Recent validation and improvements of Geant4 standard EM package at low energies

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(on behalf of the G4AI team)

Abstract

Geant4 photo-absorption ionisation (PAI) and the Moller-Bhahba standard models were extended in the low energy region. The models show good agreement with the experiment (dE/dx)for the electron energy interval 0.01 - 10 MeV. Ionisation distribution along step is discussed in terms of the Γ-distribution. Geant4 models for bremsstrahlung were tested versus experimental data and the prediction of the PENELOPE as well as EGS4 packages for the electron energy interval 1-15 MeV.

1 Outline

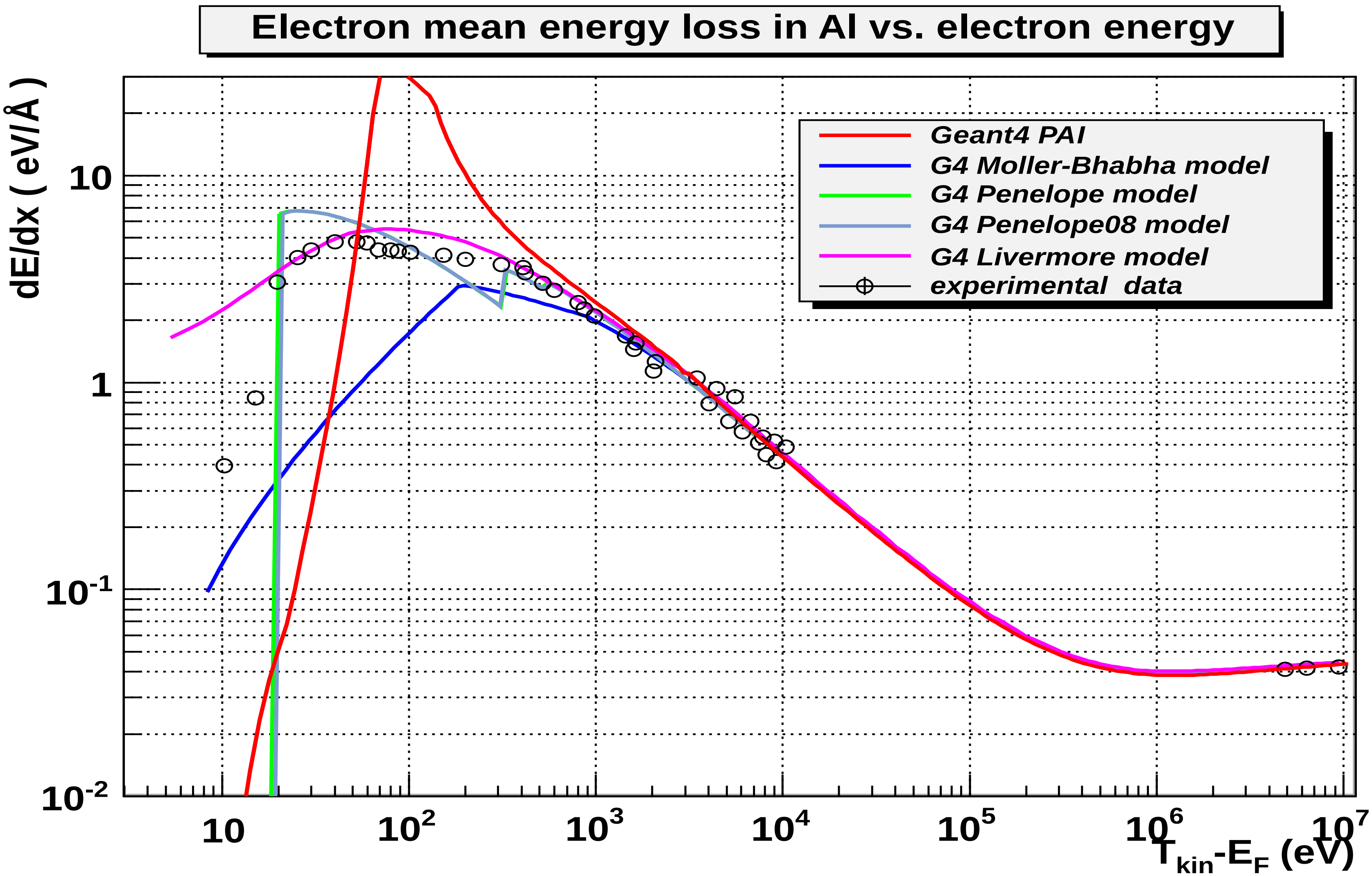
1. Geant4 PAI model extension to low energy region.
2. Comparison with experimental data for dE/dx in the case of electrons and protons.
3. Ionisation along step in Geant4 class G4ElectronIonPair. Proposal to improve the sampling of ionisation along step.
4. Comparison with experimental data for the bremsstrahlung spectrum at different angles.
5. Conclusions.

