FLUKA

LANZHOU UNIVERSITY

Exercise: Materials

23rd FLUKA Beginner's Course
Lanzhou University
Lanzhou, China

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Exercise: Materials
Objectives

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 **only** and not representative of a real scenario.

Exercise: Materials

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 &
```

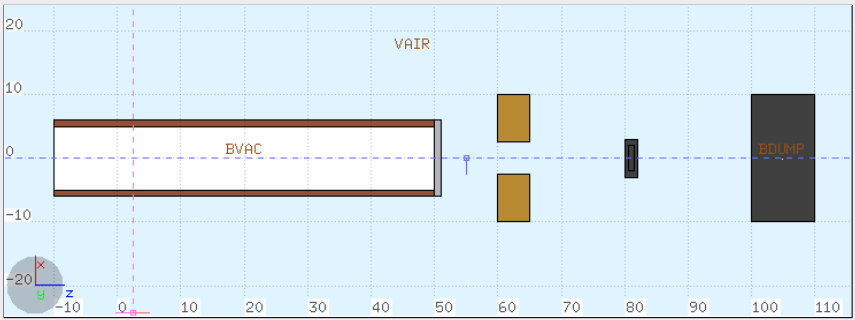
but you can always work on the input file directly with your preferred editor.

Exercise: Materials

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.

Geometry layout - Take your time to explore the input...

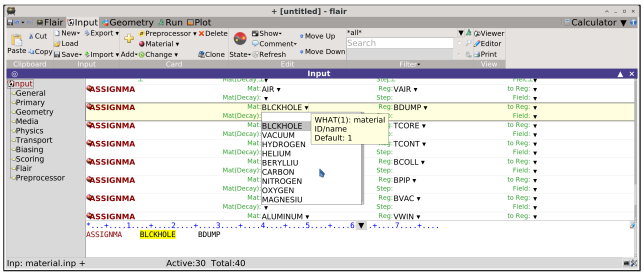
Beam direction →



Exercise: Materials

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:



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: Materials

Now add a comletely new material:

1.2 Add MATERIAL Molybdenum, Z=42 and density 10.22 g/cm^3, 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
```

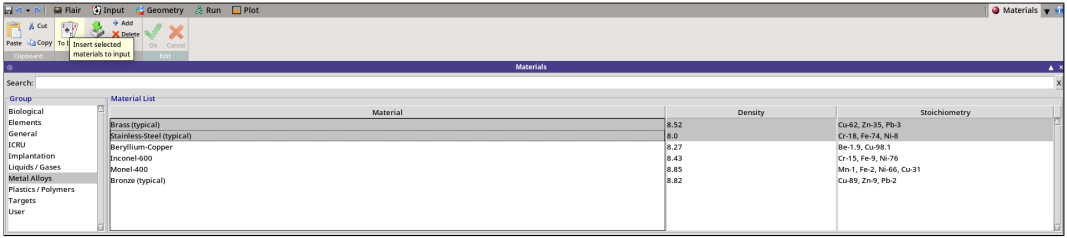
Do not place material cards between GEOBEGIN and GEOEND commands

[1] sometimes names are important, wait for the Neutron lecture

Exercise: Materials

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.



A compound definition always requires a material card:

```
MATERIAL                                    8.0                                                 Stainles
COMPOUND    18.0    CHROMIUM    74.0    IRON    8.0    NICKEL                                   Stainles
```

Exercise: Materials

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.

