

# Low Energy Neutrons

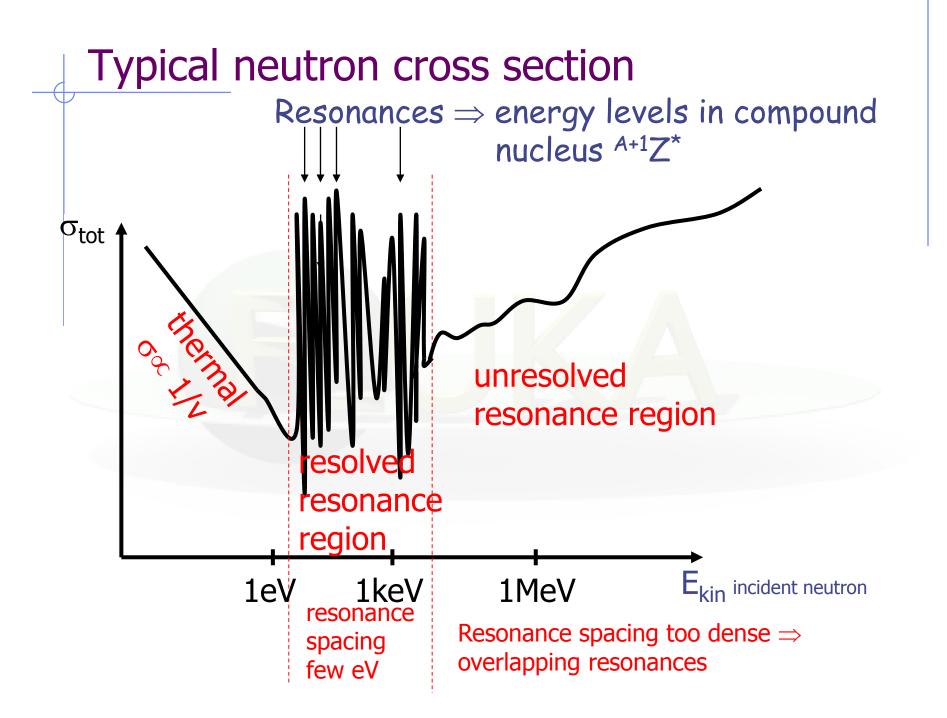
FLUKA Beginner's Course

#### Introduction

- In FLUKA we call neutrons below 20 MeV low energy neutrons
- Neutron interactions at higher energy are handled by FLUKA nuclear models
- Transport and interactions of neutrons with energies below
  20 MeV are handled by a dedicated library

#### Why are low Energy Neutrons special?

- The neutron has no charge → can interact with nuclei at low energies, e.g. meV
- Neutron cross sections (σ) are complicated → cannot be calculated by models → we rely on data files



#### **Evaluated Nuclear Data Files**

- Evaluated nuclear data files (ENDF, JEFF, JENDL...)
  - typically provide neutron  $\sigma$  (cross sections) for E<20MeV for all channels
  - $\sigma$  are stored as continuum + resonance parameters

#### Point-wise and Group-wise cross sections

- In neutron transport codes in general two approaches are used: point-wise ("continuous" cross sections) and group-wise transport
- Point-wise follows cross section precisely but it can be time and memory consuming
- Group approach is widely used in neutron transport codes because it is fast and gives good results for most application

Complex programs (NJOY, PREPRO...) convert ENDF files to point-wise or group-wise cross sections, including Doppler broadening etc.

