McDeLicious Workshop

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What is McDeLicious code

• McDeLicious code

was developed to enable a proper representation of the d-Li neutron source term in Monte Carlo transport calculations for IFMIF

- It is enhancement (set of subroutines) to MCNP5 with ability to sample the generation of d-Li source neutrons on the basis of tabulated double-differential d + ^{6,7}Li cross-sections:
 - modelling of deuteron beam configuration, orientation and profile
 - modelling of deuteron slowing down in the Lithium
 - sampling of source neutrons using evaluated d+ ^{6,7}Li data

History of McDeLicious code development

- 1999: McDeLi (*P. Wilson, Report FZKA 6218, 1999*)

 enhancement to MCNP-4a to sample the generation
 of d-Li source neutrons on the basis of <u>embed analytical formulas</u>
 representing direct deuteron striping (Serber model) and compound reactions
- 2001: McDeLicious (S.P.Simakov et al. J.Nucl.Mat.307-311(2002)1710, FZKA 6743)

 enhancement to MCNP-4b,c to sample the d-Li source neutrons
 on the basis of tabulated double-differential d + ^{6,7}Li cross-sections
 for deuteron energies up to 50 MeV
 (evaluated by A. Konobeyev et al., NSE 139 (2001)1)
- 2005: McDeLicious-05 compilation with <u>MCNP-5</u> and use tabulated double-differential cross-sections from <u>updated</u> <u>d + ^{6,7}Li evaluation</u> (made by P. Pereslavtsev et al., J.Nucl.Mat.367-370(2007)1531)

D-Li Neutron Source Term:

validation against measurements performed at accelerators with - thin Li-target - double differential cross sections - thick Li-target - integrated & differential neutron yields

Double differential cross sections /thin Li-target/: new measurements and new d + ^{6,7}Li data evaluation

Ed = 17 MeV Exp.: P.Bem et al. NPI EXP(EFDA)-05/2004 Exp.: M.Hagiwara et al. Fus.Sci.Tech.48(2005)1320



Evaluation by P. Pereslavtsev et al., JNM 367-370(2007)1531

Neutron yield from thick Li-target: available experiments

No	First Author,	Laboratory,	Tar-	E _d ,	Q,	E _{thr} ,
	Year of Publ.	Country	get	MeV	degrees	MeV
1	V.K. Daruga	Inst. of Physics &	Li	22	0°	1.8
	1968	Power Eng., Russia				
2	A.N. Weaver	Livermore	Li	5, 9, 14,	3.5°, 10°, 18°, 25°, 32°	2.5
	1972	Laboratory, USA		16, 19		1.6
3	A.N. Goland	Naval Research	Li	13.4, 19,	0°, 5°, 10°, 15°, 20°	3
	1975	Laboratory, USA		25, 29, 34		
4	H.I. Amols	Fermi National	Li	35	0°	5
	1976	Laboratory, USA	_			
5	C.E. Nelson	Triangle University,	'Li	8, 12, 15	0°, 10°, 20°, 30°, 45°	1
	1977	USA	_			
6	M.A. Lone	Chalk River Labo-	'Li	14.8, 18,	0°, 10°, 20°, 30°, 40°	0.3
	1977	ratory, Canada		23		
7	M.J. Saltmarsh	Oak Ridge	Li	40	0°, 7°, 15°, 30°, 45°, 60°,	2
	1977	Laboratory, USA			90°	
8	D.L. Johnson	University of	Li	35	0°, 4°, 8°, 12°, 20°, 30°,	1
	1979	California, USA			45°, 70°, 105°, 150°	
9	M. Sugimoto	Japan Energy	Li	32	0°,5°,10°,15°,20°,30°, 40°,	1
	1995	Research Institute,			50°, 60°, 70°, 80°, 90°,	
		Japan			100°, 110°,120°, 130°,	
					140°, 150°	
10	M. Baba	Tohoku University,	Li	25, 40	0°,5°,10°,15°,20°,25°,30°,	1
	2003	Japan			40°,45°,60°,90°, 110°	
11	P. Bém	Nuclear Physics	Li	16.3, 17.0	0°	3
	2003	Institute, Rez				

Thick Li-target neutron source: Forward Neutron Yield



Thick Li-target neutron source: Angular Neutron Yield



13-14.03.2008

Thick Li-target neutron source: Energy-Angular Yield



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D-Li Neutron Source Term:

simulation of IFMIF source



Dual deuteron beam spatial profile: each 40MeV @125 mA

Full Footprint: 20×5 cm²

Reduced Footprint: 4×5 cm²



- d-beam current density variation inside the beam foot print amounts up to 20%;
- d-beam current density gradient at the beam foot print edges (10 to 90)% per 1.5 cm
- d-beam current density 3-d distribution based on results obtained ~10 years ago!