2 dE/dx for electrons in different targets

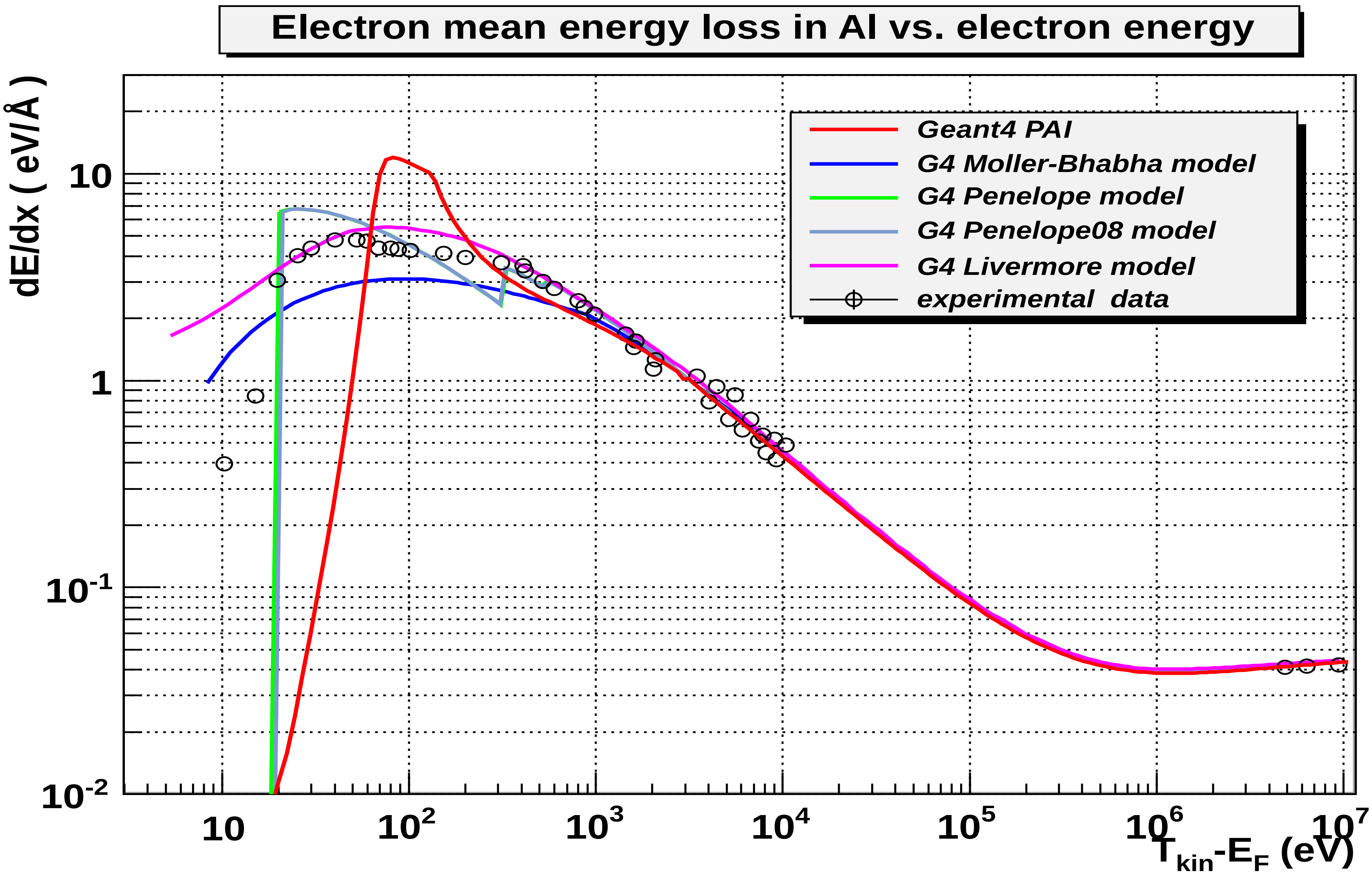
Experimental data for Al, Au, Cu and Si are compilation from [1]. The data for liquid water, hydrogen, nitrogen, oxygen and carbon dioxide are compilation from [2]. Geant4 models are: PAI, Bhabha, Penelope (Penelope08) and Livermore.

3 dE/dx for protons in different targets

Experimental data are compilation from [3]. Geant4 models are: PAI, Bragg.