#### **Group Transport Technique**

- The energy range of interest is divided in a given number of discrete intervals ("energy groups"). Each group is identified by a number <u>increasing</u> with <u>decreasing</u> energy. Group 1 is the group of highest energy (in the present FLUKA library, energies between 19.64 and 20 MeV)
- Elastic and inelastic reactions are not simulated as exclusive processes, but by group-to-group transfer probabilities (downscattering matrix)
- Downscattering matrix: if a neutron in a given group undergoes a scattering event and loses energy, it will be transferred to a group of lower energy (each of the lower energy groups having a different probability)
- If the neutron does not lose enough energy to be in another group, it will stay in the same group (in-scattering)
- In the thermal region neutrons can gain energy. This is taken into account by an upscattering matrix, containing the transfer probability to a group of higher energy

#### Group wise treatment

- Convert  $\sigma$  to energy groups like histograms, the energy width is different for each group in order to better represent resonances
- Each group *i* contains the <average>  $\sigma_i$ :

$$<\sigma_{i}>=\frac{\int_{E_{i,low}}^{E_{i,high}}\sigma(E)\Phi(E)\,dE}{\int_{E_{i,low}}^{E_{i,high}}\Phi(E)\,dE}$$

where  $\Phi$  is the fluence

- Advantage: fast
- Disadvantage: effects like self shielding are not accurately reproduced (see later), angular distributions replaced by a discrete number of angles (3 in FLUKA) conserving their first n moments (6 in FLUKA)

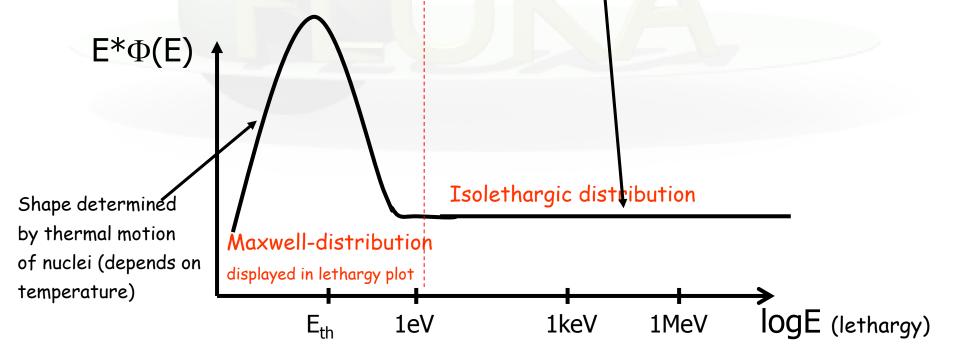
## Fluence

• An assumption is needed about the neutron spectrum to be used as a weighting function for calculating the average cross section on each group

For instance it can be shown that in most cases, between 1 eV and 1 MeV:

$$\Phi(E)dE = C\frac{dE}{E}$$
 ( $\frac{1}{E}$  spectrum)

In any case, the error is small if the group width is small



#### Angular distribution <sup>[1/2]</sup>

• The probability distribution of the scattering angle for each groupto-group transfer is represented by a Legendre polynomial expansion truncated at the (N+1)<sup>th</sup> term:

$$\sigma_s(g \to g', \mu) = \sum_{i=0}^N \frac{2i+1}{4\pi} \operatorname{P}_i(\mu) \, \sigma_s^i(g \to g')$$

 $\mu = \overline{\Omega} \cdot \overline{\Omega}' = \text{scattering angle}$ 

where N = chosen Legendre order of anisotropy

#### Angular distribution <sup>[2/2]</sup>

- In FLUKA, N=5
- The scattering angular probabilities are obtained by a discretization of a P5 Legendre polynomial expansion of the actual scattering angular distribution which preserves its first 6 moments.
- Result of this P5 expansion is a set of 3 discrete polar angle cosines and 3 corresponding probabilities, i.e. for a given transfer  $g \rightarrow g'$  only three values are possible for the polar angle
- The azimuthal angle is sampled from a uniform distribution and can have any value between 0 and  $2\pi$

# Self shielding

- The group structure is necessarily coarse with respect to the resonance structure in many materials
- A resonance in a material present in a dilute mixture or as a small piece cannot affect much a smooth neutron flux (socalled "infinite dilution")
- But if an isotope exhibiting large resonances is very pure or is present with a large fractional abundance, it can act as a "neutron sink", causing sharp dips in the neutron spectrum corresponding to each resonance  $\rightarrow$  an apparent decrease in  $\sigma$
- This effect, which results in a lower reaction rate  $\sigma \Phi$ , is called *self-shielding* and is necessarily lost in the process of cross section averaging over the width of each energy group, unless a special correction is made

