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GEANT4 SIMULATION OF ENERGY LOSSES OF SLOW HADRONS

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Abstract

The algorithm of the simulation of energy losses for hadrons with kinetic energy down to few eV is described. The details of its implementation in Geant4 are discussed. The comparison of the results of simulation with the experimental data is presented.

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1 Introduction

GEANT4 [1] is a toolkit for Monte Carlo particle transport simulation for a wide range of applications and it is based on the Object Oriented technology. The transparency of the physics implementation allows a rigorous procedure in validating the physics results. The flexibility of the GEANT4 design hence allows simulation of physical processes in such diverse fields as high energy physics, space and cosmic ray applications, nuclear and radiation computations, as well as heavy ion and medical applications.

In high energy physics the precise hadron energy losses in matter are important for hadrons with more than a few MeV kinetic energy. In a number of other applications, on the other hand, the precise simulation of energy loss and stopping of lower-energy protons and ions in matter is one of the main requirements for the simulation tool. In medical research, especially in hadron irradiation treatment, very precise simulation of the energy loss of both the incident particles and their secondary particles in tissue is required. To maximise patient safety, accurate knowledge is required of the 3-D distribution of the radiation dose within small volumes, implying low energy production thresholds and small step lenghts in the simulation.

In space instrumentation, on the other hand, reduction in component size has led to higher susceptibility to the so-called Single Event Phenomena (SEP). These phenomena are primarily due to incident protons and ions in space, and are characterised by large energy deposits in small sensitive volumes, particularly near the end of the particle track. Such phenomena usually cause memory bit-flips, and may result either in a temporary operational glitch of an instrument or the spacecraft or, in the worst case, in the loss of the entire mission.

Another example of a low-energy application is the particle-induced X-ray emission (PIXE). This is an analytical method for identifying the composition of a target material by irradiating it with low-energy charged particles, usually protons or alpha particles, inducing X-ray fluorescence emission. The part of the emission emerging from the topmost layer of the target can be observed, and is characteristic of the elements present in the target material. PIXE methods have found wide applications in mineralogy, archaeology, as well as in astrophysical research. Simulation tools capable of accurately treating the electromagnetic interactions of the incident hadrons below few MeV will be highly useful in the analysis of PIXE spectra.

In this report we describe the GEANT4 physical model of the electromagnetic interaction of protons and other hadrons with matter to low energies. This represents an extension of the GEANT4 physics models with respect to the previous development versions (identified in the following as ”GEANT4 beta”).

2 Energy Loss of Fast Hadrons

Relativistic charged hadrons moving through matter lose energy primarily by ionisation. The mean value of the energy loss (stopping power) is given by the Bethe-Bloch formula [4],

$$-\frac{dE}{dx} = N_{el}\frac{Z_h^2}{\beta^2}\left[\ln\left(\frac{2m_e\beta^2\gamma^2T_{max}}{I^2}\right) - 2\beta^2 - \delta - 2\frac{C_e}{Z}\right], \quad (1)$$

where N_{el} is the electron density of the medium, Z_h is the electric charge of the hadron, β, γ are the kinematic variables of the hadron, m_e is the electron mass, I is the average ionisation potential of the atom, δ is the so-called density correction term, C_e/Z is the so-called shell correction term, Z is the atomic number, T_{max} is the maximum energy transfered from a hadron to a free electron,

$$T_{max} = \frac{2m_e(\gamma^2-1)}{1+2\gamma\frac{m_e}{M}+(\frac{m_e}{M})^2}, \quad (2)$$

where M is the hadron mass.

The density effect becomes important at high energy because of the polarisation of the medium by a relativistic charged particle. The shell correction term takes into account the fact that, at low energies for light elements, and at all energies for heavy ones, the probability of hadron interaction with inner atomic shells becomes small. The implementation of the density effect term and of the shell correction term in GEANT4 is described in detail in Ref.[2]. The accuracy of the Bethe-Bloch formula with correction terms mentioned above is estimated as 1 % for energies between 6 MeV and 6 GeV [4]. The parametrisation of the shell correction term used in the beta version of GEANT4 became inaccurate [2] at lower energies and should not be used. This paper describes the parametrisations implemented in GEANT4 to handle the low energy range correctly.

A principal improvement in the simulation of hadrons energy loss in GEANT4 [2] in comparison with GEANT3 [3] is a unified simulation of the ionisation process. For charged hadrons, ionisation is relevant both as parametrized energy loss with fluctuations and as delta ray production. In a given medium a kinetic cut-off energy T_c for delta-electrons production is defined. If $T_c < T_{max}$ the formula (1) for the mean value of the energy loss becomes:

$$-\frac{dE}{dx} = N_{el}\frac{Z_h^2}{\beta^2}\left[\ln\left(\frac{2m_e\beta^2\gamma^2T_c}{I^2}\right) - \beta^2(1+\frac{T_c}{T_{max}}) - \delta - 2\frac{C_e}{Z}\right]. \quad (3)$$

The difference between expressions (1) and (3)

$$-\left(\frac{dE}{dx}\right)_\delta = N_{el}\frac{Z_h^2}{\beta^2}\left[\ln\frac{T_{max}}{T_c} - \beta^2\left(1-\frac{T_c}{T_{max}}\right)\right] \quad (4)$$

represents the average energy deposit per unit length leading to delta ray production.

Since $M \gg m_e$, the ionisation loss does not depend on the hadron mass, but on its velocity. Therefore the energy loss of a charged hadron with kinetic energy T is the same as the energy loss of a proton with the same velocity. The corresponding kinetic energy of the proton T_p is

$$T_p = T\frac{M_p}{M}. \tag{5}$$

Hence we will discuss below only the simulation of proton energy loss, keeping in mind that the average ionisation of any hadron at any energy can be derived from the proton ones.

3 Energy Losses of Slow Hadrons

For a velocity of a charged hadron $\beta < 0.05$, corresponding to 1 MeV for protons, formula (1) becomes inaccurate. In that case the velocity of the incident hadron is comparable to the velocity of atomic electrons. At very low energies, when $\beta < 0.01$, the model of a free electron gas [5] predicts the stopping power to be proportional to the hadron velocity, but it is not as accurate as the Bethe-Bloch formalism.

The intermediate region $0.01 < \beta < 0.05$ is not covered by theories at all. In this energy interval there is the Bragg's peak of ionisation loss. The energy loss of low-energy protons is of great interest for basic and applied physics. Thousands of publications [7] exist with experimental data on the stopping power of different absorbers and on phenomenological analysis of the data. In the beta version of GEANT4 a simple phenomenological parametrisation was chosen [2], based only on three parameters for each atom.

The practical importance of the stopping power data for different applications required detailed reviews, which have been done by J.F. Ziegler and collaborators [8,10]. They established standard procedures to average the data from different experiments and to find out universal fitting functions depending on few phenomenological parameters which describe the stopping power for protons from 1 keV to 100 MeV.