Exercise: Materials

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

```
$FLUPRO/flutil/rfluka -N0 -M3 yourmaterial
```

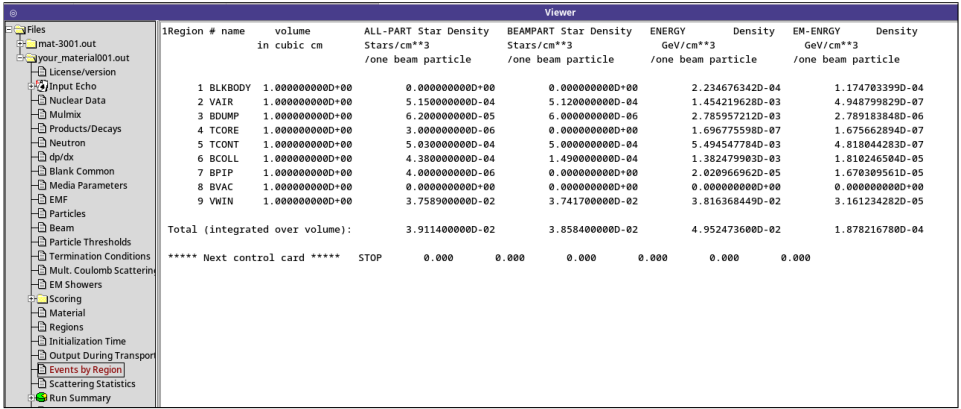
Suggestion

You can use this relaxing time to look into the FLUKA manual - open FM.pdf in your 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.*

Exercise: Materials

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:




```
1Region # name      volume          ALL-PART Star Density   BEAMPART Star Density   ENERGY        Density   EM-ENRGY      Density
                  in cubic cm       Stars/cm**3             Stars/cm**3               GeV/cm**3               GeV/cm**3
                                    /one beam particle      /one beam particle      /one beam particle      /one beam particle

     1 BLKBODY  1.000000000D+00        0.000000000D+00         0.000000000D+00         2.234676342D-04         1.174703399D-04
     2 VAIR     1.000000000D+00        5.150000000D-04         5.120000000D-04         1.454219628D-03         4.948799829D-07
     3 BDUMP    1.000000000D+00        6.200000000D-05         6.000000000D-06         2.785957212D-03         2.789183848D-06
     4 TCORE    1.000000000D+00        3.000000000D-06         0.000000000D+00         1.696775598D-07         1.675662894D-07
     5 TCONT    1.000000000D+00        5.030000000D-04         5.000000000D-04         5.494547784D-03         4.818044283D-07
     6 BCOLL    1.000000000D+00        4.380000000D-04         1.490000000D-04         1.382479903D-03         1.810246504D-05
     7 BPIP     1.000000000D+00        4.000000000D-06         0.000000000D+00         2.020966962D-05         1.670309561D-05
     8 BVAC     1.000000000D+00        0.000000000D+00         0.000000000D+00         0.000000000D+00         0.000000000D+00
     9 VWIN     1.000000000D+00        3.758900000D-02         3.741700000D-02         3.816368449D-02         3.161234282D-05

 Total (integrated over volume):        3.911400000D-02         3.858400000D-02         4.952473600D-02         1.878216780D-04

 ***** Next control card *****   STOP       0.000       0.000       0.000       0.000       0.000       0.000
```

Exercise: Materials

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})
  - You need 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?

Exercise: Materials

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 ^{100}Mo is employed** - we will hereby attempt to define a material with 99% of ^{100}Mo and 1% of ^{98}Mo.

How to create this material featuring a custom isotopic composition?

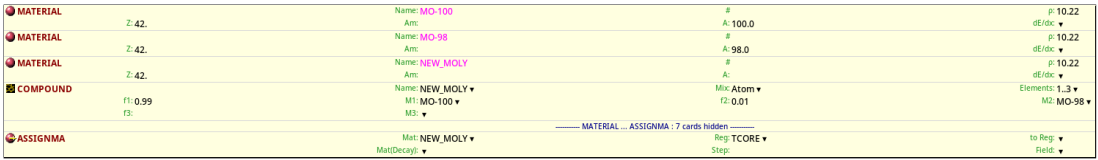
1. Explicitly define ^{100}Mo and ^{98}Mo as a single materials MO-100 and MO-98, their WHAT(6) values 100 and 98, respectively.
2. Create a new material, e.g. new_moly, required to define a compound.
3. Introduce a compound card and assign '0.01' to your Mo-98 material and '0.99' to Mo-100. Make sure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

Exercise: 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:



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