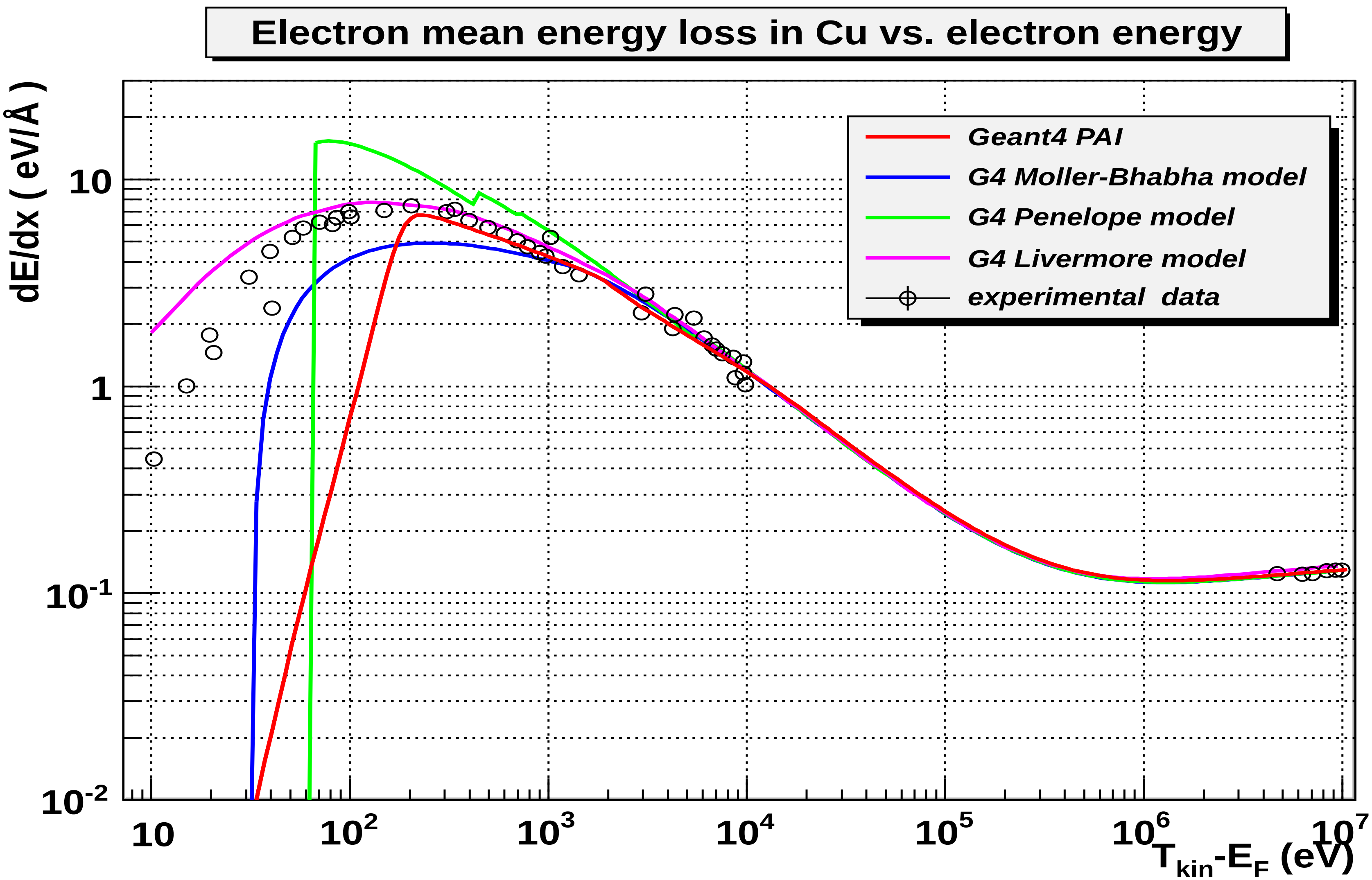


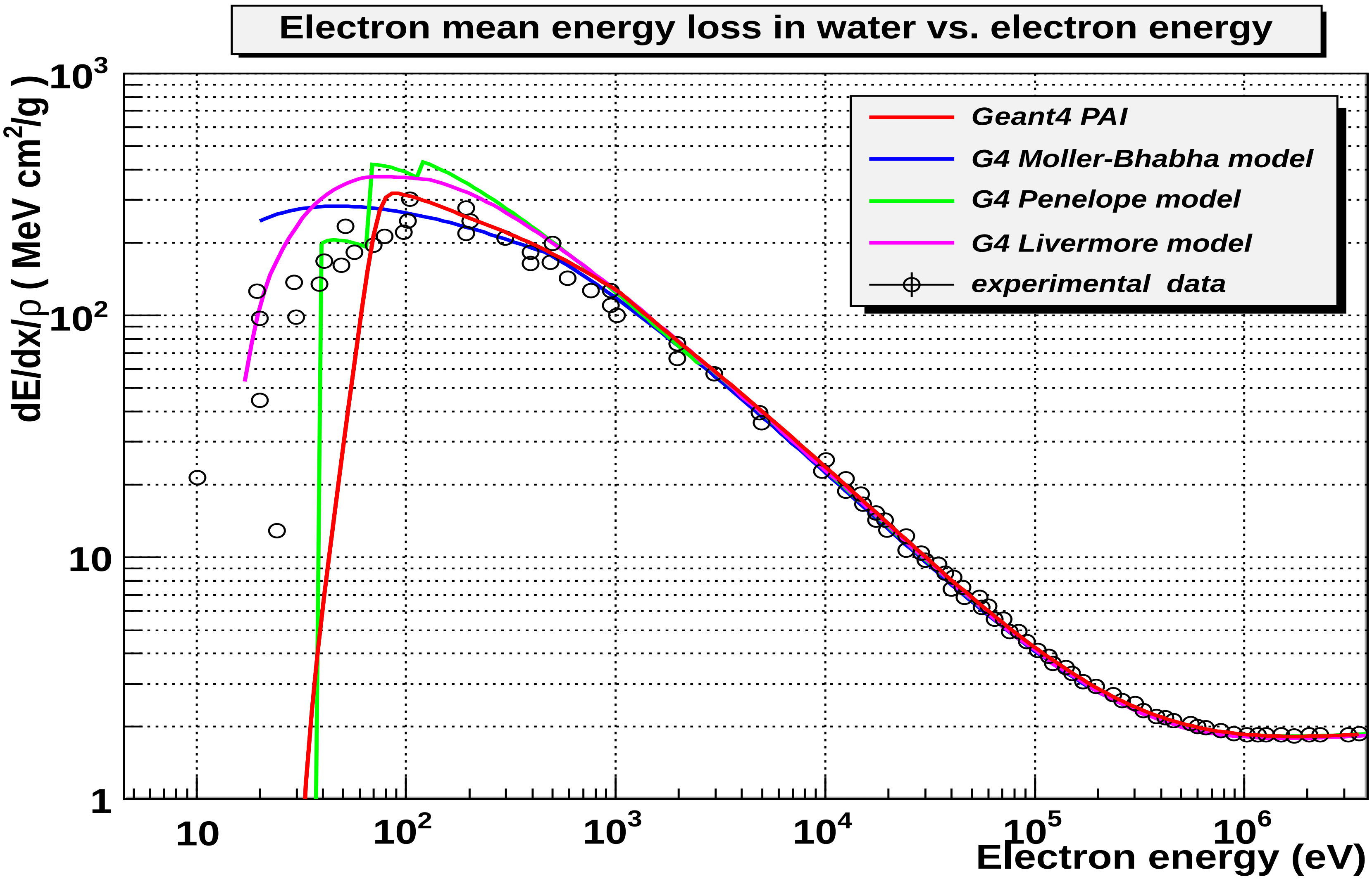
Old PAI and Moller-Bhabha models.



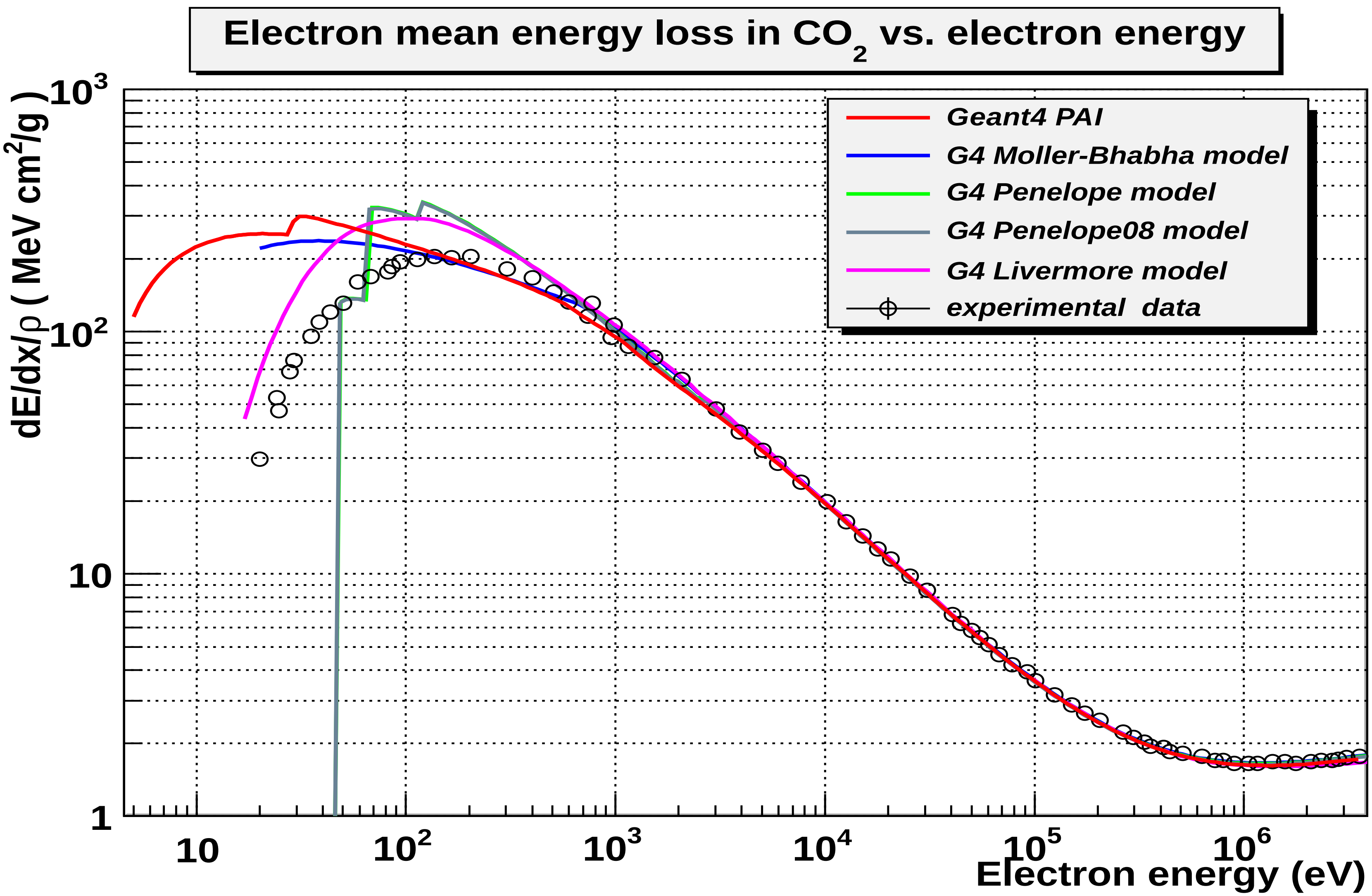
In PAI: $\{1 - \exp[-\beta/(\alpha a(Z))]\}$, $a(Z)$ is parametrised.