In order to increase the precision of the GEANT4 simulation, a new version of parametrisation of energy losses was developed. In this approach a user will have the possibility to choose the method adopted to parametrize the stopping power for slow protons. As a next step after the beta version, the following parametrisation from the review [8] was implemented in GEANT4:

$$S_e \;=\; A_1 E^{1/2}, \qquad\qquad 1\ keV < T_p < 10\ keV,$$

$$
\begin{aligned}
S_e &= \frac{S_{low}S_{high}}{S_{low}+S_{high}}, && 10\ keV < T_p < 1\ MeV,\\
S_{low} &= A_2 E^{0.45},\\
S_{high} &= \frac{A_3}{E}\ln\left(1+\frac{A_4}{E}+A_5 E\right),\\
S_e &= \frac{A_6}{\beta^2}\left[\ln\frac{A_7\beta^2}{1-\beta^2}-\beta^2-\sum_{i=0}^{4}A_{i+8}(\ln E)^i\right],\ 1\ MeV < T_p < 100\ MeV,
\end{aligned}
\tag{6}
$$

where S_e is the electronic stopping power in $[eV/10^{15}atoms/cm^2]$, $E = T_p/M_p[keV/amu]$, A_i are twelve fitting parameters found individually for each atom for atomic numbers from 1 to 92. This parametrisation is used in the interval of proton kinetic energy

$$T_1 < T_p < T_2, \tag{7}$$

where $T_1 = 1\ keV$ is the minimal kinetic energy of protons in the tables of Ref.[8], T_2 is an arbitrary value between 2 MeV to 100 MeV, since in this range both the parametrisation (6) and the Bethe-Bloch formula (1) have practically the same accuracy and are close to each other. In the current implementation of this parametrisation the value $T_2 = 2\ MeV$ was chosen.

To avoid problems in computation and to provide a continuous dE/dx function, the factor

$$F = \left(1 + B\frac{T_2}{T_p}\right) \tag{8}$$

is multiplied by the value of dE/dx for $T_p > T_2$. The parameter B is determined for each element of the material in order to provide continuation at $T_p = T_2$. The value of B for different atoms is usually less than 0.01. For the simulation of the stopping power of very slow protons the model of free electron gas [5] is used

$$S_e = A\sqrt{T_p},\ \ T_p < T_1. \tag{9}$$

The parameter A is defined for each atom by requiring the stopping power to be continuous at $T_p = T_1$.

Note that, if the cut kinetic energy is small ($T_c < T_{max}$), then the average energy deposit giving rise to delta electron production (4) is subtracted from the value of the stopping power S_e, which is calculated by formulas (6) or (9).

Since Ref.[8] (identified in the following as Ziegler1977) provides both the table of the fitting parameters and the one of the stopping powers, it is possible to perform a cross check of the computation algorithm (Fig.1). The role of shell effects is demonstrated in Fig.2 where the stopping power is shown for different proton kinetic energies.

In Figs.3-5 the energy dependence of the stopping power for aluminum, iron and lead are shown. The new GEANT4 parametrisation based on tables obtained from the data [8] well reproduces the stopping powers published in [8]. The beta version of GEANT4 qualitatively reproduced the Bragg's peak of ionisation but the height of the peaks for different atoms could not reproduce the data exactly, while the current GEANT4 implementation correctly matches the data (figs.3-5).

The alternative parametrisation of protons energy loss based on ICRU report [11] is available in GEANT4 too. This parametrisation includes also the more recent sets of data from J.F. Ziegler [9]. The parametrisation formulae in ref.[11] are the same as (6) for the kinetic energy of protons $T_p < 1\ MeV$, but the values of the parameters are different. This is also the case for the output values of the stopping power (figs.6-8). Note, that this difference is much smaller than that between the parametrisations (6) and the GEANT4 beta version. Further analysis will be performed in future to estimate the accuracy.

4 Energy losses of Hadrons in Compounds

To obtain energy losses in a mixture or compound, the absorber can be thought of as made up of thin layers of pure elements with weights proportional to the electron density of the element in the absorber (Bragg's rule)

$$\frac{dE}{dx} = \sum_i \left(\frac{dE}{dx}\right)_i, \tag{10}$$

where sum is taken over all elements of the absorber, i is the number of element, $(\frac{dE}{dx})_i$ is calculated according to the equation (3).

Bragg's rule is very accurate for relativistic particles when the interaction of electrons with a nucleus is negligible. But at low energies the accuracy of Bragg's rule is limited because the energy loss to the electrons in any material depends on the detailed orbital and excitation structure of the material. There is a lot of experimental data demonstrating the breakdown of Bragg's rule for hydrocarbons [6]. At the same time, the experimental data for compounds with heavy elements [6] show that Bragg's rule is valid with accuracy better than 1 %. Therefore the stopping power in the absorber depends on the detailed structure of the absorber. To take this fact into account, a new attribute of the material class is introduced in GEANT4: the chemical formula. The chemical formula of the material is used in GEANT4 in the following way:

- if the data on the stopping power for a compound as a function of the proton kinetic energy is available, then the direct parametrisation of the data for this material is performed;

- if the data on the stopping power for a compound is available for only one incident energy, then the computation is performed based on Bragg's rule and chemical factor for the compound is taken into account;

- if there is no data for the compound the computation is performed based on Bragg's rule.

In Ref.[11] the detailed data on energy losses for the 11 compounds is reported as a function of the proton kinetic energy. The parametrisation is implemented in GEANT4. In the review [6] stopping power data are presented for fixed energies: for protons with kinetic energy of 125 keV and for He^4 ions with kinetic energy of 500 keV in the 53 different compounds. It is shown that for all energies the stopping power S_e in a compound for protons with kinetic energy T_p can be expressed as

$$S_e(T_p) = S_{Bragg}(T_p)\left[1 + \frac{f(T_p)}{f(125\ keV)}\left(\frac{S_{exp}(125\ keV)}{S_{Bragg}(125\ keV)} - 1\right)\right], \qquad (11)$$

where $S_{exp}(125\ keV)$ is the experimental value of the energy loss for the compound for $125\ keV$ protons or the reduced experimental value for He ions, $S_{Bragg}(T_p)$ is a value of energy loss calculated according to Bragg's rule, $f(T_p)$ is a universal function which describes the disappearance of deviations from Bragg's rule for higher kinetic energies. The proposed form of this function [6] is the following:

$$f(T_p) = \frac{1}{1 + \exp\left[1.48(\frac{\beta(T_p)}{\beta(25\ keV)} - 7.0)\right]}, \qquad (12)$$

where $\beta(T_p)$ is the relative velocity of the proton with kinetic energy T_p. The energy dependence of this function is shown in Fig.9.

The importance of this "chemical effect" for slow protons is demonstrated in Fig.10 for ionisation by protons in water. In the Bragg's peak the value of this effect is more than 10 %. The differences between the J.F. Ziegler and the ICRU parametrisations as implemented in GEANT4 are quite small. The same small difference of these parametrisations for methane can be seen in Fig.11 too.

5 GEANT4 Implementation of Energy Losses of Slow Hadrons

For the implementation of energy losses of slow hadrons in GEANT4 a new class **G4hLowEnergyIonisation** has been designed. This class is based on the standard GEANT4 class **G4hIonisation** [2]. Both classes inherit from the same class **G4hEnergyLoss**. The user has the choice to include one of these classes in his **G4PhysicsList**. If the new class

is chosen, then it's possible to choose the parametrisation model. The model is defined by the void member function **SetStoppingPowerTableName("TheTableName")**.

Table 1: The list of different parametrisations available in GEANT4.

Name	Particle	Source
UrbanModel	proton	GEANT4 beta version [2]
Ziegler1977H	*proton*	J.F. Ziegler parametrisation [8]
Ziegler1977He	He^4	J.F. Ziegler parametrisation [10]
ICRU_R49p	proton	ICRU parametrisation [11]
ICRU_R49He	He^4	ICRU parametrisation [11]

The advantage of such a design is that the implementation of a new parametrisation, for example based on new data, is straightforward: the new parametrisation must just satisfy the standard interface to the class, but internally the method of parametrisation and number of parameters are individually selectable without any constraint.
In Table.1 the list of all available parametrisations is shown. The detailed comparisons of the results of the J.F. Ziegler's parametrisation [8] and the ICRU's parametrisations [11] will be addressed in further publications.
The "chemical effect" is also implemented. If the user chooses the **ICRU_R49p** parametrisation and specifies in his GEANT4 detector definition a material with its chemical formula and this formula coincides with one of the 11 names included in the list of the ICRU model (table 2), then **ICRU_R49p** parametrisation of this material is used. In opposit case if the chemical formula coincides with one of the 53 names included in the list of the **G4hLowEnergyIonisation** class (table 3) then the parametrisation of energy losses is performed using the Bragg's rule and chemical correction factor is taken into account. This factor is working independently for all available parametrisations.

