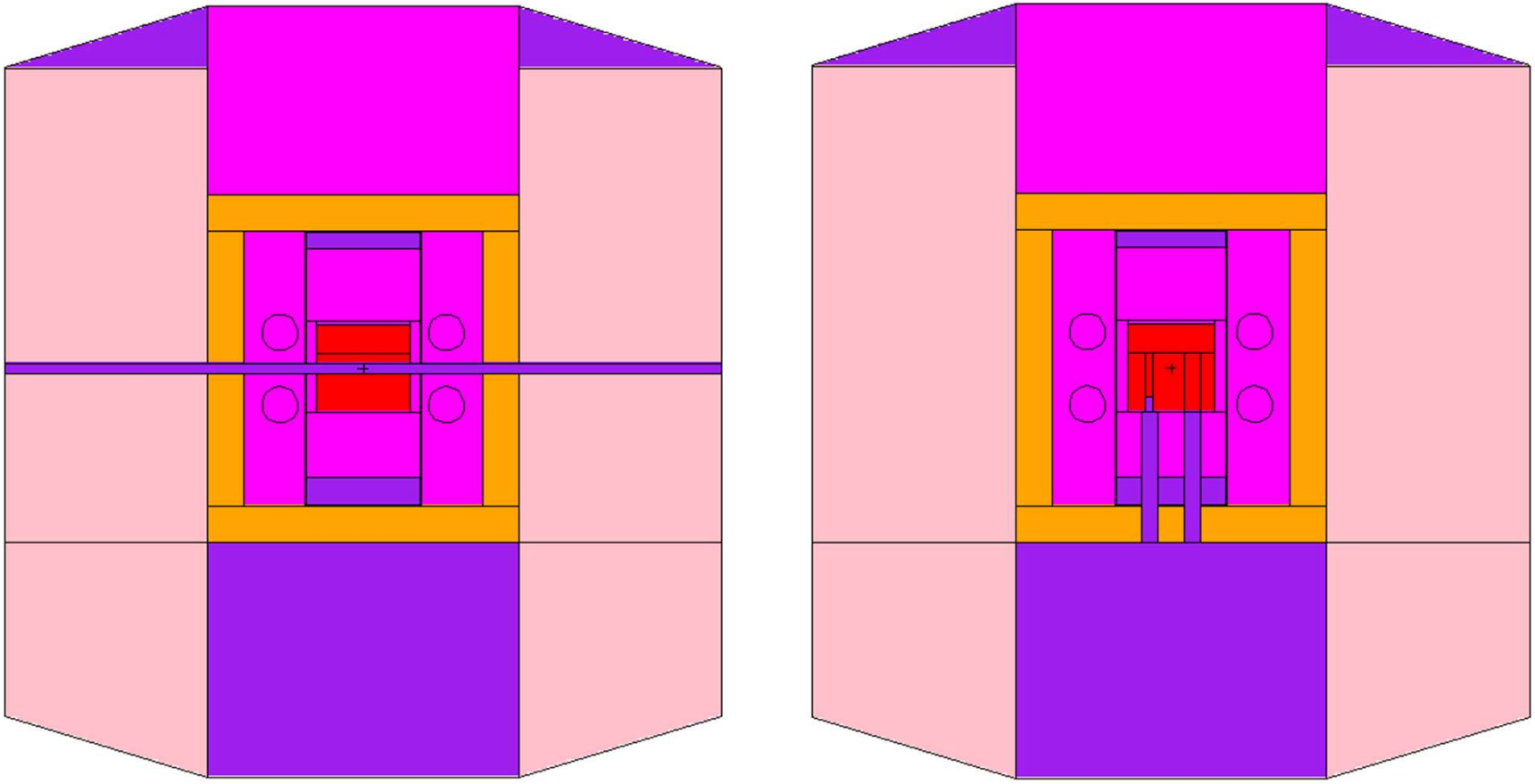
AGN-201K

- The McCARD execution line has the following form:

  Form: McCARD (-i [*input file*]) (-o [*output file*])

input file	The default file name is *INPUT*.
output file	The default file name is *OUTPUT*.