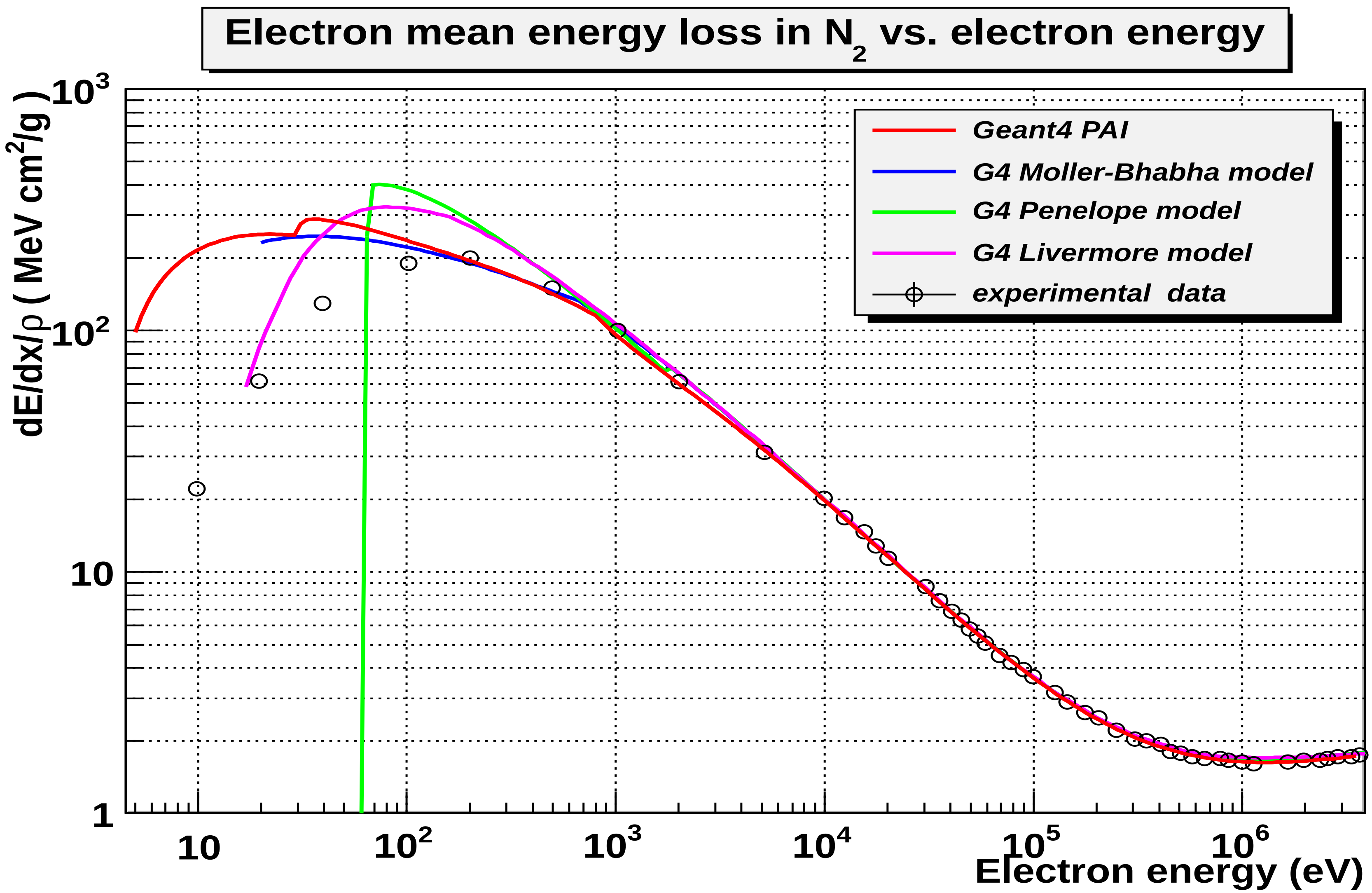
In Moller-Bhabha: low energy $0.25 \rightarrow 0.025$ keV.