Deuteron slowing down and energy deposition in Li-jet



- Deuteron track length reach 2.1 cm;
- Peak Energy Deposition is 150 kW/cc at the depth of 2.0 cm (at the end of d-track) (without incident deuteron energy smearing 1000 kW/cc !)
- Average energy deposition in Li jet = (40 MeV x 250 mA=10,000 kW)/(20x5x2 cc) =50 kW/cc



Deuteron collisions and Neutron productions probabilities in Li-jet

- First deuteron collision in Li-jet dominates
- Second collisions most probably are an elastic scattering

which conserves incident deuteron direction within 1° and energy

- Every <u>100 deuterons</u> with 40 MeV produce in Li-jet: <u>7.2 neutrons</u> and <u>1.2 gammas</u>

D-Li Neutron Spectra: thick target measurements in laboratory do show a 14 MeV peak !



Neutron Spectra at well defined angles:

Peak at energy 15 MeV is clearly visible in well fine angle geometry. This peak is reproduced by 2005 updated d-Li evaluation within 10%



Neutron spectra inside the Test Cell



Neutronics calculations do predict smoothed (no peaks) energy distribution all over the IFMIF test cell

Li-jet nuclear responses: Tritium and Be-7 Inventories

Test Cell & Li -loop



<u>³H and ⁷Be production rates in Li-loop sub-systems</u> (calculated by the McDeLicious code)

Loop component	Mass, kg	Reaction	Inventory	Rate, g/fpy
Li jet	1	d + Li d + Li	⁷ Be ³H	1.5 6.0
		<u>n + Li</u>	³ H	0.4
Li injection tank	18	n + Li	³ H	0.2
Li quench tank	1200	n + Li	³ Н	1.0
Li drain tubes	3	n + Li	³ Н	0.1
Total			³ H	7.7

D-Li collision in jet is a main source of Tritium and Be-7 inventories in the Li-Loop

S.P. Simakov et al., JNM 329-333(2004)213

MCNP geometry model for the IFMIF test cell /latest version - md34/

developed by F. Wasastjerna VTT Processes, Helsinki, Finland

F. Wasastjerna, Ann. of Nucl. Energy 35(2008)438-445

MCNP geometry Model



13-14.03.2008

MCNP geometry Model (continued)

HFTM /Vertical cut/

HFTM, MFTM, LFTM /Horizontal cut/



MCNP geometry Model (continued)

HFTM, MFTM, LFTM /Horizontal cut/

Test Cell and Walls /Vertical cut/



Evaluated cross sections data

for neutron transport and nuclear responses calculations in the IFMIF

Neutron Cross-Sections E ³ 20 MeV - General purpose data ENDF evaluations -

- IFMIF project
 - ¹H, ⁵⁶Fe, ²³Na, ³⁹K, ²⁸Si, ¹²C, ⁵²Cr, ⁵¹V, ^{6,7}Li, ⁹Be (INPE/FZK)
 - ^{180,182-184,186}W, ¹⁸¹Ta (EFF/JEFF)
- LANL 150 MeV data files (ENDF/B-VI.6 or B-VII)
 - ^{1,2}H, ¹²C, ¹⁶O, ¹⁴N, ²⁷AI, ^{28,29,30}Si, ³¹P, ⁴⁰Ca, ^{50,52,53,54}Cr, ^{54,56,57,58}Fe, ^{58,60,61,62,64}Ni, ^{63,65}Cu, ⁹³Nb, ^{182,183,184,186}W, ^{196,198, 199, 200, 201, 202, 204}Hg, ^{206, 20, 208}Pb, ²⁰⁹Bi
- NRG evaluations
 - ^{40,42-44,46,48}Ca, ⁴⁵Sc, ⁴⁶⁻⁵⁰Ti, ^{54,56-,58}Fe, ^{70,72-74,76}Ge, ^{204,206-208}Pb, ²⁰⁹Bi
- JENDL-HE data file
 - ¹H, ^{12,13}C, ¹⁴N, ¹⁶O, ²⁴⁻²⁶Mg, ²⁷AI, ²⁸⁻³⁰Si, ^{39,41}K, ^{40,42-46,48}Ca, ⁴⁶⁻⁵⁰Ti,⁵¹V, ^{50,52-54}Cr, ⁵⁵Mn, ^{54,56-58}Fe, ⁵⁹Co, ^{58,60-62,64}Ni, ^{63,65}Cu, ^{64,66-68,70}Zn, ^{90-92,94,96}Zr, ⁹³Nb, ^{180,182-184,186}W, ^{196,198-202,204}Hg
- Few other evaluations
 - KAERI (¹²C, ²⁷AI, ⁵⁶Fe, ²⁰⁸Pb), BNL (¹²C, ⁵⁶Fe, ²⁰⁸Pb, ²⁰⁹Bi), IPPE (²³²⁻²³⁸U, ^{237,239}Np, ²³⁶⁻²⁴⁴Pu)

