The geant4 isotope production model

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Abstract

Neutron induced isotope production is one of the main sources for activation of detector materials in LHC detectors, and important studies have been undertaken, to evaluate the amount of activation of the CMS detectors during the running of LHC. We present an Object Oriented isotope-production model that can be registered to the geant4 hadronic shower framework. We investigate the quality to which this tool can reproduce the cross-sections for isotope production in neutron-induced reactions. We describe workings of the model, and show results found, focussing on typical calorimeter and tracker materials.

Keywords: Activation, simulation, Geant4

1 The Model

The model under investigation is running in parasitic mode to the GEANT4[1] transport models, and can be used in conjunction with any set of models for final state production and inclusive cross-sections. It uses data driven modeling. It is targeted to allow for detailed isotope production studies, covering most of the spallation neutron energy spectrum. It is based on evaluated neutron scattering data below neutron kinetic energies of 20 MeV, and a combination of evaluated data and extrapolations at energies up to 100 MeV. The extrapolations take the form of

$$\sigma_{reac.} = F(E_n)\pi p_1^2 \ln(N)\left[1 + A^{1/3} - p_2(1 - 1/A^{1/3})\right].$$

Here F is the low energy correction factor, N the number of neutrons, A the nuclear mass number, E_n the neutron kinetic energy in GeV, and p_1 and p_2 are model parameters that have been fitted to experimental data. For details, please see [2]. The total cross-section is assumed to follow the energy dependence of the reaction cross-section above 20 MeV neutron kinetic energy. The upper limit of applicability of the model is 100 MeV neutron kinetic energy. In detail it targets the following set of requirements:

- Detailed simulation of isotope production cross-sections in the spallation neutron energy range.
- Provide information on which model produced a particular isotope.
- Provide information on the target material.
- Provide information on energy and direction of the projectile.
- Provide information on time and location of production.

The following evaluated data libraries form the basis of the GEANT4 neutron transport and activation data library G4NDL0.2:

- Brond-2.1[8]
- CENDL2.2[7]
- EFF-3[9]

- ENDF/B-VI.0[4]
- ENDF/B-VI.1
- ENDF/B-VI.5
- FENDL/E2.0[11]
- JEF2.2[10]
- JENDL-FF[5]
- JENDL-3.1
- JENDL-3.2
- MENDL-2[12]

This G4NDL selection was guided in large parts by the FENDL2.0 selection. Additions to and small modifications of this selection were possible due to the structure of the GEANT4 neutron transport code and the use of the file system to maximise the flexibility of the data formats. In addition, the MENDL data sets are included.

The implementation of the sampling of the ENDF-B VI data formats in GEANT4 is completely general with the exception of the generalised R-matrix representation, and can be used to run against any pre-processed evaluated data library that initially conforms with the ENDF-B VI data formats. The data are supplemented with data on the nuclear excitation levels that originate from the ENSDF evaluated data library.

2 Materials

The evaluation of the code uses mainly the most abundant materials of CMS calorimetry. We investigate lead, copper, zinc, and tungsten. We add silicon as one important material from the inner detector of CMS. This selection of materials is by no means complete, and more materials can be investigated in subsequent work.

We restrict ourselves to the naturally occuring isotopes[3]:

- Lead: $^{204}_{82}$Pb 1.4(1)%, $^{206}_{82}$Pb 24.1(1)%, $^{207}_{82}$Pb 22.1(1)%, $^{208}_{82}$Pb 52.4(1)%
- Tungsten: $^{180}_{74}$W 0.12(1)%, $^{182}_{74}$W 26.50(16)%, $^{183}_{74}$W 14.31(4)%, $^{184}_{74}$W 30.64(2)%, $^{186}_{74}$W 28.43(19)%
- Copper: $^{63}_{29}$Cu 69.17(3)%, $^{65}_{29}$Cu 30.83(3)%
- Zinc: $^{64}_{30}$Zn 48.63(60)%, $^{66}_{30}$Zn 27.90(27)%), $^{67}_{30}$Zn 4.10(13)%, $^{68}_{30}$Zn 18.75 (51)%, $^{70}_{30}$Zn 0.62(3)%
- Silicon: $^{28}_{14}$Si 92.2297(7)%, $^{29}_{14}$Si 4.6832(5)%, $^{30}_{14}$Si 3.0872(5)%

3 Results

In order to evaluate the code, we have generated 10^6 single interactions for each isotope at neutron energies of 0 MeV to 100 MeV in steps of 10 MeV, adding 1 MeV and 99 MeV at the borders of applicability of the model.

Figures 1 shows an example of the simulated cross-section in comparison to evaluated data from the MENDL collection, using 10^6 events for each energy isotope combination. A systematic error of 15% was added to the simulation results, to take the error in the extrapolation of the total cross-sections into account. For the full paper and a more complete set of comparison, see[13].

The number of different isotopes the code can produce is very high, and the results are limited by statistics for the very rarely produced isotopes. We add in the following the limit on the number of different isotopes produced by the code in the case of infinite statistics.

