FLUKA



Exercise: Materials

23rd FLUKA Beginner's Course Lanzhou University Lanzhou, China June 2–7, 2024



Learn how to...

- 1 ... assign materials to objects
- 2 ... define your own compound material
- 3 ... edit the input file
- 4 ... change the isotope content in a material

Disclaimer

The example provided is intended to be used for educational purposes \underline{only} and not representative of a real scenario.



Copy the input file from the material.inp in a newly created directory and change its name:

mkdir new_materials
cd new_materials
cp \$coursepath/Exercises/Material_exercise/material.inp .
mv material.inp yourmaterial.inp

We recommend that you open the with *flair* to visualize the geometry

```
flair yourmaterial.inp &
```

but you can always work on the input file directly with your preferred editor.



The input details a fictional Mo target irradiation setup to produce ^{99m}Tc via the 100 Mo(p,2n) 99m Tc reaction, which has a peak cross-section at \sim 15 MeV.





Beam Dump, Target Core and Container Regions, named BDUMP, TCORE and TCON respectively, are currently all assigned a "BLCKHOLE" material.

1.1 Start by assigning a material of your choice to the beam dump from the

pre-defined material list:

#		+ [untit	ed] - flair		A = 0 K
🖬 🕶 🖛 🛤 🖬 🕼 İn	put Geome	try &Run 💷 Plot			🔅 Calculator 🔻 📢
A Cut Load	Export • 4dd•6	Preprocessor • XDelete Material • Comment• Comm	tove Up *all* Search tove Down	▼ A @Viewer P 2Editor tu ⊴Print	
Clipboard Ir	nput	Card Edit	Filte	View	
0			Input		▲ ×
General	ASSIGNMA	MatiAIR • MatiDecavit •	Reg: VAIR	to Reg: • Field: •	
Geometry	ASSIGNMA	Mat:BLCKHOLE Mat(Decay)	Reg: BDUN	P v to Reg: v Field: v	
Physics	ASSIGNMA	Mat. BLCKHOLE Mat(Decay):VACUUM	ID/name	E • to Reg: • Field: •	
Biasing	ASSIGNMA	Mat HYDROGEN Mat(Decay): HELIUM	Step:	T • to Reg: • Field: •	
Flair	ASSIGNMA	Mat/BERYLLIU Mat/Decay2/CARBON	Reg: BCOL Step:	to Reg: • Field: •	
Preprocessor	ASSIGNMA	Mat NITROGEN Mat(Decay) OXYGEN	Reg: BPIP Step:	to Reg: • Field: •	
	ASSIGNMA	Mat MAGNESIU Mat(Decay): •	Reg: BVAC Step:	 to Reg: Field: 	
	ASSIGNMA	Mat:ALUMINUM	Reg: VWIN	 to Reg: • 	
	ASSIGNMA	SLCKHOLE BDUMP	3+6 ▼ .+7	+	
Inp: material.inp +	+	Active:30 Total:40			#X

Bonus points look into the manual for the predefined material list and assign one of them to the dump region by editing the input directly e.g.

ASSIGNMA TUNGSTEN BDUMP

Exercise Material



Now add a comletely new material:

- 1.2 Add MATERIAL Molybdenum, Z=42 and density 10.22 g/cm³, give to it the name MOLYBDEN ¹
- 1.2 Modify ASSIGNMAT to assign MOLYBDEN as the material to TCORE

Bonus points Edit the input directly e.g.:

 MATERIAL
 42
 10.22
 MOLYBDEN

 ASSIGNMA
 MOLYBDEN
 TCORE

Do not place material cards between GEOBEGIN and GEOEND commands

¹sometimes names are important, wait for the Neutron lecture



Compound material are materials made up of more than one element. Some of them materials can be found in the Flair material library

1.3 Find brass and stainless steel; add them to your input and replace the materials in BCOLL and BPIP regions, respectively. Feel free to modify them.