6 Conclusion

The first version of a precise parametrisation methods for low energy hadron ionisation losses based on experimental data has been implemented in GEANT4. The accuracy of this method is significantly higher than the one in the GEANT4 beta version and allows GEANT4 to match both ICRU's and Ziegler's evaluated data. The design of the new method provides wide possibilities to continuously improve the accuracy of simulations, by using new experimental data and new parametrisation of the data itself.

Table 2: The list of chemical formulas of compounds for which **ICRU_R49p** has parametrisations.

Number	Chemical formula
1.	AlO
2.	C_2O
3.	CH_4
4.	(C_2H_4)_N-Polyethylene
5.	(C_2H_4)_N-Polypropylene
6.	(C_8H_8)_N
7.	C_3H_8
8.	SiO_2
9.	H_2O
10.	H_2O-Gas
11.	Graphite

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Table 3: The list of chemical formulas of compounds for which the “chemical effect” is calculated for any parametrisations available in GEANT4.

Number	Chemical formula	Number	Chemical formula
1.	H_2O	28.	C_2H_6
2.	C_2H_4O	29.	C_2F_6
3.	C_3H_6O	30.	C_2H_6O
4.	C_2H_2	31.	C_3H_6O
5.	C_H_3OH	32.	C_4H_10O
6.	C_2H_5OH	33.	C_2H_4
7.	C_3H_7OH	34.	C_2H_4O
8.	C_3H_4	35.	C_2H_4S
9.	NH_3	36.	SH_2
10.	C_14H_10	37.	CH_4
11.	C_6H_6	38.	CCLF_3
12.	C_4H_10	39.	CCl_2F_2
13.	C_4H_6	40.	CHCl_2F
14.	C_4H_8O	41.	(CH_3)_2S
15.	CCl_4	42.	N_2O
16.	CF_4	43.	C_5H_10O
17.	C_6H_8	44.	C_8H_6
18.	C_6H_12	45.	(CH_2)_N
19.	C_6H_10O	46.	(C_3H_6)_N
20.	C_6H_10	47.	(C_8H_8)_N
21.	C_8H_16	48.	C_3H_8
22.	C_5H_10	49.	C_3H_6-Propylene
23.	C_5H_8	50.	C_3H_6O
24.	C_3H_6-Cyclopropane	51.	C_3H_6S
25.	C_2H_4F_2	52.	C_4H_4S
26.	C_2H_2F_2	53.	C_7H_8
27.	C_4H_8O_2		

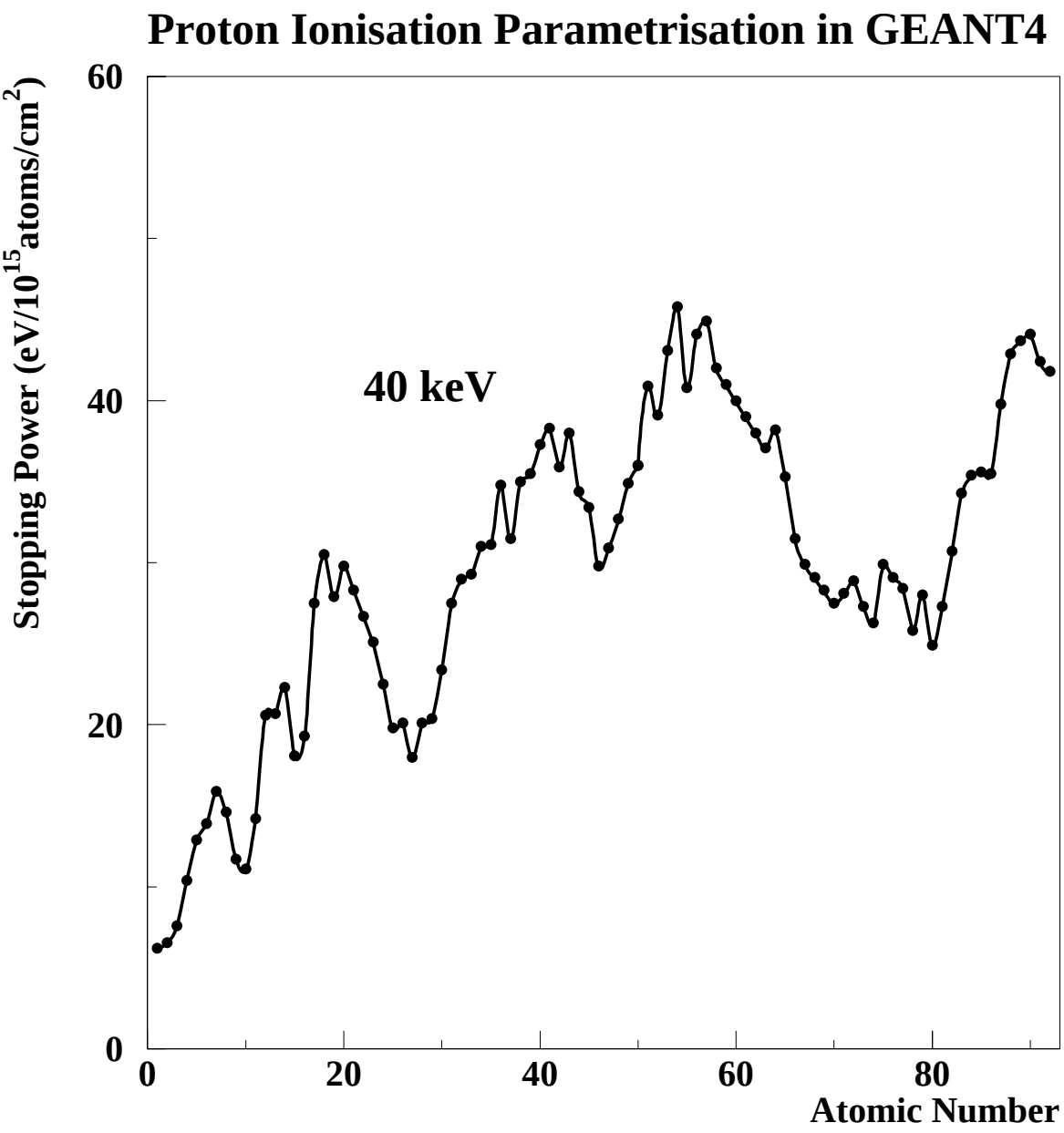

Figure 1: Cross check of the implementation of the stopping power parametrisation. Solid line - parametrised stopping power for 40 keV protons in all atoms with $Z < 93$, points - averaged data on stopping power.

