

Accurate Monte Carlo modeling of biomedical cyclotrons: optimization of FLUKA physics and transport parameters for dosimetry, shielding and activation calculations

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ALMA MATER STUDIORUM ~ UNIVERSITÀ DI BOLOGNA

IL PRESENTE MATERIALE È RISERVATO AL PERSONALE DELL'UNIVERSITÀ DI BOLOGNA E NON PUÒ ESSERE UTILIZZATO AI TERMINI DI LEGGE DA ALTRE PERSONE O PER FINI NON ISTITUZIONALI



Outline

- Introduction
- Creation and validation of a Monte Carlo model of a biomedical cyclotron:
 - Modeling
 - Optimization of the MC model
 - Production of ¹⁸F
 - Measurements of the ambient neutron dose equivalent
- > Applications:
 - Production of medical radioisotopes
 - Planning of a new cyclotron facility
 - Assessment of air activation: production of ⁴¹Ar
 - Modeling of a proton therapy degrader
- General problems encountered during MC modeling



Cyclotrons in medical field





Cyclotrons in medical field





FLUKA in Medical Physics

Prediction of ⁸⁹Zr production using the Monte Carlo code FLUKA

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Applied Radiation and Isotopes 69 (2011) 1134-1137

Clinical CT-based calculations of dose and positron emitter distributions in proton therapy using the FLUKA Monte Carlo code

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² CERN, 1211 Geneva 23, Switzerland

Phys. Med. Biol. 52 (2007) 3369-3387

Estimation of neutron production from accelerator head assembly of 15 MV medical LINAC using FLUKA simulations

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Nuclear Instruments and Methods in Physics Research B 269 (2011) 3261-3265



FLUKA Benchmarks

That's the point

FLUKA: Performances and Applications in the Intermediate Energy Range A. Fassò A. Ferrari, J. Ranft, P.R. Sala

planned in the near future. Shielding designers are confronted with a double challenge, due to *i*) the lack of reliable data in the energy range 20 MeV–1 GeV (source terms, attenuation lengths, angular and energy distributions of secondary particles) and *ii*) the difficulty of assessing correctly the large shield thicknesses required by the high beam intensity of most of the planned facilities. Compared with both the

Recently, new possibilities have emerged in this domain with the improvements of the code FLUKA in the range of energies below 1 GeV. For many years that program has been known as one of the main tools for designing shielding of proton accelerators in the multi-GeV energy range (its hadron event generator [10] has been adopted by the majority of the existing high-energy transport codes [11, 12, 13], including those used for particle physics simulations [14, 15]). In the last years, however, FLUKA has gone through an important process of transformation which has converted it from a specialized to a multi-purpose program, not restricted to a limited family of particles or to a particular energy domain.

Nuclear Instruments and Methods in Physics Research A 562 (2006) 814-818

Validation of the FLUKA Monte Carlo code for predicting induced radioactivity at high-energy accelerators

M. Brugger, A. Ferrari, S. Roesler*, L. Ulrici

Phys. Med. Biol. 55 (2010) 5833-5847

Benchmarking nuclear models of FLUKA and GEANT4 for carbon ion therapy

Nuclear Instruments and Methods in Physics Research A 581 (2007) 511–516 FLUKA Monte Carlo simulations and benchmark measurements for the LHC beam loss monitors T T Böhlen^{1,2}, F Cerutti¹, M Dosanjh¹, A Ferrari¹, I Gudowska², A Mairani³ and J M Quesada⁴

L. Sarchiapone^{a,*}, M. Brugger^a, B. Dehning^a, D. Kramer^a, M. Stockner^b, V. Vlachoudis^a



FLUKA Benchmarks





PET/SPECT cylotrons (10-70 MeV)

Proton Therapy cyclotrons



Ion Therapy cyclotrons (250 MeV) (400 MeV)



TRIUMF cyclotron (500 MeV)



Proton Synchrotron Booster (CERN) (1.4 GeV)