### The FLUKA Low Energy Neutron Library [1/3]

- FLUKA uses the multigroup transport technique
- The energy boundary below which multigroup transport takes over depends in principle on the cross section library used. In the present library it is 20 MeV.
- Both fully biased and semi-analog approaches are available
- Number of groups: 260 of approximately equal logarithmic width, the actual energy limits of each group can be found in the manual (or can be printed to \*.out file)
- N.B. the group with the highest energy has the number 1, the group with the lowest energy has number 260
- 31 thermal groups, with 30 upscattering groups
- Energy range of library: 0.01 meV 20 MeV

### The FLUKA Low Energy Neutron library [2/3]

- Based on recent versions of evaluated nuclear data files: ENDF/B-VI.8, ENDF/B-VII.0, Jendl-3.3, Jendl-3.4, Jeff-3.1,...
- About 270 isotopes/materials available
- Almost all materials available at 2 temperatures: 87K, 296K
- Some also at 4K, 120K, 430K
- Doppler broadening at the relevant temperature is taken into account
- The library handles also gamma generation, energy deposition by kerma factors, residual nuclei production, secondary neutrons, fission neutrons
- For some isotopes/materials: self-shielding, molecular binding, correlated gamma generation, point-wise transport
- NB: Because of the group technique the energy of a transported neutron below 20 MeV is only defined within the resolution of the groups

### The FLUKA Low Energy Neutron library [3/3]

Energy weighting:

- Averaging inside each energy group according to the following weighting function. In order of increasing energy:
  - a Maxwellian at the relevant temperature in the thermal range
  - a 1/E spectrum in the intermediate energy range

But it is important to realize that the groups in the present library are very narrow! Therefore the energy weighting is not very important

#### Gamma generation

- Gamma generation from  $(n,x\gamma)$  reactions is possible only for those elements for which data are available in the evaluated nuclear data files (see manual for a complete list)
- Gamma generation is performed by a multigroup scheme as well
- Number of gamma groups: 42
  - NB number of γ groups different from number of neutron groups!
- Energy range: 1keV 50 MeV
  - NB γ energy range different from neutron energy range!
- The actual energy of the generated photon is sampled randomly in the energy interval corresponding to its gamma group
- Exception: 2.2 MeV from  $H(n,\gamma)^2H$  reaction, 478 keV photon from  ${}^{10}B(n, \alpha\gamma)$  and gamma cascades from  $Cd(n,\gamma)$  and  $Xe(n,\gamma)$
- Capture gammas as well as gammas from inelastic reactions like (n,n') are included
- The neutron library only creates gammas, the transport is done by the EMF module (like all other gammas in FLUKA)

#### **Energy deposition**

 Energy deposition by neutrons below 20 MeV is estimated by means of kerma factors

- For some materials with gamma production the kerma values of some groups (mainly at high energies) are problematic (see manual). The reason is inconsistent data in the evaluated data files. Effort was addressed to apply corrections to improve the situation but there are still some materials with problematic kermas.
- The user should check carefully the results of simulations with these materials. However, the effect should vanish in a typical simulation.

#### Secondary and Fission Neutrons

- Neutrons from (n,xn) reactions are taken into account implicitly by a group-dependent non-absorption probability, i.e. a factor by which the weight of a neutron is multiplied after a collision
- If the only possible processes are scattering and capture the nonabsorption probability is smaller than 1. If also (n,2n) is possible, the factor is bigger than 1
- Fission neutrons are treated separately by a group-dependent fission probability
- Fission neutrons are emitted isotropically with an energy sampled from a fission spectrum appropriate for the isotope and neutron energy
- The fission neutron multiplicity was obtained separately from the evaluated data files
- The fission fragments are not transported, their energy is deposited at the spot