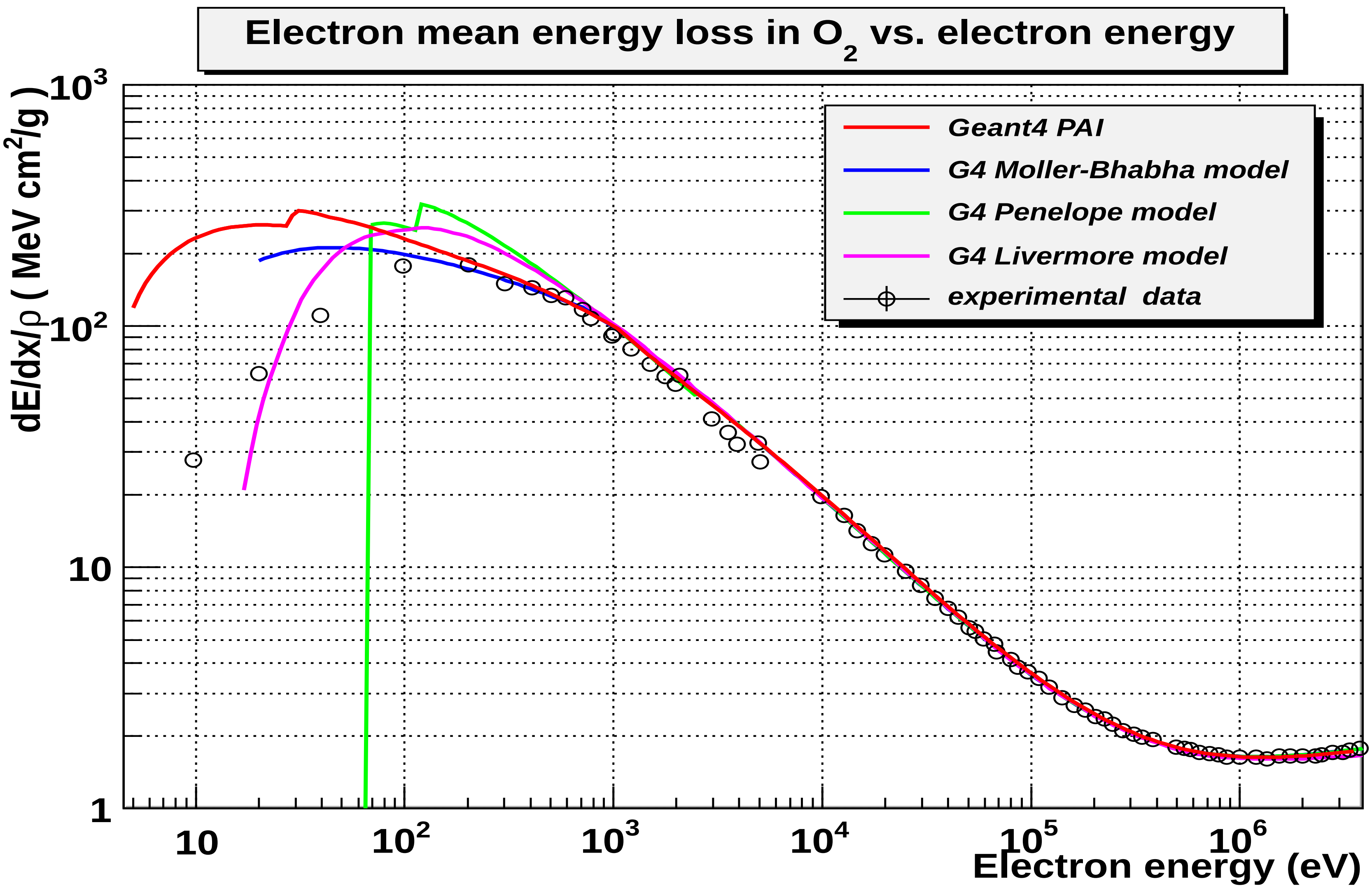

Electron mean energy loss in Cu vs. electron energy
dE/dx (eV/Å)
10
1
10-1
10-2
10
10²
10³
10⁴
10⁵
10⁶
10⁷
T kin-E F (eV)
Geant4 PAI
G4 Moller-Bhabha model
G4 Penelope model
G4 Livermore model
experimental data

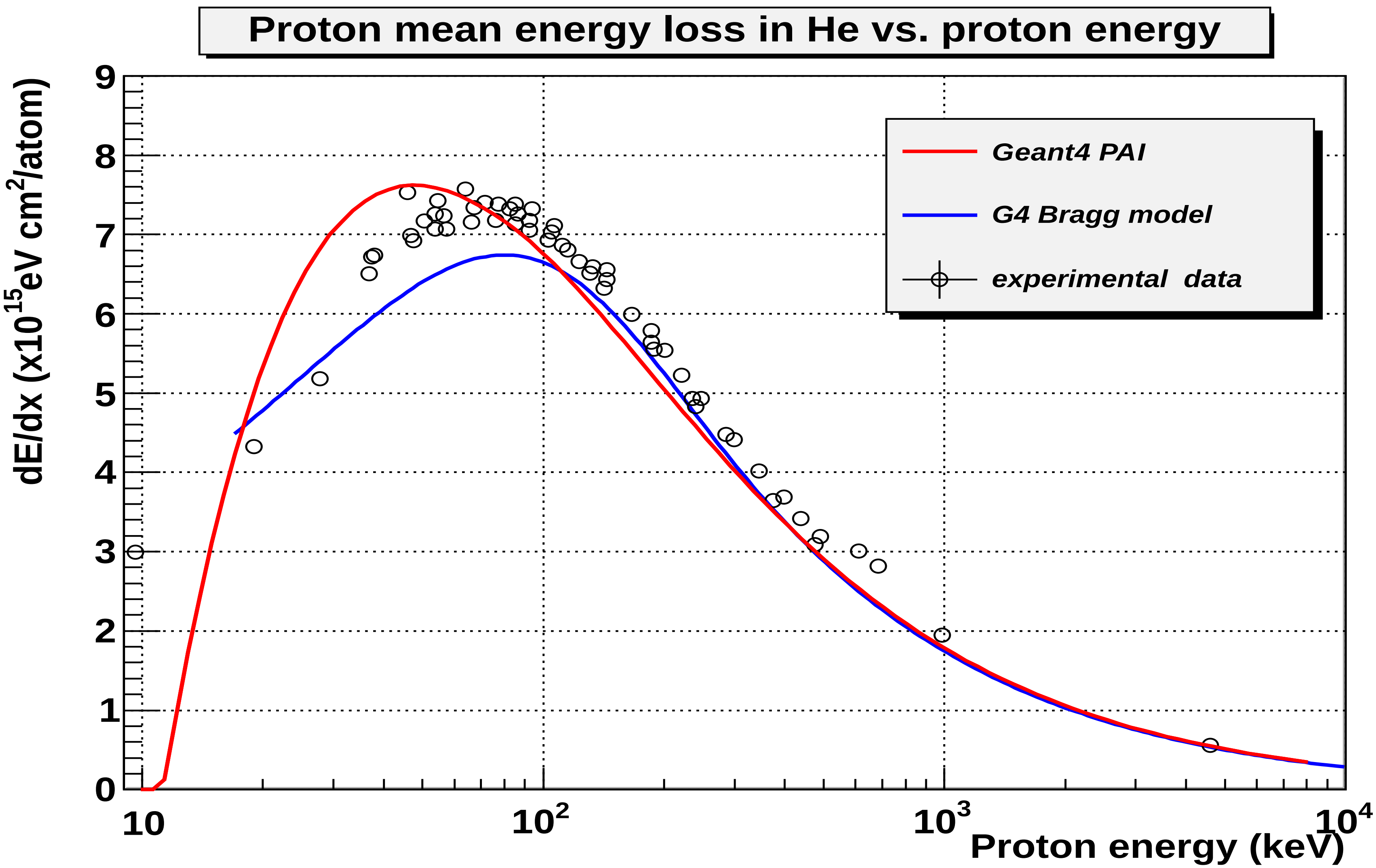


Electron mean energy loss in water vs. electron energy
dE/dx/ρ (MeV cm²/g)
10³
10²
10
1
10
10²
10³
10⁴
10⁵
10⁶
Electron energy (eV)
Geant4 PAI
G4 Moller-Bhabha model
G4 Penelope model
G4 Livermore model
experimental data