- Lead: $^{204}_{82}$Pb: 122, $^{206}_{82}$Pb: 125, $^{207}_{82}$Pb: 123, $^{208}_{82}$Pb: 123
- Tungsten: $^{180}_{74}$W: 122, $^{182}_{74}$W: 124, $^{183}_{74}$W: 128, $^{184}_{74}$W: 86, $^{186}_{74}$W: 86

- Copper: $^{63}_{29}$Cu: 100, $^{65}_{29}$Cu: 102
- Zinc: $^{64}_{30}$Zn: 96, $^{66}_{30}$Zn: 103, $^{67}_{30}$Zn: 105, $^{68}_{30}$Zn: 105, $^{70}_{30}$Zn: 110
- Silicon: $^{28}_{14}$Si: 73, $^{29}_{14}$Si: 75, $^{30}_{14}$Si: 76

The maximum ΔA for which the cross-sections are simulated with better than O(10%) precision is 22 for Lead, 21 for Tungsten, 20 for Copper, 21 for Zinc, and 16 for Silicon.

Taking into account that typical pre-compound and neutron transport models can describe the isotope production cross-sections at sizable ΔA to within 50%, the results of the comparison are very satisfactory. In all cases investigated, a precision of O(5%) is reached in the description of neutron induced isotope production cross-sections in CMS materials, and the threshold and double threshold production behaviours are simulated correctly, with a systematic error of 15% on the absolute normalisation.

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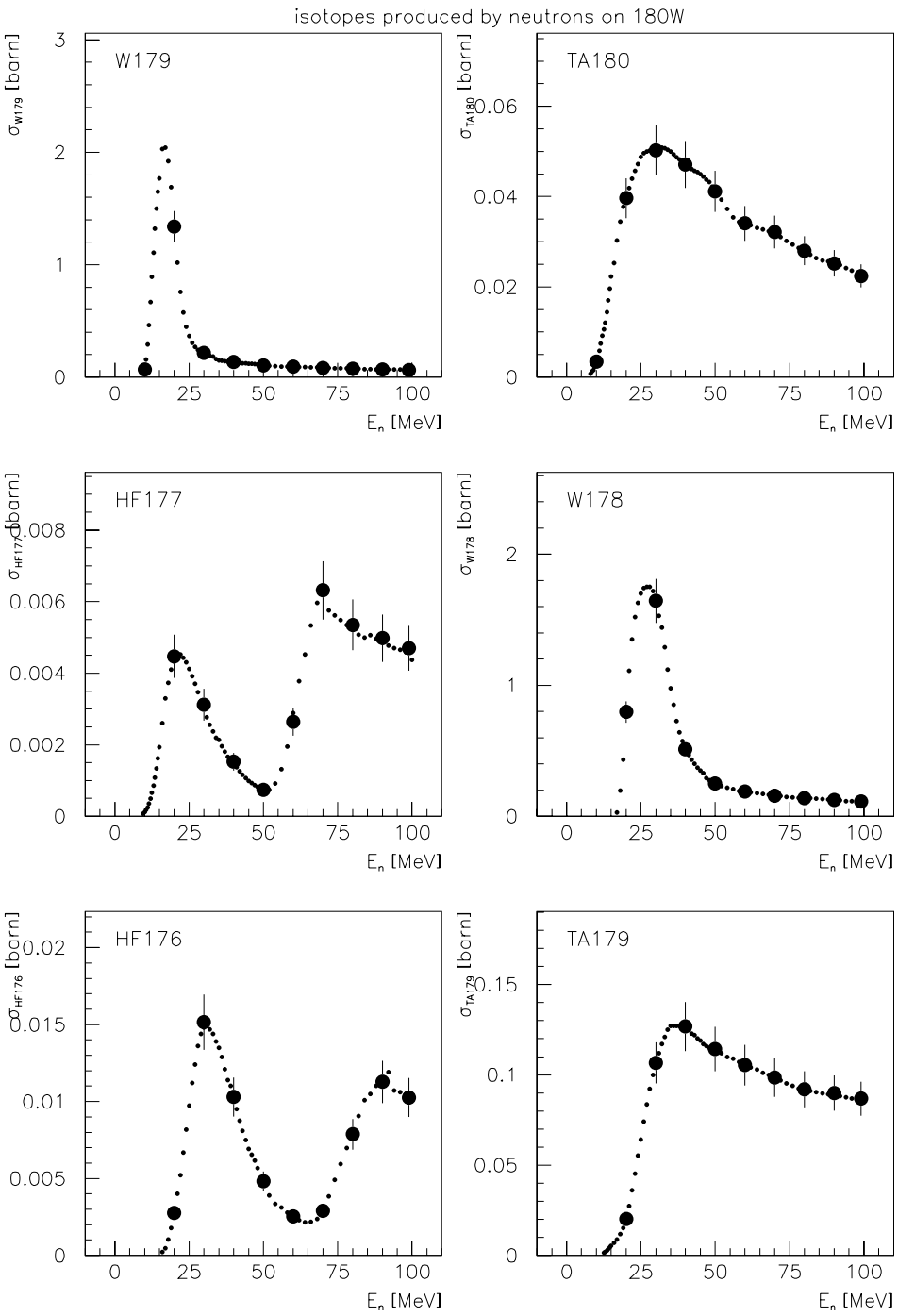

Figure 1: Isotope production cross-sections for neutron induced production of important isotopes as simulated using the isotope-production code in GEANT4. Large points are simulation results, small points are evaluated data from the MENDL2 data library.