Proton Synchrotron

(CERN)

(25 GeV)



LHC (CERN) (4 TeV)

Energy ↔ Velocity





Bike (15-70 km/h)

Sport Car



Kimi Raikkonen (F1 GP Monza 2005 370.1 km/h)

Maglev Train (China 2003, 501 km/h)





F-14 TOMCAT (980-2400 km/h)

ISS (~ 27500 km/h)

Millennium Falcon Speed of Light

Sources:

ISS: http://www.esa.int/Our Activities/Human Spaceflight/International Space Station/ISS International Space Station

CERN acceleratos: http://home.web.cern.ch/about/accelerators

(250 km/h)

- TRIUMF: www.triumf.ca
- Maglev: http://en.wikipedia.org/wiki/Maglev
- Kimi: http://www.formulapassion.it/2014/08/f1-monza-record-del-tempio-della-velocita/
- F14: http://www.museumofflight.org/aircraft/grumman-f-14a-tomcat

Note: (WRONG) Assumption 1 MeV = 1 km/h1 MeV proton $\rightarrow \sim 50 \times 10^6$ km/h



GE PETtrace cyclotron

3D Monte Carlo model of the ¹⁸F⁻ target (GE Healthcare, Uppsala, Sweden) 3D Monte Carlo model of the PETtrace cyclotron (GE Healthcare, Uppsala, Sweden)



Model of the Bunker



Section of the FLUKA Monte Carlo model and comparison with the original technical drawing of the bunker.



Model of the Bunker



3D Monte Carlo model of the S. Orsola-Malpighi cyclotron vault. Detail of the pipes that contain the delivery lines, the RF cables, the control cables, etc.



Validation: Production of ¹⁸F

Three different set of defaults, predefined transport settings for the most common problems, were compared to find the optimal combination of physical and transport parameters and cpu-time usage.

- > NEW-DEFA in which reasonable minimal set of physical mechanisms are enabled;
- HADROTHE for hadrotherapy calculations;
- PRECISO for maximum precision simulations.



 Processor:
 i7-3630QM

 N° core:
 4 (8 thread)

 N° runs:
 8

The saturation yield for the very well-known reaction ${}^{18}O(p,n){}^{18}F$ calculated with FLUKA was compared with the experimental value and the recommended saturation yield (A₂) in the IAEA database for medical radioisotopes production. A target of a water solution (1.3 g) 97% enriched in ${}^{18}O$ and a 16,5 MeV pencil beam were simulated in a geometry independent case.



Validation: Production of ¹⁸F

$$A(EOB) = A_{sat} \cdot \left(1 - e^{-\lambda \cdot t_{irr}}\right)$$

$$Y = \frac{A_{sat}}{I_{irr}} = \frac{A(EOB)}{I_{irr} \cdot (1 - e^{-\lambda \cdot t_{irr}})}$$

<u>Note:</u>

• Y corresponds to IAEA A₂ value

• $A(EOB)=A(1h-1\mu A)$ corresponds to IAEA A₁ value

DEFAULTS	NEW-DEFA	NEW-DEFA	NEW-DEFA	HADROTHE	HADROTHE	PRECISIO	PRECISIO
TRANSPORT	PART-THR: as default (10 MeV)	PART-THR: 0.1 MeV	PART-THR: 1 MeV for protons	PART-THR: as default (0.1 MeV)	PART-THR: 10 MeV	PART-THR: as default (0.1 MeV)	PART-THR: 10 MeV
Simulation Time [h]	1.05	5.04	3.12	25.17	3.43	25.48	2.26
Ysat ¹⁸ F [MBq∕µA]	6521 ± 6	13166 ± 9	13161 ± 9	13169 ± 10	6508 ± 5	13200 ± 10	6486 ± 6
A ₂ /Y _{FLUKA}	2.01 ± 0.20	0.99 ± 0.10	0.99 ± 0.10	0.99 ± 0.10	2.01 ± 0.20	0.99 ± 0.10	2.02 ± 0.20
<u>Note:</u> 10 ⁹ primary	y particles simulate	ed.	Υ _{exp} [MBq/μA]	Y _{exp} /Y _{FLUKA}			
			8600 ± 400	0.65 ± 0.03			