#### Charged particle generation

- Recoil protons from hydrogen and protons from <sup>14</sup>N(n,p) are produced and transported explicitly (i.e. like other protons)
- That means that detailed kinematics of elastic scattering, continuous energy loss with energy straggling, delta ray production, multiple and single scattering, are all taken into account
- If point-wise transport has been requested,  $\alpha$  and <sup>3</sup>H fragments from neutron capture in <sup>6</sup>Li and <sup>10</sup>B can also be transported explicitly Note that for this purpose you cannot use the cross sections of natural Li and B, but you must define a compound of <sup>6</sup>Li and <sup>7</sup>Li, or one of <sup>10</sup>B and <sup>11</sup>B
- All other charged secondaries produced in low energy neutron reactions are not transported but their energy is deposited at the point of interaction using kerma factors

#### Residual nuclei production

- Residual nuclei: nuclei that are the result of a reaction and are at rest, e.g. <sup>28</sup>Al after a neutron capture reaction of <sup>27</sup>Al
- For all materials data are available for estimating residual nuclei production by low energy neutrons. Command RESNUCLEi allows to request separately residual nuclei from low energy neutrons and from high energy particles
- For Ti, Ga the residual nuclei information is based on different evaluations than the transport

# Using the Low Energy Neutron Library

#### **Available Materials**

#### • Section 10.4.1.2 of manual gives a list of available materials

#### • Example:

	Material	Temp.	Origin	RN	Name	Identifiers		Gam	
9Be	Beryllium 9	296K	ENDF/B-VIIR0	Y	BERYLLIU	4	9	296	Y
9Be	Beryllium 9	87K	ENDF/B-VIIR0	Y	BERYLLIU	4	9	87	Υ
В	Natural Boron	296K	ENDF/B-VIIR0	Y	BORON	5	-2	296	Y
В	Natural Boron	87K	ENDF/B-VIIR0	Y	BORON	5	-2	87	Y
10B	Boron 10	296K	ENDF/B-VIIR0	Y	BORON-10	5	10	296	Y
10B	Boron 10	87K	ENDF/B-VIIR0	Y	BORON-10	5	10	87	Y
11B	Boron 11	296K	ENDF/B-VIIR0	Y	BORON-11	5	11	296	Y
11B	Boron 11	87K	ENDF/B-VIIR0	Y	BORON-11	5	11	87	Y
С	Free gas natural Carbon	296K	ENDF/B-VIIR0	Y	CARBON	6	-2	296	Y
С	Graphite bound nat. Carbon	296K	ENDF/B-VIIR0	Y	CARBON	6	-3	296	Y
С	Free gas natural Carbon	87K	ENDF/B-VIIR0	Y	CARBON	6	-2	87	Y
Ν	Natural Nitrogen	296K	ENDF/B-VIIR0	Y	NITROGEN	7	-2	296	Y
N	Natural Nitrogen	87K	ENDF/B-VIIR0	Y	NITROGEN	7	-2	87	Y
14N	Nitrogen 14	296K	ENDF/B-VIIR0	Y	NITRO-14	7	14	296	Y
14N	Nitrogen 14	87K	ENDF/B-VIIR0	Y	NITRO-14	7	14	87	Y
160	Oxygen 16	296K	ENDF/B-VIR8	Y	OXYGEN	8	16	296	Υ
160	Oxygen 16	87K	ENDF/B-VIR8	Y	OXYGEN	8	16	87	Y
19F	Fluorine 19	296K	ENDF/B-VIR8	Y	FLUORINE	9	19	296	Y
19F	Fluorine 19	87K	ENDF/B-VIR8	Y	FLUORINE	9	19	87	Y
23Na	Sodium 23	296K	JENDL-3.3	Y	SODIUM	11	23	296	Y
23Na	Sodium 23	87K	JENDL-3.3	Y	SODIUM	11	23	87	Y
Mg	Natural Magnesium	296K	JENDL-3.3	Y	MAGNESIU	12	-2	296	Y
Mg	Natural Magnesium	87K	JENDL-3.3	Y	MAGNESIU	12	-2	87	Y
27AI	Aluminium 27	296K	ENDF/B-VIIR0	Y	ALUMINUM	13	27	296	Y
27AI	Aluminium 27 SelfShielded	296K	ENDF/B-VIIR0	Y	ALUMINUM	13	1027	296	Y