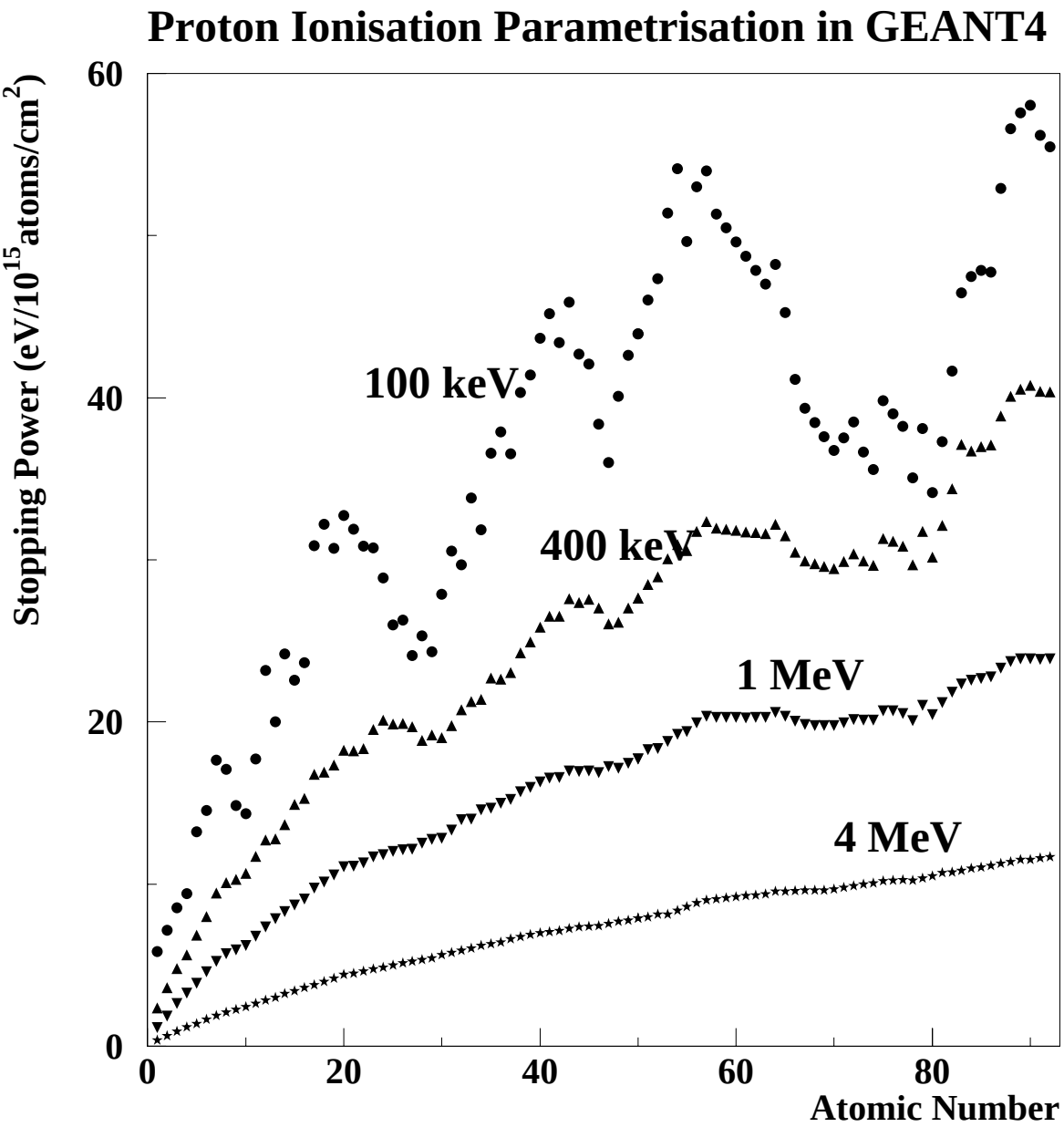

Figure 2: Stopping power in all atoms with $Z < 93$ for various proton energies.

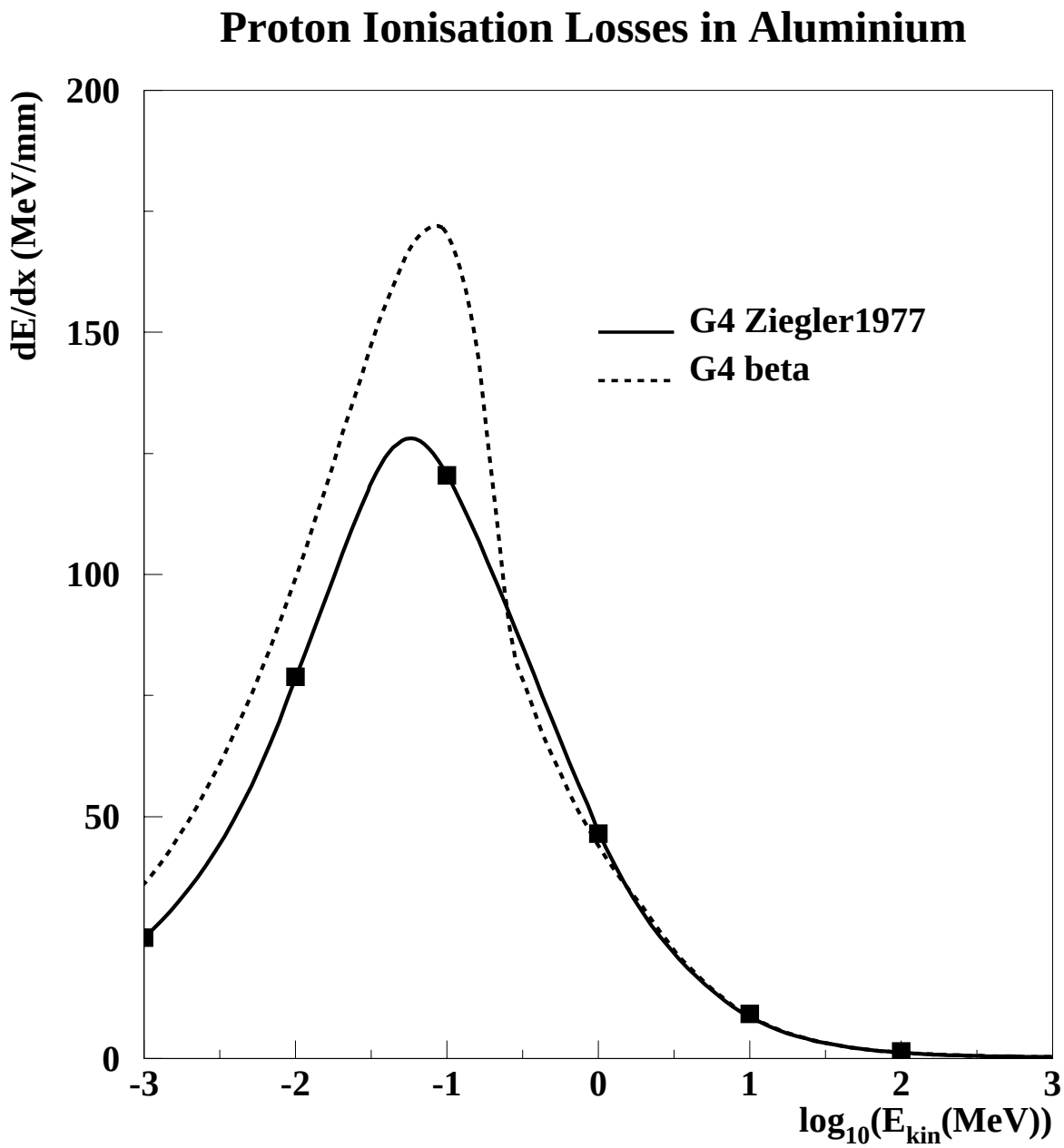

Figure 3: Ionisation of protons in aluminum. Points - averaged data on stopping power.