<u>*Ref.*</u> Infantino, A., Marengo, M., Baschetti, S., Cicoria, G., Longo Vaschetto, V., Lucconi, G., Massucci, P., Vichi, S., Zagni, F., Mostacci, D., 2014. Accurate Monte Carlo modeling of cyclotrons for optimization of shielding and activation calculations in the biomedical field. Radiation Physics and Chemistry, Manuscript submitted for publication.



Validation: neutron dose

R. Gallerani et al. *Neutron production in the operation of a 16.5 MeV PETtrace cyclotron*. Progress in Nuclear Energy. 50, 939-943, **2008**.





Validation: neutron dose



- ✓ Measurements performed at the same points as in *R. Gallerani et al.*
- ✓ A neutron rem-counter FHT-752 (Thermo Scientific) based on a BF₃ proportional-counter and a PEmoderator, calibrated in H*(10).
- ✓ A set of 12 dosimeters for fast neutrons (CR-39).
- ✓ Irradiation tests were conducted with values of integrated current between 0.005 and 0.0016 µAh.





Results of the Simulations



Assessment of the neutron dose field around the GE PETtrace cyclotron. Left: Neutron dose field over the bunker (5 cm pitch cartesian mesh). Right: Detail of the neutron dose field around the cyclotron (cylindrical mesh)

Simulations vs. Measurements



Simulations vs. Measurements



Note: Monte Carlo uncertainties have a stochastic nature (random uncertainties)



Input Parameters

DEFAULTS: NEW-DEFA.

- > Transport of electrons, positrons and photons enabled
- Low energy neutron (≤20 MeV) transport on down to thermal energies included;
- Delta ray production enabled
- Heavy particle bremsstrahlung activated with explicit photon production above 1 MeV;
- Heavy particle e+/e- pair production activated with full explicit production
- ... and more

PHYSICS & TRANSPORT:

- Coalescence and Evaporation enabled;
- > EMFCUT (e & γ thresholds)
- Protons transported down to 1 MeV;
- FLUKAFIX set to 0.01 (not always)
- > Irradiation profile of 1h @ 1μ A proton current.

<u>SCORING:</u>

- ✓ DOSE-EQ from neutrons/photons (USRBIN)
- ✓ Activation (RESNUCLE)
- ✓ Proton/Neutron spectra (USRTRACK)
- Proton current (USRBDX)
- **PRIMARY:** 10⁹ primary particles simulated.





Production of radioisotopes

Prediction of ⁸⁹Zr production using the Monte Carlo code FLUKA

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Applied Radiation and Isotopes 69 (2011) 1134–1137 BEAM Aluminum Degrader 300 µm Yttrium Foil Copper backing *YTALYS YFLUKA *Y_{exp} Y_{TALYS}/Y_{FLUKA} Isotope Y_{exp}/Y_{FLUKA} [MBq/µA] $[MBq/\mu A]$ [MBq/µA] Zr-89 2200 ± 200 2400 ± 200 1.09 ± 0.15 2300 ± 200 1.07 ± 0.16

<u>*Ref:</u> A. Ciarmatori, G. Cicoria, D. Pancaldi, A. Infantino, S. Boschi, S. Fanti, M. Marengo. *Some experimental studies* on ⁸⁹Zr production. Radiochimica Acta, 99, 1-4, **2011**.



MATERIAL

LOW-MAT

MATERIAL

◇LOW-MAT

MATERIAL

LOW-MAT

MATERIAL

COMPOUND

Z: 42.

Z: 42.