RN: residual nuclei

Gam: Gamma production

Name: name to be used in LOW-MAT card

Identifiers: to be used in LOW-MAT card

### Using the Low Energy Neutron Library

- How to activate low energy neutron transport?
  - Implicit: giving a DEFAULTS cards (except with default EM-CASCA), or not giving a DEFAULTS card at all

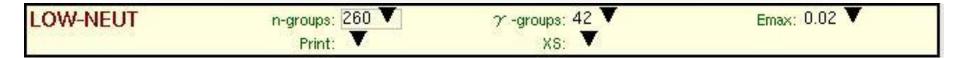
That means: you are using the library in almost any simulation (unless you are using the default EM-CASCA or you have switched it off explicitly with a LOW-BIAS or PART-THR card)

- Explicit: giving a LOW-NEUT card
  - NB you don't need it in most practical cases! (See below)
- What must the user do?
  - To set correspondence between the actual material and the material in the low neutron library (LOW-MAT card), if not done by default.
    - NB you don't need it in most practical cases!
  - To set transport thresholds with PART-THR, if defaults are not ideal for the actual problem
  - To request special features like point wise cross sections or cross section printing (LOW-NEUT)

#### Input Cards: LOW-NEUT [1/4]

This card activates low-energy neutron transport.

- WHAT(1): number of neutron groups of the library
  - Default: 260
- WHAT(2): number of gamma groups of the library
  - Default: 42
- WHAT(3): maximum energy (in GeV) of the library
  - Default: 0.02
- WHAT(5): number of thermal groups
  - Default: 31



 The defaults for WHAT(1) - WHAT(3) and WHAT(5) are fine. The only reason for changing them would be if using a different library (there was one until recently, but it has been suppressed)

Don't use them!

#### Input Cards: LOW-NEUT [2/4]

- WHAT(4): printing flag, neutron cross section information is written to \*.out file
  - 0.0 Minimum
  - 1.0 integral cross sections, kerma factors and probabilities
  - 2.0 additionally downscattering matrices and gamma matrices
  - 3.0 additionally scattering probabilities and angles
  - 4.0 residual nuclei information
  - Default: 0.0 (minimum)

LOW-NEUT	n-groups: Print:	260 🗸	γ -groups: 42 ▼ XS: ▼	Emax: 0.02 🔻
		Minimum Integral XS +Downscatter +Angles	S hidden	

#### Input Cards: LOW-NEUT [3/4]

#### The output for WHAT(4) = 1

- Group energy limits, average energies, velocities and momenta, thermal velocities, gamma group limits
- For each material: availability of residual nuclei information (the line: "RESIDUAL NUCLEI INFORMATIONS AVAILABLE" indicates the possibility to use option RESNUCLEi with WHAT(1)= 2.0
- for each neutron energy group in each material:
  - SIGT = total cross section
  - **SIGST** = "scattering" cross section:  $\sigma(n,n) + 2\sigma(n,2n) + 3\sigma(n,3n)$
  - PNUP = upscatter probability, is 0.0 in non thermal groups
  - PNABS = Probability of Non-ABSorption (= scattering)
    PNABS = SIGST/SIGT, and can sometimes be> 1 because of (n,xn) reactions
  - GAMGEN = GAMma GENeration probability = gamma production cross section divided by SIGT and multiplied by the average number of  $\gamma$  per (n,  $\gamma$ ) reaction
  - NU\*FIS = fission neutron production = fission cross section divided by SIGT and multiplied by v, the average number of neutrons per fission
  - EDEP = Kerma contribution in GeV per collision
  - PNEL, PXN, PFISS, PNGAM = partial cross sections, expressed as probabilities (*i.e.*, ratios to SIGT). In the order: non-elastic, (n,xn), fission, (n,gamma)