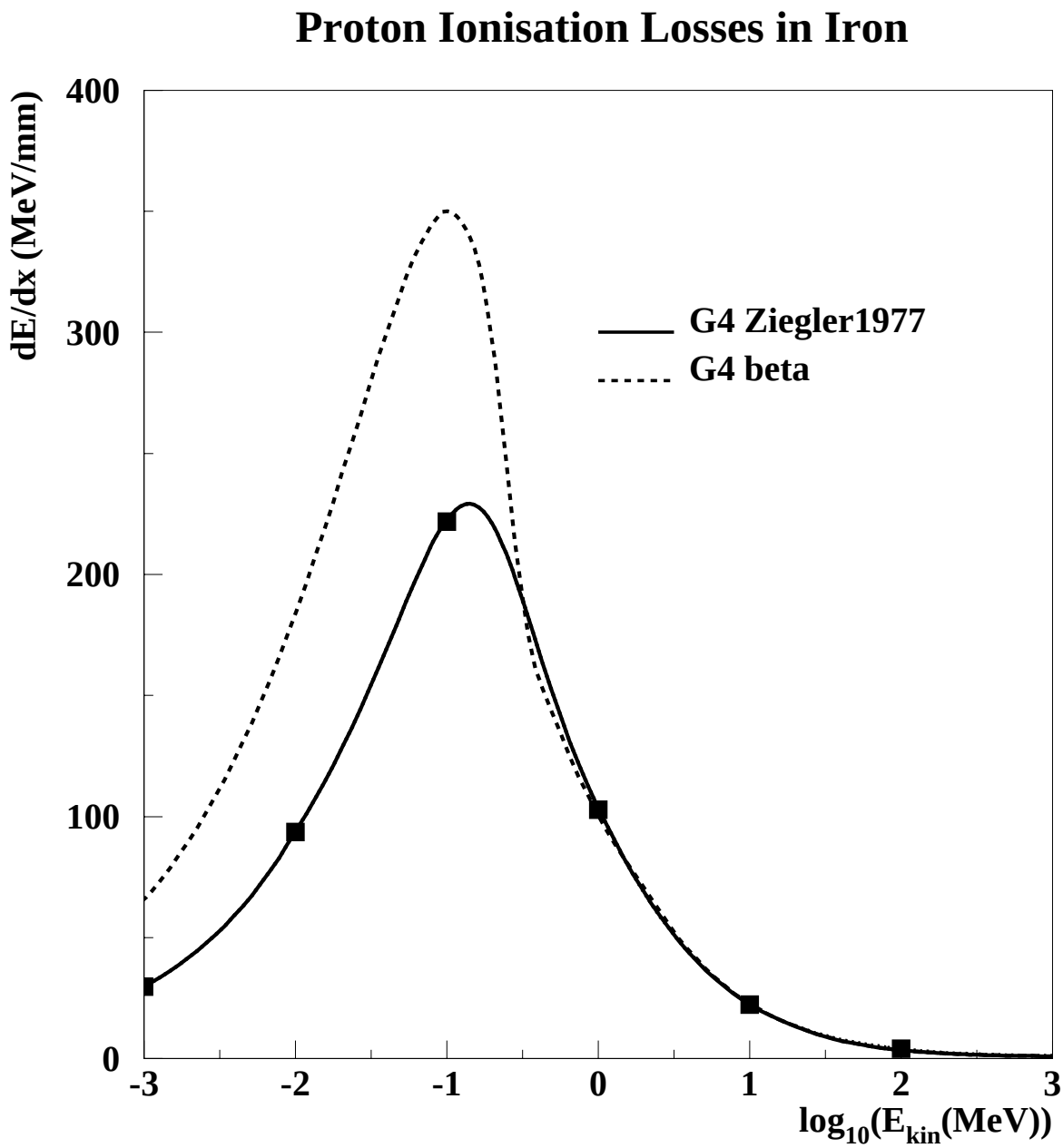

Figure 4: Ionisation of protons in iron. Points - averaged data on stopping power.

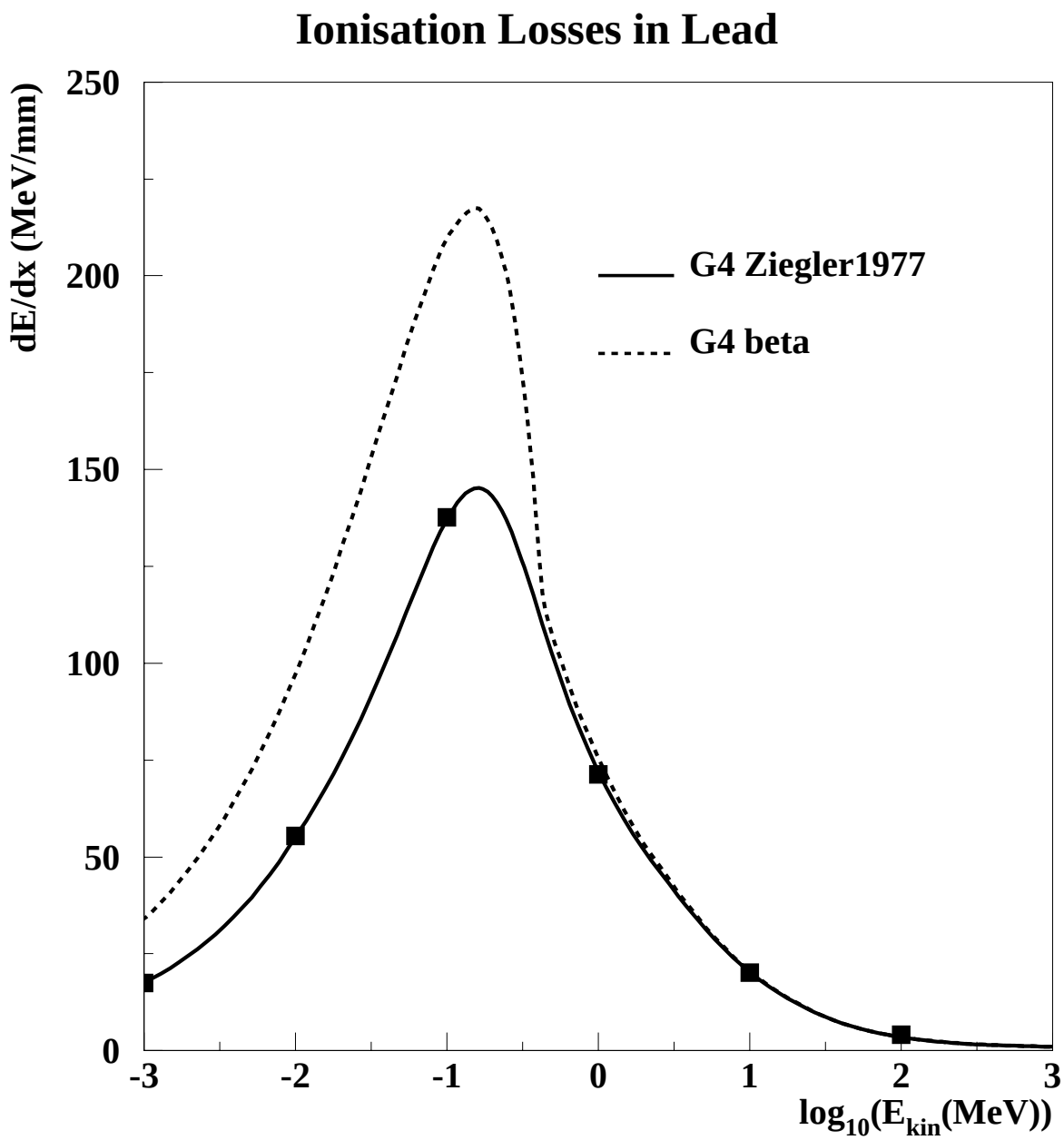

Figure 5: Ionisation of protons in lead. Points - averaged data on stopping power.