Z: 42.

f1:14.84

f3: 15.92

f5:9.55

f7:9.63

Production of ^{99m}Tc

Simulation setup

- 100 µm thick ^{nat}Mo foil
- > 100 μ m thick 99.01 % enriched ¹⁰⁰Mo foil

Mat: 98Mo 🔻

Mat: 99Mo V

Mat: 100Mo 🔻

ame: Monat T

M1:92Mo v

M3:95Mo

M5:97Mo 🔻

M7: 100Mo

- 1 mm thick ^{nat}MoO₃ pellet
- 1 mm thick 99.01 % enriched ¹⁰⁰MoO₃ pellet (including impurities reported in the batch certificate)

A: 98

A: QC

A: 100

Mix: Mass 🔻

12:9.25

f4:16.68

f6:24.13

LowMat: Mo. Natural Molybdenum (2), 296K V

^{lat:} Mo. Natural Molybdenum (2), 296K ▼

Mat: Mo. Natural Molybdenum (2), 296K 🔻



Target assembly for irradiation of MoO₃ pellets

 $\label{eq:bound} \begin{array}{l} \underline{\textit{Beam parameters:}}\\ FWHM_x=0.71 \ \text{cm}, \ FWHM_{\Delta E}=0.0785 \ \text{MeV},\\ FWHM_{\Delta \Phi}=0.001 \ \text{mrad} \\ On \ average \ 79.8 \ \% \ of \ the \ proton \\ current \ extracted \ hits \ the \ target \\ material \ (~20 \ \% \ on \ the \\ collimator). \end{array}$



p: 10.22

p: 10.22

p: 10.22

ρ: 10.22 dE/dx: ▼

M2:94Mo

M4:96Mo

M6:98Mo

dE/dx: 🔻

dE/dx: 🔻

dE/dx: 🔻

Elements: 7.9

Solid target station and target assembly employed in preliminary tests: 100 μ m thick foil of ^{nat}Mo

Production of ^{99m}Tc



WHAT(2) = flag for "patching" isomer production, while waiting for a better production model <u>Source:</u> FLUKA manual 2011, RADDECAY card.

"Patching isomers" in FLUKA will simply split the production of a specific isotope in (half-half) between ground and isomeric state (if it exists)".



Production of ^{99m}Tc

PRELIMINARY RESULTS

	100 μm thick ^{nat} Mo foil experimental values	100 μm thick ^{nat} Mo foil Monte Carlo simulations*	Ratio Exp/FLUKA		
Isotope	Y _s (MBq/μA)	Y _s (MBq/μA)			
Tc-99m	$(1.102 \pm 0.015) \cdot 10^2$	$(7.30499 \pm 0.00018) \cdot 10^{1}$	1.51 ± 0.02		
Tc-97m	$(1.7 \pm 0.9) \cdot 10^2$	$(1.81584 \pm 0.00004) \cdot 10^2$	0.9 ± 0.5		
Tc-96m	$(3.75 \pm 0.13) \cdot 10^2$	$(1.53227 \pm 0.00004) \cdot 10^2$	2.45 ± 0.08		
Tc-96	$(3.88 \pm 0.04) \cdot 10^2$	$(2.84431 \pm 0.00003) \cdot 10^2$	1.364 ± 0.014		
Tc-95m	$(1.66 \pm 0.02) \cdot 10^2$	$(1.63320 \pm 0.00004) \cdot 10^2$	1.016 ± 0.012		
Tc-95	$(4.48 \pm 0.05) \cdot 10^2$	$(4.79743 \pm 0.00012) \cdot 10^2$	0.934 ± 0.010		
Tc-94m	$(2.62 \pm 0.05) \cdot 10^2$	$(8.9225 \pm 0.0002) \cdot 10^{1}$	2.94 ± 0.06		
Tc-94	$(1.60 \pm 0.02) \cdot 10^2$	$(4.25356 \pm 0.00010) \cdot 10^2$	0.376 ± 0.005		
Tc-93m	$(1.12 \pm 0.04) \cdot 10^{1}$	$(1.75946 \pm 0.00004) \cdot 10^{1}$	0.64 ± 0.02		
Tc-93	$(6.09 \pm 0.10) \cdot 10^{1}$	$(9.5201 \pm 0.0002) \cdot 10^{1}$	0.725 ± 0.011		
Tc-92	$(2.9 \pm 0.6) \cdot 10^2$	$(2.27032 \pm 0.00005) \cdot 10^2$	1.3 ± 0.3		
Nb-95	$(1.20 \pm 0.04) \cdot 10^{1}$	3.34993 ± 0.00005	3.58 ± 0.12		
Nb-92m	3.96 ± 0.14	7.02240 ± 0.00017	0.56 ± 0.02		
Mo-99	6.18 ± 0.10	2.95731 ± 0.00007	2.09 ± 0.03		