Transport cross sections and nuclear responses

Evaluated neutron cross sections (LANL – solid, INPE/FZK – dash)

 10^{5} Flux [10¹¹/MeV/cm²/s] ⁵⁶Fe Neutron Flux in HFTM 10 10^{3} σ(n,dpa) 10^{2} $\sigma(n.tot)$ 10 10^{0} $\sigma(n, x\gamma)$ σ(n,xp 10^{-1} 10^{-2} $\sigma(n,x\alpha)$ σ [b], 10^{-3} $\sigma(n,\gamma)$ 10° 0.01 0.1 1E-3 10 100 Energy, MeV

Responses in HFTM/IFMIF vs. Libraries (uncertainties due to XS data)

Parameter	LANL	INPE	Differ.
dpa-rate, 1/fpy	31.1	33.6	8 %
Heating, W/cm3	16.9	19.7	16 %
H-production, appm/fpy	1602	1767	10 %
He-production, appm/fpy	345	396	13 %
n-flux, 10 ¹⁴ /cm2/s	7.05	7.43	5 %
γ -flux, 10 ¹⁴ /cm2/s	3.38	3.59	6 %

Expected uncertainties of IFMIF nuclear responses due to the transport cross sections data amounts at least (5 - 15)%

Iron Transmission Benchmark Experiment



Gas (He) production cross-sections in Iron



INPE-FZK looks more preferable than LA-150 (?!)

Transport and nuclear response cross sections files for IFMIF

High Energy Files (up to 150 MeV)	Fusion Energy Files (up to 20 MeV)
LA-150 library (extension = 24c), xsdir = iedirLA	JENDL-FF library (extension = 41c)
n + 1-H-1, H-2	n + 22-Ti-46, Ti-47, Ti-48, Ti-49, Ti-50
n + 4-Be-9	
n + 6-C-nat	(better to replace by JEFF-3.1, < 200 MeV
n + 8-O-16	
n + 13-Al-27	ENDE/B-VI library (extension = 60c)
n + 14-Si-28, Si-29, Si-30	n + 16-S-32
n + 20-Ca-nat	
n + 24-Cr-50, Cr-52, Cr-53, Cr-54	(better to replace by ENDE/B-V/II < 20 MeV/
n + 26-Fe-54, Fe-56, Fe-57	
n + 28-Ni-58, Ni-60, Ni-61, Ni-62, Ni-64	
n + 29-Cu-63, Cu-65	
n + 74-w-182, W-183, W-184, W-186	

IFMIF Energy domain Files (up to 50 MeV)

INPE/FZK library (extension = 95c)				
from file wq_Li6 and wq_Li7 (xsdir_wq_Li6_Li7)				
from file iexs2 (bin) or iexs1 (ASCII, xsdir =iedir1)				

McDeLicious:

programming details

McDeLicious Logic Structure

1. <u>Main subroutine **source** lib-05.F90</u> does following:

- calls subroutine load(filename,..) which uploads in memory the ACE files with d-⁶Li and d-⁷Li cross sections
- reads beam parameters from the McDelicious input file such as number of beams, declination angle, d-beam spatial profile parameters, deuteron incident energy, Li-jet density, entrance surface and target cell
- calls subroutine **yield_Ed**(..) which calculates deuteron range in Li media, total neutron yield and prepares the tables for deuteron track sampling

McDeLicious Logic Structure (continued)

