International Atomic Energy Agency

INDC(NDS)-295

INDC INTERNATIONAL NUCLEAR DATA COMMITTEE

Atomic and Molecular Data Needs for Monte Carlo Track Structure Calculations of Radiation Induced Damage in Biological Substances

Summary Report of an IAEA Consultants' Meeting

Vienna, Austria, November 11-12, 1993

Prepared by

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January 1994

IAEA NUCLEAR DATA SECTION, WAGRAMERSTRASSE 5, A-1400 VIENNA

Printed by the IAEA in Austria
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Abstract

The proceedings and the results of the IAEA Consultants' Meeting on "Atomic and molecular data needs for Monte Carlo track structure calculations of radiation induced damage in biological substances" (November 11-12, 1993, Vienna) are described. The meeting conclusions regarding the data status, further data needs for improving the atomic physics of Monte Carlo codes, organizational steps for establishing an internationally recommended atomic database for track structure calculations and the role of the IAEA in this effort are presented.

The scope and objectives of an IAEA Co-ordinated Research Programme, to be initiated as soon as possible, are outlined

Contents

1. INTRODUCTION

The Consultants' Meeting on "Atomic and Molecular Data Needs for Monte Carlo Track Structure Calculations of Radiation Induced Damage in Biological Substances" (November 11-12, 1993, IAEA Headquarters, Vienna) has been organized by the IAEA Atomic and Molecular (A+M) Data Unit as a natural next step after the successful completion of the IAEA Co-ordinated Research Programme (CRP) on "Atomic and Molecular Data for Radiotherapy" (1989-1993). The basic idea for organizing this meeting was to define an Agency atomic and molecular data programme in the area of radiation biology which would take full advantage of the well established collaborative links of the Agency's Nuclear Data Section (NDS) with both the radiobiological and atomic physics research communities, and of the existing atomic collision databases and data processing capabilities of the NDS A+M Data Unit. Because of the large amount of required A+M data, its potential to approach the physics of the onset and dynamical evolution of radiation induced biological effects on a subcellular level and its relevance to the DNA radiation damage studies, the Monte Carlo track structure calculations and analysis method was selected as an appropriate subject for focussing the Agency A+M data activities in the radiobiological area. The objectives of the Meeting were set to:

(i) analyze the status of A+M data currently used in Monte Carlo codes for track structure calculations from the point of view of their completeness and accuracy;

(ii) identify the specific A+M data needs for improvement of the predictive power of Monte Carlo track structure calculation codes;

(iii) formulate the programmatic scope of an international effort, co-ordinated by the Agency, aimed at establishing an international reference A+M database for predictive Monte Carlo track structure calculations.

The meeting Agenda (see Appendix 1) was composed in such a way as to fully reflect these objectives. Five prominent world leading experts in the field, with extensive experience either in the development and use of Monte Carlo codes or in A+M data generation (compilation, evaluation) for these codes, were invited to participate in the Meeting (see Appendix 2). Part of the staff of IAEA A+M Data Unit and Nuclear Data Section also took part in the meeting discussions.

2. BRIEF MEETING PROCEEDINGS

After the introductory remarks of the scientific secretary (R K Janev) regarding the meeting objectives, and the adoption of the Meeting Agenda, the work of the meeting under the co-chairmanship of Dr Paretzke and Dr Inokuti, proceeded along the following principal items:

- Review and analysis of the atomic and molecular physics content of present Monte Carlo codes for track structure calculations, including interacting species, collision processes, energy ranges, data accuracy, etc.;

- Required improvements in the A+M physics base of Monte Carlo codes (from the point of view of the physical processes involved, completeness and quality of required data, data presentation and formatting, etc),

- Definition of the scope, methods and participants of an international, Agency co-ordinated activity, for establishing of a recommended international database for highly accurate Monte Carlo track structure calculations, with an ultimate goal to provide a tool for describing the radiation damage effects on the scale of subcellular structures (e.g. DNA).

The first day of the meeting was devoted to analysis of the A+M physics and data content of existing Monte Carlo codes. The discussion was focussed on a selected group of target materials of prime radiobiological interest (liquid and vaporized water, carbon, DNA, proteins) and on the most relevant radiation agents (X-rays, electrons, protons, alpha particles, carbon ions) with energies ranging from about 1 eV (for the electrons) and 1 keV (for other projectiles) up to 100 MeV (100 MeV/amu for the heavy projectiles) The meeting limited the scope of elementary processes between interacting species to those involved in the "physical stage" of the radiation damage process, i e. excluding the processes in the "chemical stage". The processes in the physical stage define the particle transport, energy deposition, and the spatial pattern of energy deposition (the track structure). The latter is closely related to the biological effectiveness of a given type of ionizing radiation. The analysis of the physics content of the existing Monte Carlo codes revealed large differences in the data used for the same type of processes (as illustrated by Dr. Terrissol). Differences among the codes exist also in the level of details at which different types of processes are described (e.g dissociation and multiple ionization channels, condensed phase effects, etc). In general, the meeting discussions showed that the present A+M data content of the Monte Carlo code is characterized by large uncertainties in the data used (except for the stopping power and total cross sections) for all relevant processes, and existence of large gaps in the database, especially for the doubly differential cross sections for the most relevant target materials, required for determination of spatial patterns of energy deposition The details of these discussions are described in the next section of this report.