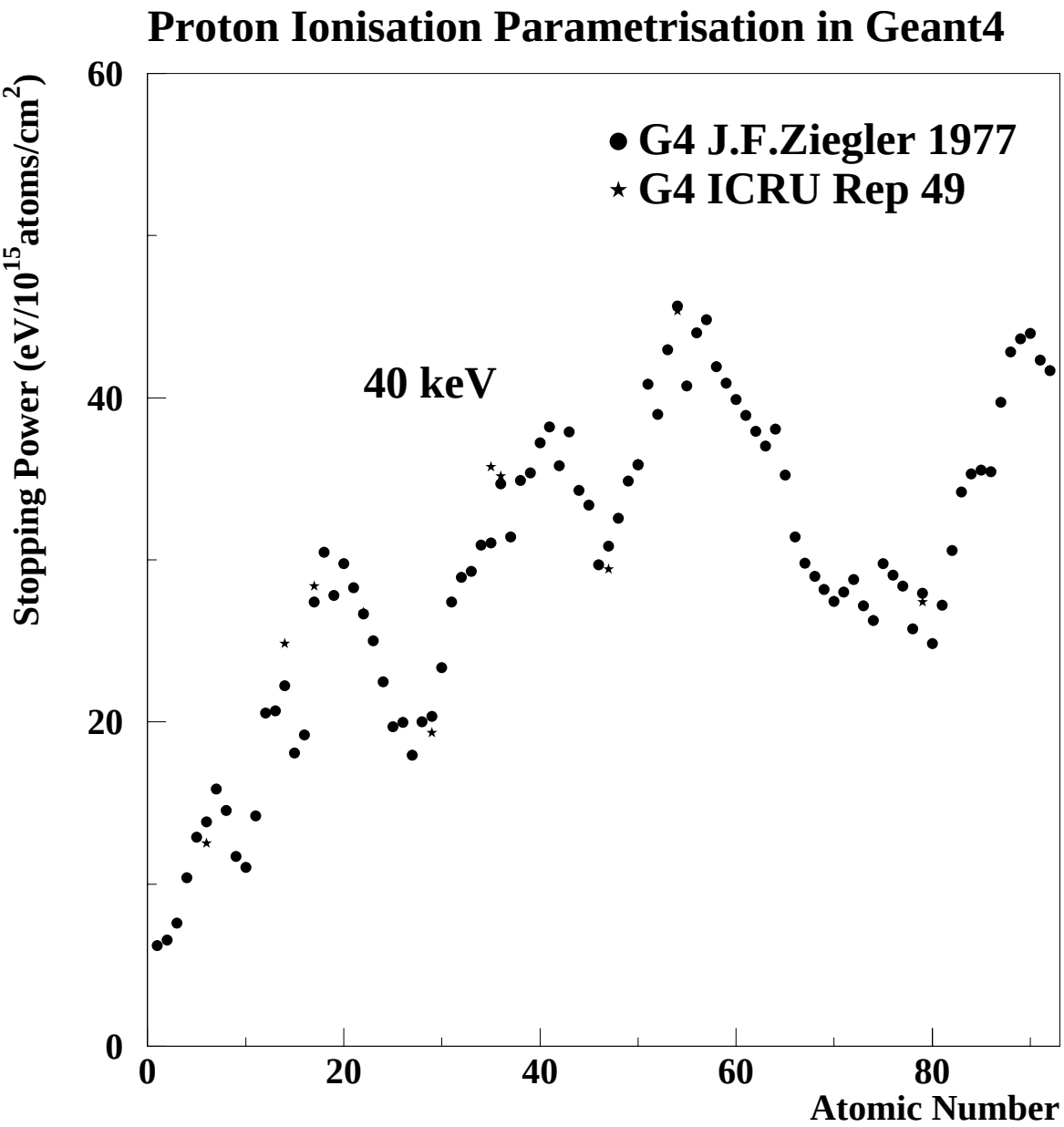

Figure 6: Comparison of two available parametrisations of the proton stopping power.

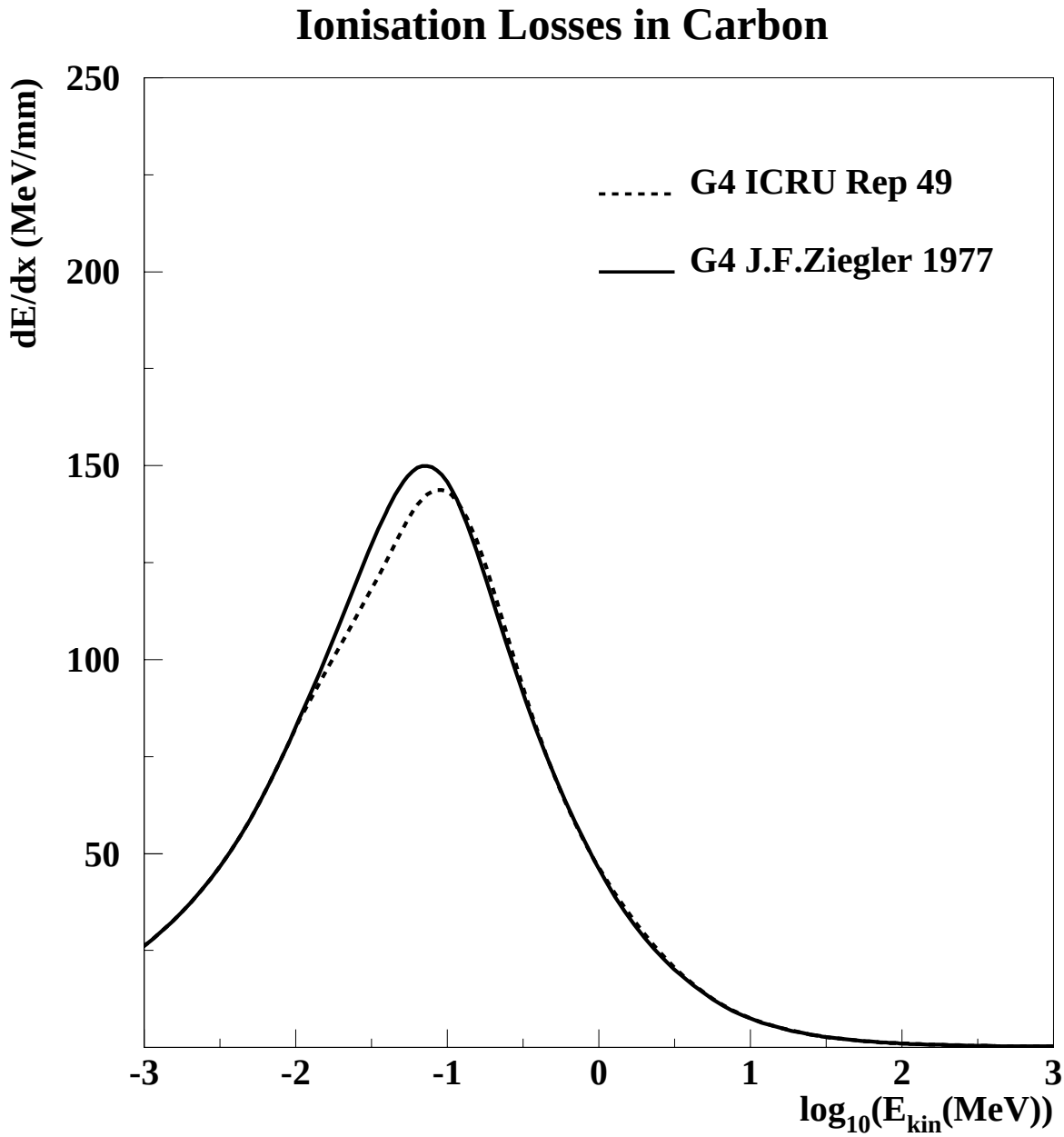

Figure 7: Comparison of two available parametrisations of the proton ionisation losses in carbon.