AGN-201K Model



McCARD INPUT

```
CEL Fuel1    Air          { -czFuel  AND -pz07  AND  +pz08                              }  TMPK T_Air       //top fuel cell
CEL Fuel2    FuelTop      { -czFuel  AND -pz08  AND  +pz09                              }  TMPK T_Fuel      //top fuel cell
CEL Fuel3    FuelTop      { -czFuel  AND -pz09  AND  +pz11
                            AND +cpzFR1  AND +cpzCR  AND +cpzSR1  AND +cpzSR2  AND +cxGlory   }  TMPK T_Fuel      //bottom

CEL FR1      FuelTop      { -cpzFR1  AND -pz09  AND +pz10                               }  TMPK T_Fuel      //fine rod(insertion)1
CEL FR2      Air          { -cpzFR1  AND -pz10  AND +pz11                               }  TMPK T_Air       //fine rod(void)2
CEL FR3      Air          { -cpzFR2  AND -pz11  AND +pz15                               }  TMPK T_Air       //fine rod(void)2

CEL CR1      FuelTop      { -cpzCR  AND -pz09  AND +pz11                                }  TMPK T_Fuel      //coarse rod(insertion)1
CEL CR2      Air          { -cpzCR  AND -pz11  AND +pz15                                }  TMPK T_Air       //coarse rod(void)2

CEL SR1_1    FuelTop      { -cpzSR1  AND -pz09  AND +pz11                               }  TMPK T_Fuel      //safety rod 1(insertion)1
CEL SR1_2    Air          { -cpzSR1  AND -pz11  AND +pz15                               }  TMPK T_Air       //safety rod 1(void)2
CEL SR2_1    FuelTop      { -cpzSR2  AND -pz09  AND +pz11                               }  TMPK T_Fuel      //safety rod 2(insertion)1
CEL SR2_2    Air          { -cpzSR2  AND -pz11  AND +pz15                               }  TMPK T_Air       //safety rod 2(void)2
```

```
SUR czFuel   CZ   12.8                 //fuel
SUR cpzFR1    CPZ  -6  6  1.5             //fine rod
SUR cpzFR2    CPZ  -6  6  2.5             //fine rod
SUR cpzCR     CPZ   6 -6  2.5            //coarse rod
SUR cpzSR1    CPZ   6  6  2.5             //safety rod1
SUR cpzSR2    CPZ  -6 -6  2.5             //safety rod2

SUR pz07    PZ 13.0
SUR pz08    PZ 12.0
SUR pz09    PZ 4.0
SUR pz10    PZ -8.0
SUR pz11    PZ -12.0
SUR pz12    PZ  -30
SUR pz13    PZ -37.8
SUR pz14    PZ -38.0
SUR pz15    PZ -48.0
```

Comparison with MCNP

❖ 계산조건

- 활성/비활성주기 : 300, 100
- 주기당 중성자수 : 100,000
- 라이브러리 : ENDF/B VII.1
- 버전 : McCARD v1.1.0.1, MCNP5

❖ 증배계수

McCARD		MCNP	
k_{eff}	SD	k_{eff}	SD
0.99980	0.00015	0.99995	0.00015

Kinetics Parameters

	β_{eff}	Rel. SD(β_{eff})	Λ_{eff}	Rel. SD(Λ_{eff})
value	7.74889×10^{-3}	0.01097	8.54603×10^{-5}	0.00291

group	$\beta_{eff,g}$	Rel. SD($\beta_{eff,g}$)	λ_g	Rel. SD(λ_g)
1	2.45228×10^{-4}	0.05528	1.24906×10^{-2}	1.32029×10^{-9}
2	1.27633×10^{-3}	0.02588	3.18194×10^{-2}	4.88681×10^{-7}
3	1.34780×10^{-3}	0.02475	1.09395×10^{-1}	5.94560×10^{-7}
4	3.47852×10^{-3}	0.01632	3.17063×10^{-1}	7.65456×10^{-7}
5	1.05101×10^{-3}	0.02933	1.35388	2.58812×10^{-7}
6	3.49999×10^{-4}	0.04817	8.64040	1.54016×10^{-6}