#### Input Cards: LOW-NEUT [4/4]

- WHAT(6): i<sub>0</sub> + 10 \* i<sub>1</sub>:
  - $i_0 = 1$ : available point wise cross sections used and explicit and correlated  ${}^{6}Li(n,\gamma){}^{7}Li$ ,  ${}^{6}Li(n,t){}^{4}He$ ,  ${}^{10}B(n,\alpha\gamma){}^{7}Li$ ,  ${}^{40}Ar(n,\gamma){}^{41}Ar$ ,  ${}^{\times}Xe(n,\gamma){}^{\times+1}Xe$  and  ${}^{113}Cd(n,\gamma){}^{114}Cd$  photon cascade requested
    - = 0: ignored
    - =< -1: resets to the default (point wise cross sections are not used)</p>
  - i<sub>1</sub> = 1, fission neutron multiplicity forced to 1, with proper weight to compensate for the "wrong" multiplicity
    - = 0, ignored
    - =< -1: resets to the default (normal fission multiplicity)</p>
  - Default = -11., unless option DEFAULTS is present with SDUM = CALORIME, ICARUS, NEUTRONS or PRECISIO, in which case the default is 1.0 (point wise cross sections are used when available and fission multiplicity is not forced)

LOW-NEUT	n-groups: 260 🔻	∽ -groups: 42	Emax: 0.02 🔻
	Print:	XS:	
	PART-THR ST	DP : 2 cards hidden -	
		Default	
		Pt-wise XS	
		Fission mult	
		Pt-XS+Fission	
		reset	

#### Input Cards: LOW-MAT<sup>[1/3]</sup>

- The LOW-MAT card sets the correspondence between FLUKA materials and the low energy neutron cross sections
- If a material has the same name as a name given in the list of low neutron materials, the correspondence between material and low energy neutron transport is set automatically, and a LOW-MAT card is not necessary. The first material with the right name is taken. This is always a material at room temperature.
- That means that for the predefined material HYDROGEN hydrogen bound in water is used, not the free gas one
- If you want to use low energy neutron transport in  $\rm H_2$  gas you have to do this explicitly by a LOW-MAT card

#### Input Cards: LOW-MAT<sup>[2/3]</sup>

- WHAT(1): Name of the material (single element/isotope only!)
  - In flair this can be chosen from a pull down menu
- WHAT(2), WHAT(3) and WHAT(4): the 3 identifiers from table 10.4.1.2 of the manual
- SDUM: name of the material from table 10.4.1.2 of the manual
- In flair there is only one pull down menu for all identifiers and the name
- If you want to use the predefined materials at a temperature different from 296K, it is mandatory to give a LOW-MAT card with the proper identifiers

#### Input Cards: LOW-MAT<sup>[3/3]</sup>

- Setting the correspondence between a material and low energy neutron transport cross sections:
  - First create the material with a MATERIAL card and give it a name in SDUM
  - Give a LOW-MAT card with WHAT(1) = the name you gave in the SDUM of the MATERIAL
  - Give in WHAT(2), WHAT(3) and WHAT(4) of the LOW-MAT card the numerical identifiers (table 10.4.1.2 in manual) of the material you want to use, be careful to use the one with the right temperature
  - Give in SDUM of the LOW-MAT card the name provided in the same table

### Example: compound at 87K

#### • Example: sodium iodide (NaI) at 87K

- Create a material sodium and give it some name (SODIU\_87), do the same with iodine (IOD\_87)
- Give a LOW-MAT card for SODIU\_87, choose the right cross sections identifiers (those for 87K) and name (see list in manual), do the same for iodine
- Create a material NAI\_87 by giving first a MATERIAL card and then a corresponding COMPOUND card with the right composition