- calls subroutine **yz_sample(...)** and samples deuteron direction and entrance point on the surface of Li target
- calls subroutine sample_Ed(...), which samples d-track length to collision and calculates this point (X, Y,Z), deuteron energy E_d and neutron weight W_n there
- samples whether isotope ⁶Li or ⁷Li a deuteron collides with
- subroutine **sample_EnAng (...)** samples neutron emission Energy E_n , polar Θ_n and azimuth φ_n Angles using tables from d-Li ACE file
- submits to MCNP parameters of generated neutron: $\{X, Y, Z\}, \{\cos_X, \cos_Y, \cos_Z\}, E_n, W_n, T_n=0$
- 2. Files <u>load_sample-05.F90</u> and <u>beam.F90</u> collect subroutines and functions mentioned above: *load, yield_Ed, sample_Ed, sample_EnAng, dedx, f_average, yz_sample, gausdev*

McDeLicious subroutines allocation and compilation with MCNP5 ones to get executable for *mpi* parallelism

- Ø Subroutine source_lib-05.F90 should replace MCNP dummy subroutine source.F90 in directory MCNP5/Source/src; files load_lib-05.F90 and beam.F90 should be allocated there too
- Ø System dependent script for MCNP5 compilation **go_pgi_mpi** (after slight modification - **go_mpi_McDeLicious-05**) should be available in directory MCNP5/Source and has to be executed
- Ø After successful compilation an executable file mcnp5.mpi will be produced which should be renamed to McDeLicious-05 and moved in your working or bin directory
- Ø To run McDelicious code one needs specific ACE files :
 - d_li6_056.ace_up50 and d_li7_056.ace_up50
 - which are the d-6,7Li evaluation processed by NJOY code

McDeLicious subroutines allocation in MCNP5 directories



	message:Datapath=~/directory_for_data	McDeLicious Input File Structure
sp	xsdir=xsdir_file_for_cross_sections	
MCNP car	empty line Cell cards empty line Surface cards empty line Materials	IFMIF Test Cell geometry and materials cards (around lines 8000 lines)
	Sp901 SP916	D-Li source specification cards (see next slide)
cards	Tally cards F6n,p cell_number 	Responses specification cards (see next slide)
MCNP	mode n,p phys:p j 1 cut:n 1j 5.0E-7 nps 1.E+7	Problem specification cards

McDeLicious Input File: D-Li Source Specification

two 40MeV d-beams declined in Horizontal plane by 10deg, 20x5cm2 Footprint С _____ C #2 c beams #1 SI901 L 1 1 \$ target number SI902 L 1 \$ beams current (only relative value has meaning) 1 \$ beams energy Ed [MeV] SI903 L 40 40 cos(x) cos(y) cos(z) cos(x) cos(y) cos(z) for beam orientation С SI904 L 0.173648 0. 0.984808 -0.173648 0. 0.984808 \$ beams 10deg in Horiz. SI905 L 100 100 \$ beam orientation vector: along X-axis for beam spatial profile for 20 x 5 cm**2 ΧοσπΧοσπ С SI906 L 9.0 0.6 1.00 9.0 0.6 1 \$ basic horizontal parameters SI907 L 2.0 0.6 1.00 2.0 0.6 1 \$ basic vertical parameters SI908 L 8.5 0.25 0.35 8.5 0.25 0.35 \$ first horizontal correction \$ first vertical correction SI909 L 0 0 0 0 0 0 SI910 L 0 10 0.2 0 10 0.2 \$ second horizontal correction 0 0 0 SI911L0 0 0 \$ second vertical correction C X Y Z X Y Z for beam centre coordinates SI912 L 0 0 -2.68 0 0 -2.68 \$ beam spot centre [cm] on Li-jet surface SI913 L 2001 \$ program cell number for Li-jet \$ target surface normal: along Z-axis SI914 L 0 0 1 \$ target density [g/cm**3], thickness [cm] SI915 L 0.512 2.50 \$ Li-6 and Li-7 relative Abundance SI916 L 0.075 0.925



 $p(x) = m^* \exp(-(x - x_0)^2 / 2s) / \sqrt{2ps}$ (+ Heaviside function for basic profile)

	Horizontal		Vertical			
	m	X ₀ , cm	σ , cm ²	m	X ₀ , cm	σ , cm ²
Basic	1.00	±9.0	0.60	1.0	±2.0	0.6
1st correction	0.35	±8.5	0.25	-	-	-
2nd correction	0.20	0.0	10.0	-	-	-