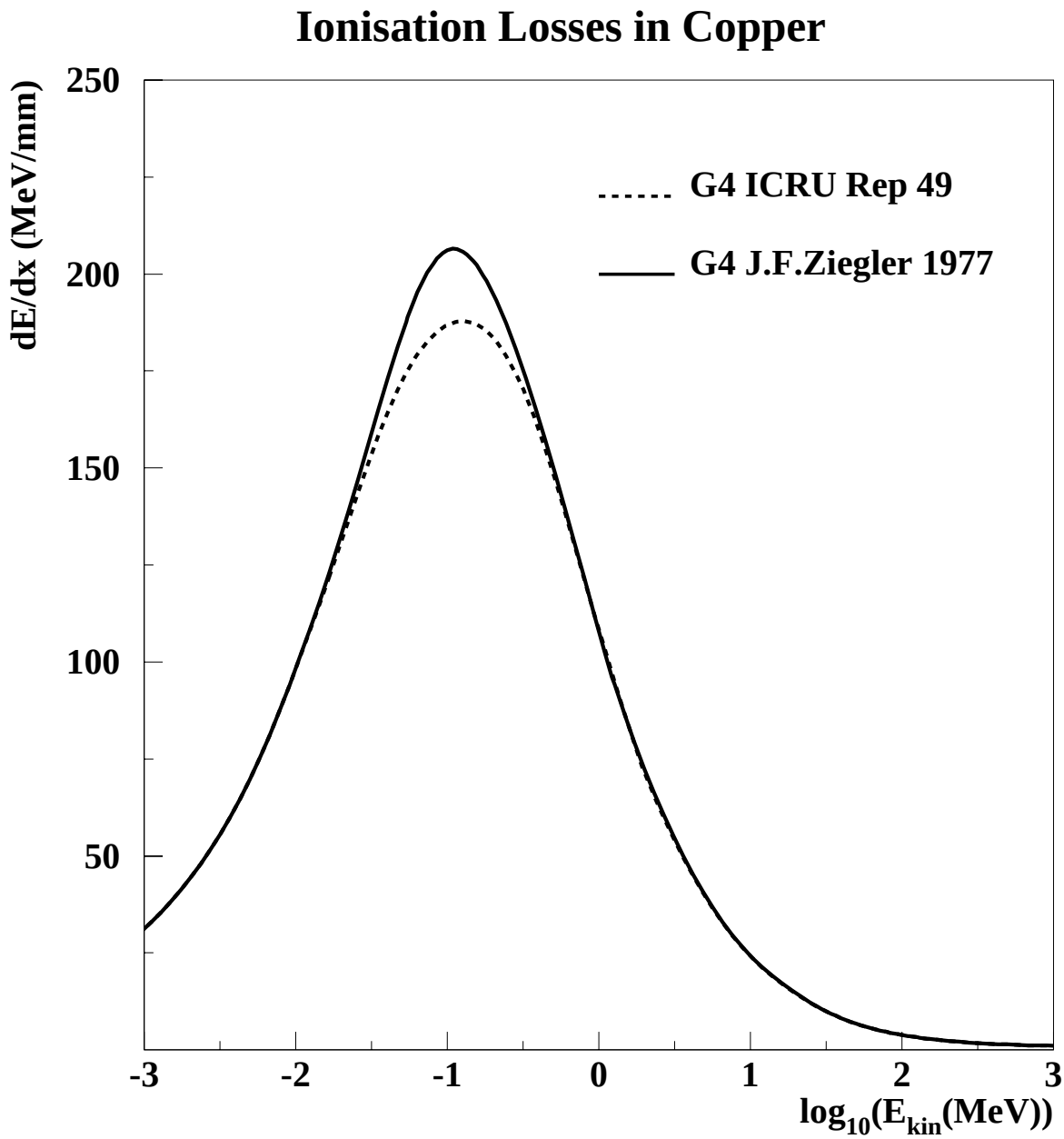

Figure 8: Comparison of two available parametrisations of the proton ionisation losses in copper.

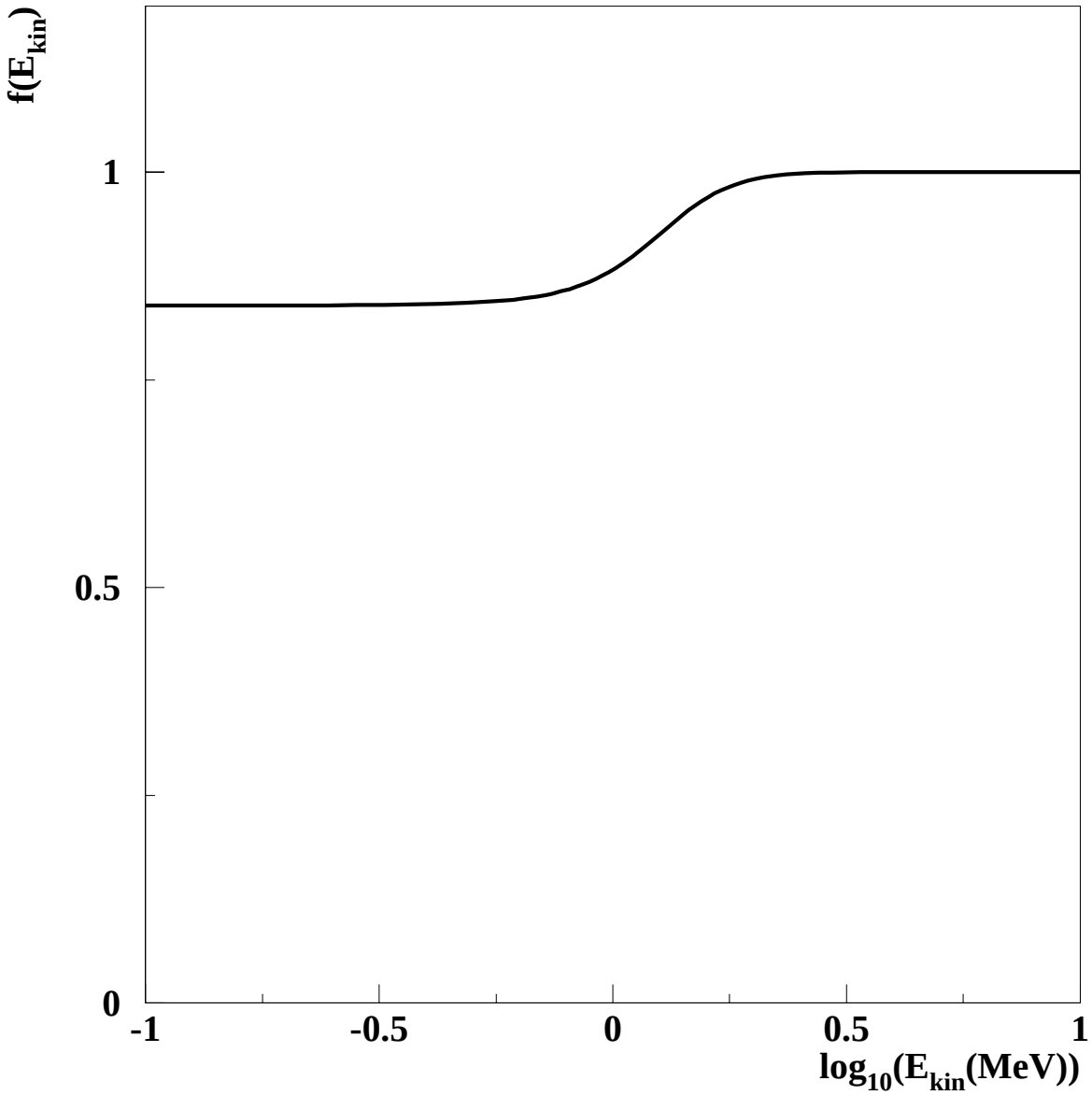

Figure 9: Dependence of the chemical effect on proton energy.