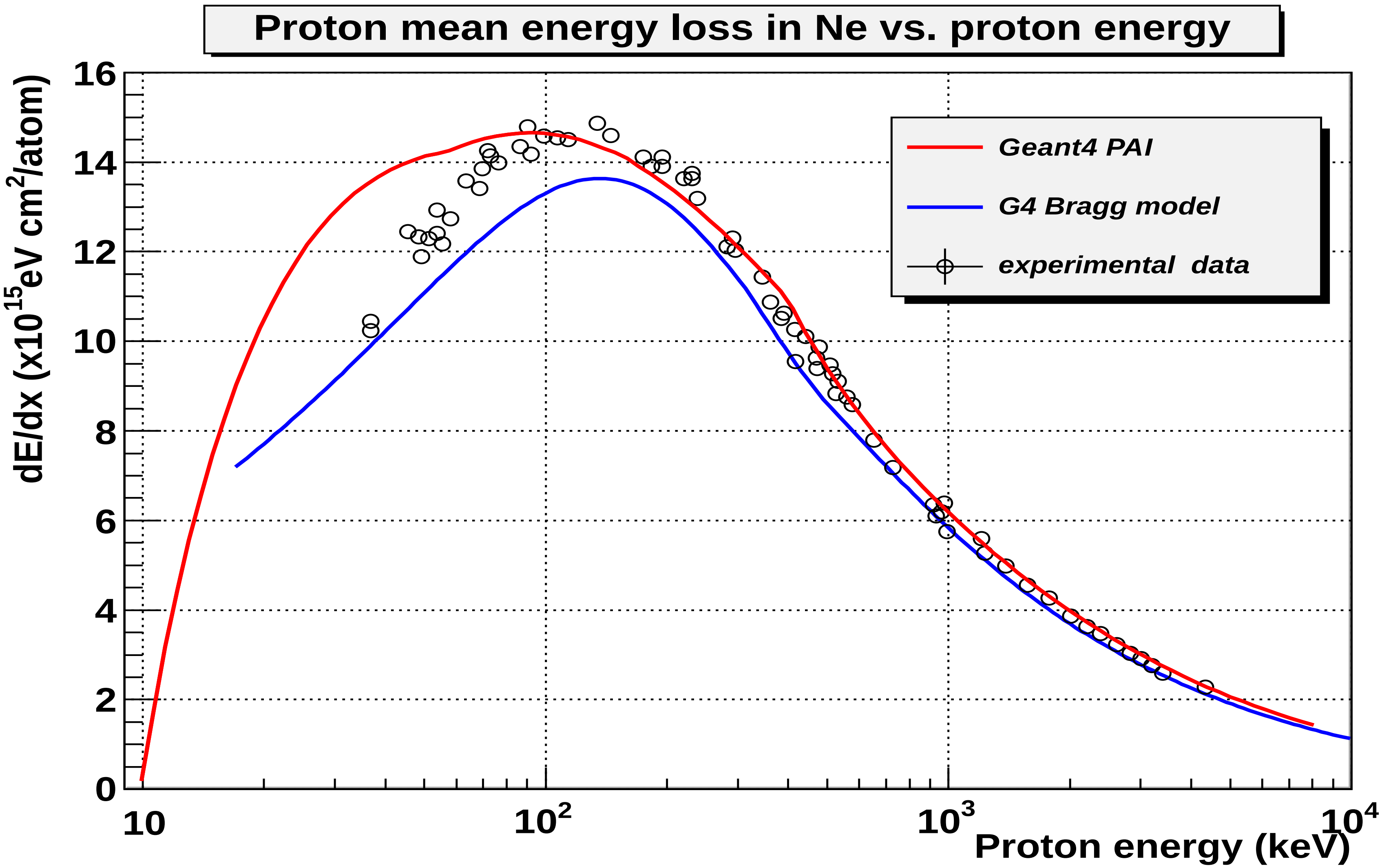

Electron mean energy loss in CO_2 vs. electron energy
dE/dx/ρ (MeV cm²/g)
Geant4 PAI
G4 Moller-Bhabha model
G4 Penelope model
G4 Penelope08 model
G4 Livermore model
experimental data
10^3
10^2
10
1
10
10^2
10^3
10^4
10^5
10^6
Electron energy (eV)


Electron mean energy loss in N_2 vs. electron energy
Geant4 PAI
G4 Moller-Bhabha model
G4 Penelope model
G4 Livermore model
experimental data
$dE/dx/\rho$ (MeV cm^2/g)
10^3
10^2
10
1
10
10^2
10^3
10^4
10^5
10^6
Electron energy (eV)


Electron mean energy loss in O_2 vs. electron energy
dE/dx/ρ (MeV cm²/g)
Electron energy (eV)
Geant4 PAI
G4 Moller-Bhabha model
G4 Penelope model
G4 Livermore model
experimental data



Proton mean energy loss in He vs. proton energy
dE/dx (x10^15eV cm^2/atom)
Proton energy (keV)
Geant4 PAI
G4 Bragg model
experimental data
0
1
2
3
4
5
6
7
8
9
10
10^2
10^3
10^4


Proton mean energy loss in Ne vs. proton energy
dE/dx (x10^15 eV cm^2/atom)
16
14
12
10
8
6
4
2
0
10
10^2
10^3
10^4
Proton energy (keV)
Geant4 PAI
G4 Bragg model
experimental data

4 Proposal to improve the sampling of ionisation along step

There were two problems in old GEANT4 code (G4ElectronIonPair::SampleNumberOfIonsAlongStep):

1. The Fano factor, F, defines the variance of ionisation distribution [4, 5], rather than the mean square root (old GEANT4 code):

   $$\langle (n - \bar{n})^2 \rangle = F\bar{n}.$$

   Here n is the ionisation, and $\bar{n} = \Delta/W$ its mean value (Δ is the energy deposited along the step, and W is the mean energy required to produce an electron-ion pair).

2. It is more safe to use the Γ-distribution (instead of Gaussian in old GEANT4 code) which provides non-negative ionisation.

New function:

```
inline G4int G4ElectronIonPair::SampleNumberOfIonsAlongStep(const G4Step* step)
{
  G4double meanion = MeanNumberOfIonsAlongStep(step);
  G4double lambda  = 1./FanoFactor;
  G4double a       = meanion*lambda;
  G4int    nion    = G4int(CLHEP::RandGamma::shoot(a,lambda) + 0.5);
  return nion;
}
```

since the Γ-distribution:

$$p(x) = \frac{\lambda^a}{\Gamma(a)} x^{a-1} \exp(-\lambda x),$$

has the mean value, $\bar{x} = a/\lambda = \Delta/W$, and the variance, $\langle (x - \bar{x})^2 \rangle = a/\lambda^2 = \bar{x}/\lambda = F\bar{x}$ (so $\lambda = 1/F$, and $a = \Delta/(WF)$). The ionisation n is defined as integer of $x + 0.5$, $n = \text{G4int}(x + 0.5)$.