P. Wilson, Report FZKA 6218, 1999

13-14.03.2008

Tallies and its normalization

Overal normalization

- All McDeLicious results (talleis) are normalized per one incident deuteron

Specific Tally normalization:

- Flux Tally (F4, F5) for Neutron and Photon [1/cm²/s]:

I [mA] * 1.E-3 / (e⁻=1.60218E-19) = 6.2415E+15 * I [mA] = 1.56045E+18 (I=250 mA)

- Heating Tally (F6:n,p) by neutrons and photons [W/g]:

I [mA] * 1.E-3 (MeV/J=1.60218E-13)/(e=1.602177E-19 C)= I [mA] *1.E+3 =2.5E+5 (I=250mA)

- Heating in material M using mean flux in Cell estimated by tally F4 [W/g]:

- F4:n cell
- FM4 I [mA] * 1.E+3 *atom/gramm_denisity M -1 -4
- F4:p cell
- FM4 I [mA] * 1.E+3 *atom/gramm_denisity M -5 -6

Tallies and its normalization (continued)

Displacement Damage Rate caused by neutrons in materials

 $Damage_Rate[dpa/fpy] = F[n/cm^2/s] \times S_{dpa}[b] \times 1.E - 24[cm^2/b] \times 3.1557E + 7[s/fpy]$

where:

 $F[n/cm^{2}/s] - neutron flux = F4[n/cm^{2}]* I [mA] * 1.E-3 / (e=1.602177E-19 C)$ $s_{dpa}[b] = 0.8 \times DE[b*MeV] / (2 \times E_{d}[eV]) - displacement cross section$ DE[MeV*b] - damage energy (available in MT=444) $E_{d} [eV] - threshold energy to displace atom in lattice (e.g., 40 eV for Fe)$

Finally:

 $Damage_Rate[\ dpa/fpy\] = (78785.2/Ed \times I[mA]) \times F4[\ n/cm^2\]$

```
Example: dpa/fpy in Iron (material M) which fills the Cell;
d-beam current I = 250 mA
F4:n Cell
FM4 4.9241E+5 M 444
```

Tallies and its normalization (continued)

<u>Gas production rate = gas atoms per 1 target atom over time unit</u>

 $Gas_Production[appm/fpy] = F[n/cm^2/s] \times \mathbf{S}_{gas}[b] \times 1.E - 24[cm^2/b] \times 3.1557E + 7[s/fpy] \times 1.E + 6[appm]$

where:

F [n/cm2/s] - neutron flux = F4[n/cm2]* I [mA] * 1.E-3 / (e=1.602177E-19 C) σ_{gas} [b]- gas production cross-section MT=203 (H) or MT=207(He)

Finally:

Gas_Production[appm/ fpy] = $(0.19696 \times I[mA]) \times F4[n/cm^2]$

Example: He [appm/fpy] in Iron (material M) which fills the Cell; d-beam current I = 250 mA F4:n Cell FM4 49.241 M 207

13-14.03.2008

Nuclear Responses in the IFMIF sub-systems



Neutron energy fluxes in the IFMIF



Neutron fluxes & dpa in the IFMIF components

IFMIF test cell sub-system	Neutron Flux, 10 ¹⁴ n/cm ² /s	Damage (Element), dpa/fpy
Li-jet back Plate (BP)	15.0	66 (Fe)
High Flux Test Module (HFTM)	7.3	20 - 55 (Fe)
Univers. Test Machine (UTM)	3.5	11 (Fe)
Tungsten Moderator (W)	2.0	1.1 (W)
Tritium Release module (TRM)	1.1	2.4 (Fe), 3.5 (Be)
Low Flux Test Module (LFTM)	0.61	0.65 (Fe)
Front wall steel liner	0.01	0.004 (Fe)

S.P. Simakov et al. Fus.Eng.Des.75-79(2005)813

Nuclear Responses in the IFMIF sub-systems /F4 mesh tallies capabilities/



13-14.03.2008

IFMIF neutronics, McDeLicious code Test Cell geometry model:

further developments



IFMIF Test Cell MCNP Model converted by McCAD from CAD



Horizontal cut at target mid-plane level



H. Tsige-Tamirat et al. Fus. Eng.Des.,82(2007)1956