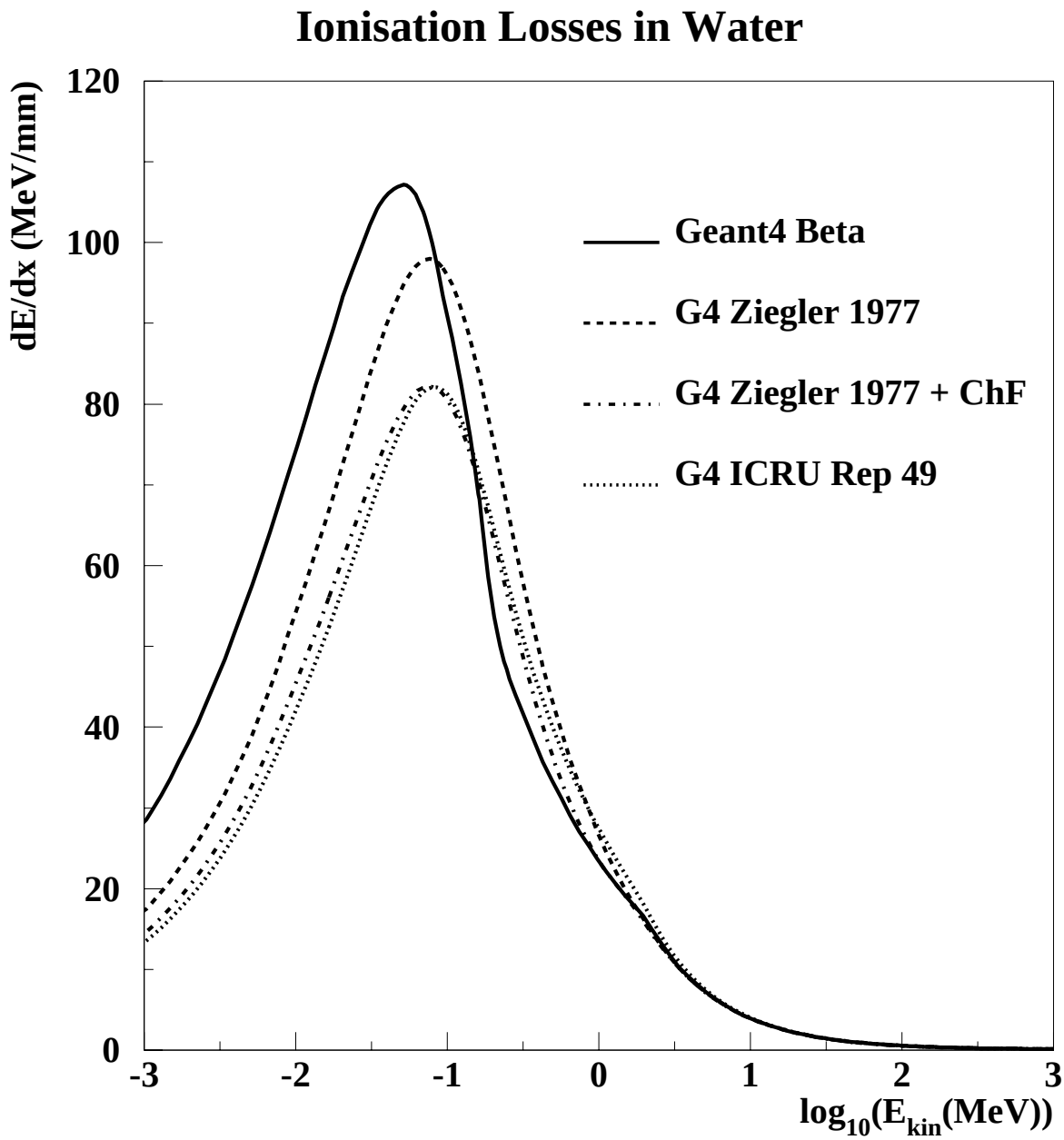

Figure 10: Comparison of different parametrisations of the proton ionisation losses in water.

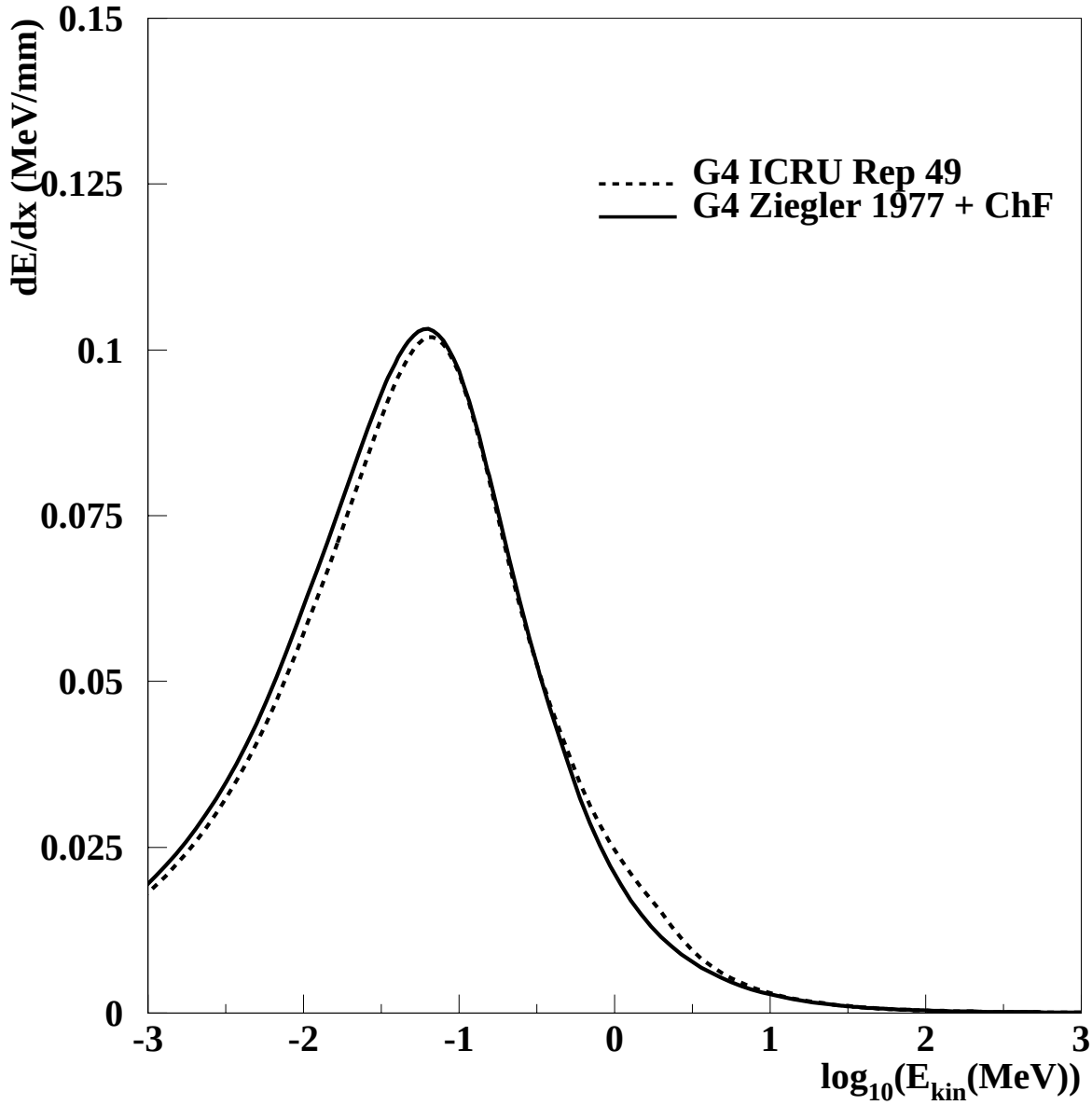

Figure 11: Comparison of two available parametrisations of the proton ionisation losses in methane.