🖽 🔊 \star 陀 🔗 Flair - 🧐	Input 🧯 Geometry 👌 Run 🔲 Plot			Materials 🔻 🚺				
Peter - La Copy To J Exert selected								
Clipboard materials	to input carr							
0	Materials		i	▲ ×				
Search:				×				
Group	/ Material List							
Biological	Material	Density	Stoichiometry					
Elements	Brass(typical)	8.52	Cu-62, Zn-35, Pb-3	E .				
General	Stainless-Steel (typical)	8.0	Cr-18, Fe-74, Ni-8					
ICRU	Beryflium-Copper	8.27	Be-1.9, Cu-98.1					
Implantation	Inconel-600	8,43	Cr-15, Fe-9, Ni-76					
Liquids / Gases	Monel-400	8.85	Mn-1, Fe-2, Ni-66, Cu-31					
Metal Alloys	Bronze (typical)	8.82	Cu-89, Zn-9, Pb-2					
Plastics / Polymers								
Targets								
User								
				1				

A compound definition always requires a material card:

MATERIAL			8.0				Stainles
COMPOUND	18.0	CHROMIUM	74.0	IRON	8.0	NICKEL	Stainles



Now to define your very own compound material:

2 Create a compound material named mybronze based on 87.5% Cu and 12.5% Sn mass contents. You should be able to calculate its density rather easily. Assign that compound material to region TCONT

Suggestion

The library does have a bronze material, albeit with a different composition. You could use that as a template for your new compound.



Run yourmaterial.inp from the terminal*, 3 cycles, 5000 primaries:

```
$FLUPRO/flutil/rfluka -NO -M3 yourmaterial
```

Suggestion

You can use this relaxing time to look into the $\rm FLUKA$ manual – open FM.pdf in your $\rm FLUKA$ installation folder or press "F1" while using flair.

*Alternatively, if you are already familiar with flair, feel free to run your FLUKA simulation through the flair interface instead.



Once a cycle run is complete, an output file is automatically created - e.g. your_material001.out - open it with a text editor and search for the following:

0				Viewer		
Files	1Region # name	volume	ALL-PART Star Density	BEAMPART Star Density	ENERGY Density	EM-ENRGY Density
mat-3001.out		in cubic cm	Stars/cm**3	Stars/cm**3	GeV/cm**3	GeV/cm**3
⊖ your_material001.out			/one beam particle	/one beam particle	/one beam particle	/one beam particle
License/version						
🕀 🕘 Input Echo	1 BLKBODY	1.00000000D+00	0.00000000D+00	0.00000000D+00	2.234676342D-04	1.174703399D-04
- 🗋 Nuclear Data	2 VAIR	1.00000000D+00	5.15000000D-04	5.12000000D-04	1.454219628D-03	4.948799829D-07
- 🗈 Mulmix	3 BDUMP	1.00000000D+00	6.20000000D-05	6.00000000D-06	2.785957212D-03	2.789183848D-06
Products/Decays	4 TCORE	1.00000000D+00	3.000000000D-06	0.000000000D+00	1.696775598D-07	1.675662894D-07
- Neutron	5 TCONT	1.00000000D+00	5.03000000D-04	5.000000000-04	5.494547784D-03	4.818044283D-07
-D dp/dx	6 BCOLL	1.000000000000+00	4.380000000-04	1.490000000D-04	1.3824799030-03	1.810246504D-05
- Blank Common	7 RPTP	1.00000000000+00	4 0000000000-05	0.0000000000+00	2.0209669620-05	1.670309561D-05
Media Parameters	8 BVAC	1.0000000000000000000000000000000000000	0,0000000000000000000000000000000000000	0.0000000000000000000000000000000000000	0 0000000000000000	0.0000000000+00
-D EME	9 VWTN	1 0000000000000000000000000000000000000	3.7589000000-02	3.741700000-02	3 8163684490-02	3 1612342820-05
-D Particles	5 1111	1.000000000000000	5.756566666-62	5.7417000000-02	5.0105004450-02	5.1012542020-05
Beam	Total (integral	ted over volume)	2 911400000 02	2 959400000-02	4 9524726880 82	1 9792167990 84
Particle Thresholds	Total (Integra	ced over vorume).	5.511400000-02	5.050400000-02	4:5524750000-02	1:0/0210/000-04
Termination Conditions	***** Neut cont	trol card *****	5TOP 8 888 8			
B Mult, Coulomb Scattering	Next com	cioi card	STOP 0.000 0	.000 0.000 0	0.000	0.000
D FM Chewart						
Carries						
LD Material						
D Designs						
Regions						
- Initialization Time						
- Output During Transport						
Events by Region						
Scattering Statistics						
🖓 🚭 Run Summary						