Target assembly: copper backing and 100μ m thick natural-Mo foil.

On Average: 0.664 ± 0.003

*Calculated convoluting the proton flux with cross section (TALYS).

G. Lucconi, F. Carnaccini, E. Galloni, A. Infantino, F. Zagni, G. Cicoria, D. Pancaldi, M. Marengo. Development of a solid target for cyclotron production of 99mTc. Eur J Nuc Med Mol Imaging 41 (Suppl 2):S151-S705 **2014**.





3D Monte Carlo model of the TR19 cyclotron (ACSI, Richmond, Canada).





Original technical drawing of the «Sacro Cuore – Don Calabria» Hospital PET facility. Negrar (VR), Italy.



Detail of the floating floor, the walls and the ducts containing the delivery lines, the RF cables, the control cables, etc.







Activation of Air: ⁴¹Ar

$^{40}Ar(n,\gamma)^{41}Ar$

 41 Ar (t_{1/2} = 109.34 min) is produced by the activation of air due to secondary thermal neutron flux during irradiation.

 $\sigma_{(n,\gamma)} \sim 660 \text{ mb } @ 0.025 \text{ eV} (ENDF/B-VII.0)$



Monte Carlo model of one of the experimental setup adopted.

Simulation setup

- ✓ Direct assessment (RESNUCLE) and convolution Fluence-Cross Section
 - Total net air volume (assessed using SimpleGeo, ~120 m³);
 - Marinelli beakers (1000 cm³) in different position;
 - Volumes of 1 m³ centered in the Marinelli's positions;

$$A_{sat} \cong \rho V \omega_x \frac{N_A}{A_x} N_P \sum_{i=260}^{1} F(E_i) \sigma_{xy}(E_i) \Delta E_i$$

"In the FLUKA neutron cross section library, the energy range up to 20 MeV is divided into <u>260</u> <u>energy groups</u> of approximately equal logarithmic width (31 of which are thermal)." <u>Source:</u> FLUKA manual 2011

Activation of Air: ⁴¹Ar

Total v	Marinelli beakers			Volumes 1m ³			
<i>C_{FLUKA}</i> [Bq/dm³*μAh]	2.18 ± 0.11	Beaker	FD/Exp	FC/Exp	Beaker	FD/Exp	FC/Exp
Cexp	0.784 ± 0.012	1	n/a	3.58 ± 0.18	1	7 ± 4	3.01 ± 0.14
[Bq/dm ³ *µAh]		2	n/a	3.51 ± 0.20	2	3.5 ± 1.2	3.13 ± 0.16
C _{FLUKA} /C _{exp}	2.78 ± 0.15	3	n/a	3.56 ± 0.19	3	3.0 ± 1.3	3.05 ± 0.14
		4	n/a	3.36 ± 0.19	4	2.6 ± 0.8	2.99 ± 0.16

Note: FD = FLUKA Direct assessment; FC = FLUKA Convolution fluence-CS

Open questions:



- What kind of CS are used for Argon selecting «AIR» as material?
- Self-Shielded case? (*Manual, 10.1.1 Possible artefacts*)

(ongoing testing...)