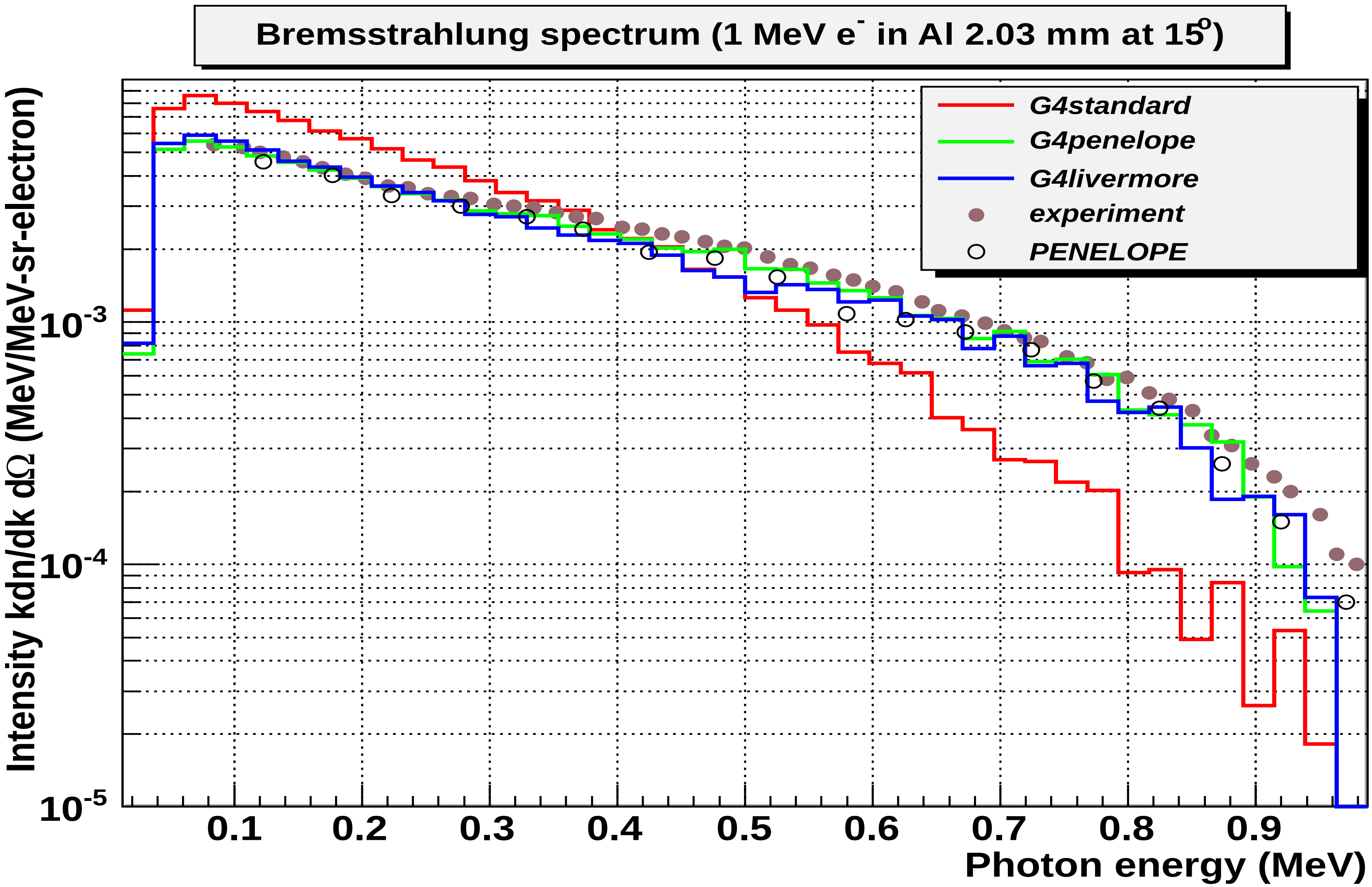
5 Geant4 bremsstrahlung model validation

1. G4eBremsstrahlungModel in the EM standard package.
2. G4PenelopeBremsstrahlungModel in the EM low energy package.
3. G4LivermoreBremsstrahlungModel in the EM low energy package.

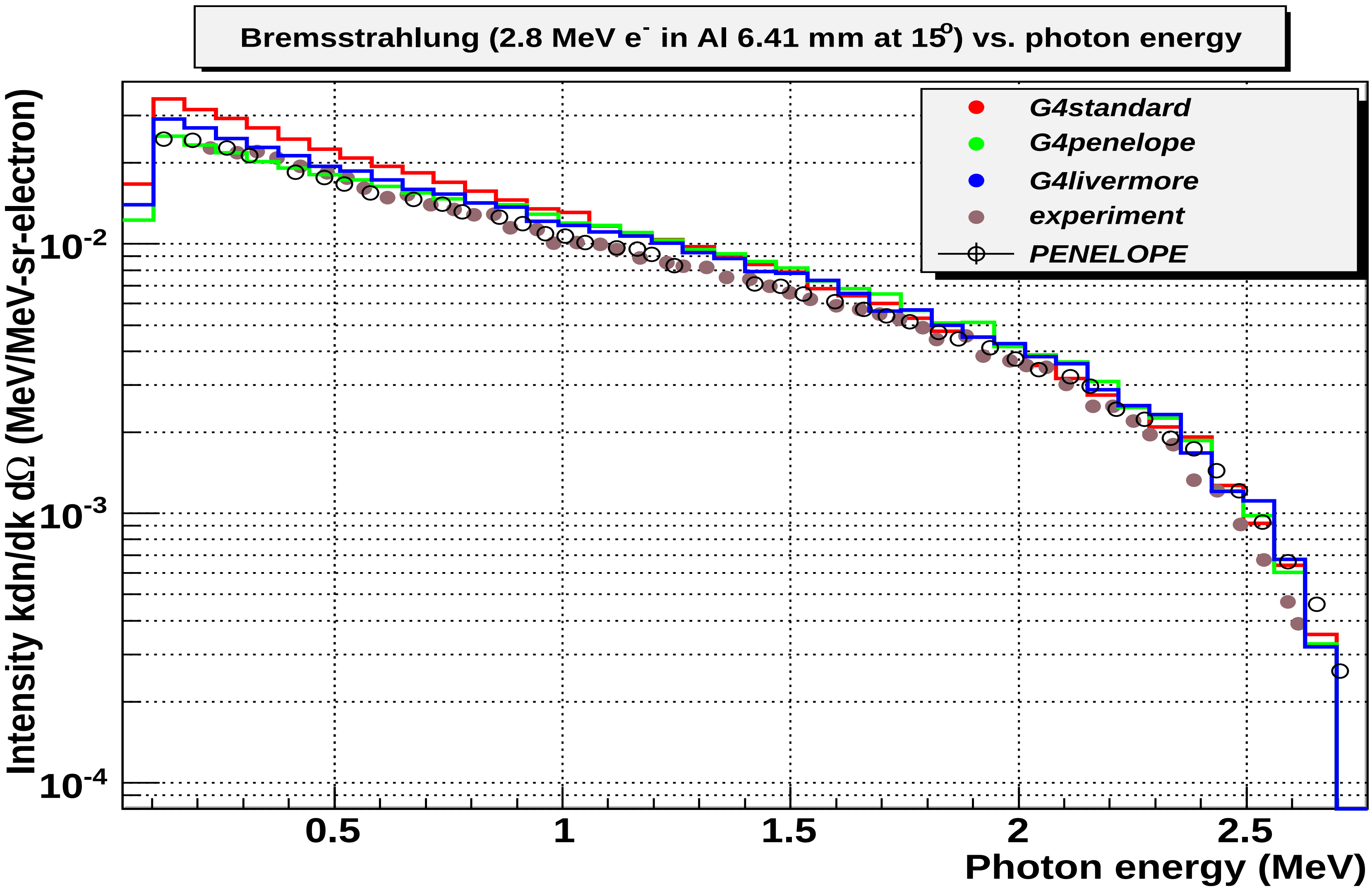
6 Bremsstrahlung produced by low energy electrons