- 3 From the output one can see that this setup is not optimized. For instance, the proton beam is not interacting with the target: i.e. TCORE BEAMPART Star Density = 0 because the vacuum window is too thick, as VWIN ENERGY Density $\approx 75\%$ of total.
- Let us edit the input and try to improve the situation by:
 - decreasing the thickness of the vacuum window to 1 mm: in the geometry section of the input search for RCC vwin and change WHAT(6) $1 \rightarrow 0.1$
 - replacing the TCONT material: e.g., with graphite (Z = 6, $\rho = 1.7$ g cm⁻³)
 - Source to define the new material graphite and assign it to TCONT
 - enhancing beam quality: in the BEAM card change WHAT(4) and WHAT(5) values from -1.0 to \rightarrow 0.5. Check the implication of the sign change in the manual.



Save your new input with a different name to avoid overriding the previous' run files and run, as before, 3 cycles of 5000 primaries.

Suggestion

While the run is ongoing, do take the time to open the edited input with flair and have a look at how it changed with respect to the previous file.

Once an output is produced, compare it with the previous example. Did it improve?



4 Natural Mo consists of several isotopes ranging in mass from 92-100 and with their respective abundances already factored in the FLUKA elemental Mo material. However, in the context of ^{99m}Tc production via proton bombardment, enriched Mo with over 99% of ¹⁰⁰Mo is employed - we will hereby attempt to define a material with 99% of ¹⁰⁰Mo and 1% of ⁹⁸Mo.

How to create this material featuring a custom isotopic composition?

- Explicitly define ¹⁰⁰Mo and ⁹⁸Mo as a single materials MO-100 and MO-98, their WHAT(6) values 100 and 98, respectively.
- 2 Create a new material, e.g. new_moly, required to define a compound.
- Introduce a compound card and assign '0.01' to your Mo-98 material and '0.99' to Mo-100. Make sure to use the same density as molybdenum for all these new materials.



Input example:

MATERIAL	42	100	10.22		MO-100
MATERIAL	42	98	10.22		MO-98
MATERIAL			10.22		NEW_MOLY
COMPOUND	0.99	MO-100	0.01	MO-98	NEW_MOLY
ASSIGNMA	NEW_MOLY	TCORE			

From the flair standpoint:

MATERIAL		Name: MO-100	8	ρ: 10.22
	Z: 42.	Am:	A: 100.0	dE/dx: 👻
MATERIAL		Name: MO-98	4 C	ρ: 10.22
	Z: 42.	Am:	A: 98.0	dE/dx: 🖷
MATERIAL		Name: NEW_MOLY	4 C	ρ: 10.22
	Z: 42.	Am:	A:	dE/dx 👻
COMPOUND		Name: NEW_MOLY	Mix Atom 🔻	Elements: 13 v
	f1:0.99	M1: MO-100 ¥	f2: 0.01	M2: MO-98 v
	f3:	M3: 🗸		
		MATER	IAL ASSIGNMA : 7 cards hidden	
ASSIGNMA		Mat: NEW_MOLY	Reg: TCORE V	to Reg: 👻
		Mat(Decay): •	Step:	Field: 🔻

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