MATERIAL		Name	SODIU_87		#	p: 0.97
Z: 11		Am	22.99		A:	dE/dx: 🔻
LOW-MAT		Mat	SODIU_87 🔻		LowMat: 23Na. Sodi	um 23, 87K 🔻
MATERIAL		Name	: IOD_87		#	ρ: <b>4.93</b>
Z: 53		Am	126.9		A:	dE/dx: 🔻
LOW-MAT		Mat	IOD_87 ▼		LowMat: 1291. lodine	e 129 (2), 87K 🔻
MATERIAL		Name	: NAI_87		#	ρ: <b>3.667</b>
Z:		Am	i:		A:	dE/dx: 🔻
COMPOUND		Name	NAI_87 ▼		Mix: Atom 🔻	Elements: 13 V
f1: 1.0	1		: IOD_87 ▼		f2: 1.0	M2: SODIU_87 V
f3: M3: 🔻						
	MATERIAL	11.	22.99	0.97		SODIU 87
	LOW-MAT	SODIU 87	11.	23.	87.	SODIUM
	MATERIAL	53.	126.9	4.93		IOD 87
	LOW-MAT	IOD 87	53.	129.	87.	129-I
	MATERIAL	200_07	55.	3.667		NAI 87
	COMPOUND	1.0	IOD 87	1.0	SODIU 87	NAI 87
	_					

### Input Cards: LOW-BIAS [1/2]

This card sets an energy cut-off during low-energy neutron transport on a region by region basis and/or non-analog absorption. <u>However, for an overall energy cut-off, it is preferable to use PART-THR</u>

- WHAT(1): number of the group to apply a transport cut-off, i.e. neutrons in groups the number of which >= WHAT(1) are not transported. Remember that the group with the highest energy has the number 1.
  - Default: 0.0 (no cut-off)
  - flair automatically matches the group number to the upper energy boundary of each group

LOW-BIAS	Ecut: 19.155 MeV 🔻	NonAnalogue: No cut-off 🔻	Survival:
	Reg: No cut-off	to Reg: 🔻	Step:
	<i>COMPO</i> 20.000 MeV	-	
	19.640 MeV		
	19.155 MeV		
	18.682 MeV		
	18.221 MeV		
	17.771 MeV		
	27.333 MeV		
requests non-analogue al low energy neutron trans	sorption and/or a region 16.905 MeV	ıg	
	+3+4.16.487 MeV	7 . + 7 +	

#### Input Cards: LOW-BIAS<sup>[2/2]</sup>

- Analog absorption: a neutron does not exist any more after an absorption process
- Non-analog absorption: the neutron is never killed at any interaction, but lives on with a lower weight, accounting for the relative probability of absorption and scattering. Capture gammas are created with a weight equal to that of the surviving neutron
- WHAT(2): Group limit for non-analog absorption (neutrons in groups >= WHAT(2) undergo non-analog absorption)
  - Default: 230 (non-analog absorption for all thermal neutrons)
- WHAT(3): non-analog survival probability
  - Default : 0.85 or 0.95, DEFAULTS-dependent)
- WARNING: Only experts should modify the non-analog absorption survival probability!
- If no LOW-BIAS card is given, non-analog absorption depends on the DEFAULTS card (see manual)
- The change of weight of the particle is taken into account (see lecture about biasing)

#### Transport cut-offs

- Transport cut off: a particle is not transported if its energy is lower than a cut off energy
- Transport cut offs for neutrons can be set to save CPU time
- Use cut offs with care, you could miss important effects like activation, dose, secondary particles,...
- For activation, thermal neutrons are very important. If you are interested in activation <u>never</u> cut off low energy neutrons!
- To set a general transport cut off for neutrons, please give the energy of the cut off in the PART-THR card, no matter if high or low energy neutrons. That was different in previous versions: the card LOW-BIAS was needed for low energy neutrons. LOW-BIAS is still needed if one wants set a cut-off region by region
- If there is no interest in low-energy neutron transport, but that feature is implicit in the DEFAULTS option chosen, it is suggested to request LOW-NEUT, and to use PART-THRes with an energy cutoff WHAT(1) = 0.020

#### Self-shielding<sup>[1/3]</sup>

Self-shielded materials in FLUKA:

- at 296K, 87K, 4K, 430K
- natA, <sup>40</sup>Ar at 296K, 87K
- natFe at 296K, 87K, 4K, 430K
- natCu at 296K, 87K, 4K, 430K
- 181 Ta at 296K, 87K
- natW at 296K, 87K, 4K, 430K
- <sup>197</sup>Au at 296K, 87K
- natPb at 296K, 87K
- 208Pb at 296K
- <sup>209</sup>Bi at 296K, 87K
  - Special case: cast iron (<sup>nat</sup>Fe +5%C) at 296K, 87K, 4K, 430K (see example further on)

### Self-shielding <sup>[2/3]</sup>

- When to use these materials?
  - Bulky (huge) pieces that are very pure (containing only one isotope)
- When not to use self-shielded materials?
  - "small" iron, copper, lead, aluminum pieces
  - Thin gold foils (but a self-shielded 100µm Au foil is available)
  - Diluted materials
- How to use self-shielded materials?
  - Define your material with a MATERIAL card
  - Give additionally a LOW-MAT card and give the proper identifiers in WHAT(2)-WHAT(4) and SDUM
  - If you have to use self-shielded and non self-shielded materials of the same element you need to define 2 different materials
  - Attention: predefined materials like iron, copper and lead are not self-shielded, you have to give a LOW-MAT card to use them self-shielded

#### Self-shielding [3/3]

- Cast iron is iron with a significant amount of carbon
- There is a self-shielded material cast iron in the low energy neutron library which is prepared to be used for creating a compound of iron and roughly 5% carbon. The amount of carbon doesn't need to be exactly 5%.
- How to create self-shielded cast iron?
  - Define a material iron called FeCarbSS (or any other name you like) with a MATERIAL card (parameters as for natural iron)
  - Insert a LOW-MAT card for FeCarbSS with the proper identifiers for cast iron in WHAT(2)-WHAT(4) and SDUM
  - Insert a MATERIAL card to declare a compound material called CastFe (or any other name you like)
  - Insert a COMPOUND card for defining CastFe as a compound of FeCarbSS and CARBON (predefined)

#### Artifacts of discrete angular distribution

- Artifacts can arise when a neutron is likely to scatter only once (thin foil, regions of low density like gases), due to the discrete angular distribution (only 3 angles are possible for each  $g \rightarrow g'$ )
- The user should be aware of such artifacts and interpret results of scattering at thin foils and gases carefully
- Because the 3 angles are different for each  $g \rightarrow g'$  and the azimuthal angle is sampled from a continuous distribution, the artifact disappears when the neutrons have the possibility of scattering two or more times.
- Information about which angles and probabilities are used for each group can be obtained by setting WHAT(4) = 3 in the LOW-NEUT card. The information is then written to the \*.out file (see manual chapter 9: Output)

#### Materials with molecular binding

- Available materials with molecular bindings at 296K:
  - H (natural isotopic amount) in  $H_2O$ ,  $CH_2$
  - <sup>1</sup>H in  $H_2O$ ,  $CH_2$
  - $^{2}D \text{ in } D_{2}O$
  - C in graphite
- Use of these materials makes the thermal neutron calculation more realistic and can affect the energy and spatial distributions
- Example: CH<sub>2</sub> (polyethylene) including molecular binding
  - Create a material hydrogen and give a corresponding LOW-MAT card that refers to H bound in  $CH_2$
  - Give a COMPOUND cart that creates CH<sub>2</sub> as a compound of bound H and normal carbon
- For hydrogen, H bound in water is the default, because it is the first in the list of low energy neutron materials



- Most of the simulations in FLUKA use the low energy neutrons, implicitly via the DEFAULTS card
- Low neutron transport in a material is enabled by a LOW-MAT card, only needed if the material's name is not one of those in the neutron cross section library, or temperature, self-shielding or molecular binding are different from the default ones
- Use self-shielded materials properly for "bulky" and "pure" (in isotopic composition) materials
- Don't give a LOW-MAT card for compounds