ASSIGNMA	N		N	Mat: AIR V lat(Decay):					Reg: A Step:	irB ▼
Material Properties										
Title: 104 Air dry (r	near sea level)									
Notes Stoichiom	etry Properties									
Composition: mass	s 🔻		S	tate: gas 🛛 🔻				Der	sity: 0.00	120484
Z	A	El		Name				F	rac	
6 7 8 18		C C N N O Ar A	arbon litrogen xyge. rgon			0.00 0.75 0.23 0.01	01248 5267 1781 2827			
Mater	rial		Temp.	Origin	RN	Name	Ide	ntifi	ers	Gam
Ar Natu	ral Argon		296K	JEFF-3.1	Y	ARGON	18	-2	296	Y
Ar Natu	ral Argon	SelfShielded	2968	JEFF-3.1	÷	ARGON	18	-4	296	÷
Ar Natu	ral Argon	SelfShielded	87K	JEFF-3.1	Ŷ	ARGON	18	-4	87	Ŷ
40Ar Argo	n 40 -		296K	JEFF-3.1	Y	ARGON-40	18	40	296	Y
40Ar Argo	n 40		87K	JEFF-3.1	Y	ARGON-40	18	40	87	Y
40Ar Argo	n 40 SelfS	hielded	296K	JEFF-3.1	Y	ARGON-40	18	1040	296	Y
40Ar Argo	n 40 SelfS	hielded	87K	JEFF-3.1	Y	ARGON-40	18	1040	87	Y





SimpleGeo ×	
Problem with line: WED CUNEO2 -12.309 -1.25 60.963 11.559 0.0 0.0 0.0 0.0 2.21 0.0 2.5 0.0 ARB, WED, RAW not yet implemented!	ATTENTION: No source primitive cuneo8 was found while trying to bu ATTENTION: No source primitive cuneo9 was found while trying to bu ATTENTION: No source primitive cuneo10 was found while trying to b
ОК	< Clear loa Close loa Close loa

Wedge and other Flair body are not (yet) implemented in SimpleGeo (and viceversa i.e. Torus)



Other incompatibilities/problems found are:

- Import of a geometry with ROT-DEFINI/translat defined
- DaVis3D: import USRBIN with $R\Phi Z$ mesh
- PIPSICAD3D: Problem in running PipsiCAD_SimpleGeo.linux interface (useful if directly implemented in Flair!!!)



3D simplified Monte Carlo model of a degrader for proton therapy applications.

Wedge thickness modelled

Outcoming Proton Energy	Crossed wedge thickness			
[IVIEV]	[cm]*			
70	16.691			
120	13.452			
140	11.816			
180	8.304			
200	5.910			

*Calculated using SRIM



Section of the FLUKA Monte Carlo model of the degrader.



Environmental neutron dose equivalent H*(10) - Ep=200MeV



Preliminary assessment of the neutron dose field around a proton therapy degrader: results obtained simulating an outcoming proton energy of 200 MeV. **PIPSICAD 3D plugin**. Tracks indicate the different particle produced during irradiation: protons (red), electrons (green), photons, (yellow) and neutrons (blue). Fade of tracks enabled.



Main problems encountered

Activation from protons below 20 MeV

- Some differences from experimental and simulated results in particular for liquid and gaseous materials
- Thermal and Fluid-dynamics effects? Chemical reactions with target material/target body? (Real) Low Energy regime?
- > Isomers: accounting a correct production branching ratio

Activation from neutrons below 20 MeV

- Production of ⁴¹Ar. Simulations convergent in the different cases but:
 - > Possible artefacts? Self-Shielding? Only a problem of the material definition?

Compatibility Flair/SimpleGeo

- Body missing between the two programs (wedges, torus, etc)
- Problems in running at best some plugins (importing R\u03c6Z mesh, running of PipsiCAD_SimpleGeo.linux interface)



Collaboration UniBo - S. Orsola

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