Experimental data for Al, from [6, 7] are evaluated versus the Geant4 models and the prediction of the PENELOPE package [8]. The bremsstrahlung intensity spectrum produced by electrons with the energies 1 and 2.8 MeV was evaluated at the angle of 15^o in aluminum with 2.03 and 6.41 mm thicknesses, respectively. The experiment with 15 MeV [9] electrons was evaluated in terms of bremsstrahlung spectrum to compare the Geant4 model predictions with the results of EGS4 simulation (Al 36.1 mm thick at 10^o).

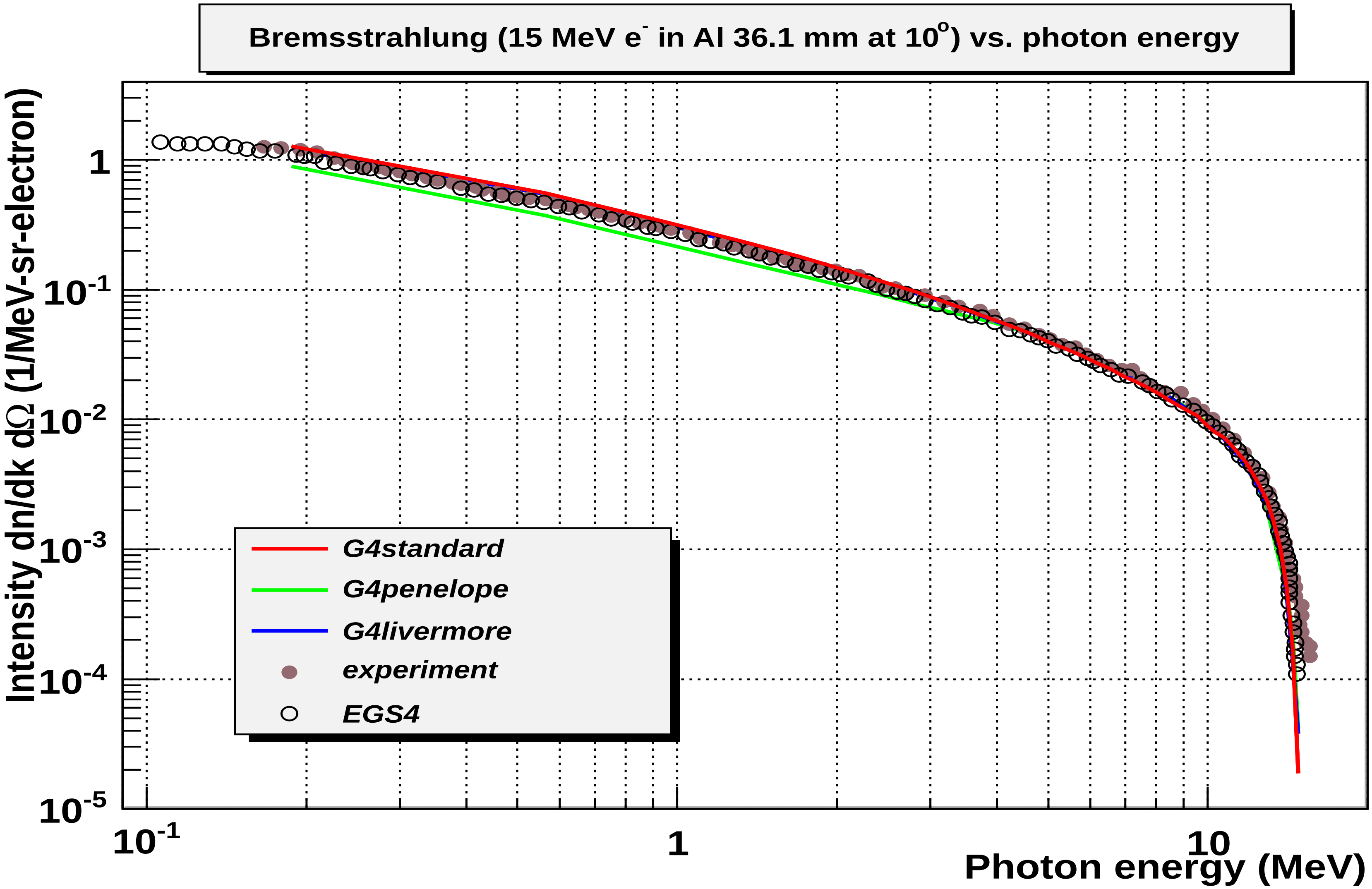
The simulation of bremsstrahlung requires high statistics to get smooth curves corresponding to the experimental measurements. A modern remote cluster of parallel processors was used in the batch mode to perform the simulation of the experimental set-ups.



Statistics is $1 \cdot 10^8$. The G4eBremsstrahlungModel overestimates the spectrum at low energies and underestimates at high energies.



Statistics is $1 \cdot 10^8$.



Statistics is $5 \cdot 10^7$.

7 Conclusions

1. The GEANT4 PAI model was extended to low energy region below the ionisation minimum. The Moller-Bhabha standard ionisation model was corrected in the low energy mode. The GEANT4 ionisation models show satisfactory agreement with dE/dx experimental data for the electron kinetic energies in the range 0.01-10 MeV.

2. The ionisation distribution along step was corrected and implemented in terms of the Γ-distribution.

3. The GEANT4 G4PenelopeBremsstrahlungModel and G4LivermoreBremsstrahlungModel models are in satisfactory agreement with experimental data and the prediction of PENELOPE and EGS4 packages.

4. For slow electrons (≤ 3 MeV), the GEANT4 G4eBremsstrahlungModel model overestimates the bremsstrahlung spectrum at fixed angle for low photon energies with more deep decreasing for high energies.

8 Acknowledgments

This work was done in close collaboration with J. Allison, A. Howard, S. Incerti, V. Ivantchenko, P. Nieminen and G. Santin. The author is thankful to them for stimulating discussions and support.

References

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