A more detailed analysis of the requirements for establishing a reasonably complete and self-consistent A+M database for Monte Carlo track structure calculations was undertaken during the morning session of the second day of the meeting These discussions which

included the purpose, scope and physical content of a desired A+M database (Drs Goodhead and Paretzke), specified data requirements (Dr. Toburen) confronted with the presently available database (Dr. Terrissol) and its assessed completeness and accuracy (Dr. Inokuti), are also reflected in the next section of this report. The meeting participants were informed about the available A+M databases in the Agency's ALADDIN database system (Dr. Botero), part of which overlaps with the required A+M data for the Monte Carlo codes

During the afternoon session of the second day of the meeting, the scope, implementation methods and potential participants of an international effort on establishing a reference A+M database for Monte Carlo track structure calculations were discussed. Based on the significant incompleteness of the presently available data and the widely recognized current need for building a powerful tool for the description of radiation damage effects on a subcellular level, the concensus of the meeting was that the establishment of such an A+M database is an urgent task of highest priority for radiobiology. The role of the IAEA in the co-ordination of such an international effort was clearly identified. In view of the existing A+M databases in the IAEA A+M Data Unit, its established relations with the atomic physics community and the international A+M Data Centre Network, and its developed data processing methods and technical capabilities, the involvement of the Agency in this international endeavour would be highly beneficial for the efficiency of the project. The scope of a proposed IAEA Co-ordinated Research Programme, including its objectives, implementation methodology and potential participants, has, therefore, been formulated and are described in section 4 of this report.

At the end of the Meeting, the meeting participants summarized the conclusions of their work and formulated a set of recommendations regarding the future Agency activities in the area of A+M data for radiobiology.

3. ATOMIC AND MOLECULAR DATA STATUS AND NEEDS FOR MONTE CARLO TRACK STRUCTURE CALCULATIONS

3.1. Introduction

Humans are exposed to radiation from a wide variety of sources, including the nuclear fuel cycle, other industrial activities, natural radioactivity and medical diagnoses and treatment Apart from rare accident scenario and radiotherapy treatment, these exposures are at low doses and usually at low dose rates. The detrimental effects of main concern are induction of cancers that occur as stochastic consequences of radiation damage to individual cells within the body, probably without any safe threshold of dose or dose rate. Risk estimates have been derived primarily from epidemiological studies of human populations exposed to external ionizing radiation at much higher doses and/or dose rates, for which statistically adequate increases in cancer incidence have been observed Extrapolation of the risk to the low levels of main practical relevance, and to other radiation types, can be done only on the basis of models of radiation carcinogenesis. Mechanistic understanding is required to develop models that have a firm foundation

Insult to cells from ionizing radiation is always in the form of structured tracks of charged particles (as primary or secondary components of the radiation field). At the low doses and dose rates of principle interest, individual cells in the body receive only single tracks, or small number of tracks, well separated in time and space from each other Therefore, crucial aspects of radiation carcinogenesis depend on the capabilities of single tracks to induce relevant subcellular damage and on any cooperative effects of subsequent tracks. In order to develop mechanistic models of radiation action, it is therefore essential to include realistic descriptions of the radiation tracks

DNA is a key molecular target for radiation damage; it is well established that radiation can bring about permanent DNA rearrangements, including mutations and chromozone aberrations involving cancer genes and others. Consequently, the track structure descriptions should have at least sufficient resolution to describe the damage processes on the scale of the DNA double helix. The chemical environment in the cell is so reactive that radiolysis free-radical products react mostly within only a few nanometres from their points of formation. Thus the radiation chemistry of DNA damage in cells is likely to be dominated by features of tracks on this scale, by direct ionizations in the DNA and in nearby molecules A particular feature of ionizing radiations is their ability to produce local clusters of ionizations and excitations on this scale, and these may lead to clustered molecular damage including DNA double strand breaks, and associated damage with varying degrees of complexity Mammalian cells are able to repair the vast majority of DNA damage, so a mechanistic description of radiation effects should include the frequency spectrum of initial damage with particular emphasis on those components that are least repairable and are most likely to lead to permanent alterations to the DNA. The required spatial resolution of the track descriptions is about 0.2 nm in order to distinguish between basic components of the DNA (such as individual bases, the sugar and phosphate moieties of the backbone) and adjacent material, such as bound water, bulk water and adjacent proteins.

Monte-Carlo methods provide a mean to describe tracks with this resolution The current status and uses of such codes has been summarized in the final document of the recently terminated IAEA CRP on Atomic and Molecular Data for Radiotherapy

3.2. Present Situation

Most of our knowledge on spatial distribution of track structure is based on Monte Carlo calculations. To obtain gross parameters or data useful for tissues, it is sufficient to use codes based on stopping power or continuous slowing down approximation, while an extensive set of differential cross sections for all possible events must be involved for the atomic or DNA level studies. However, the complexity of this latter biological structure makes such simulation very difficult, or even impossible, because of the lack of mentioned differential cross-sections. At present, to model biological effects, all Monte Carlo track structure codes use particle transport in water. But a complete set of doubly differential cross-sections for electrons in liquid water still does not exist, and assumptions or extrapolations must be used.

Even when the cross-sections are available, different codes are built with different data sets. The reasons are not always evident and probably lie in the structure of the computer codes used, the hypotheses done in establishing the computational algorithms, or in the adopted energy range. A clarification of this aspect is needed

As an illustrative example, one can see in Tables 1-3, various cross-sections and assumptions used for the track structure simulation in liquid water, which is most often used as a tissue equivalent. The reading of the table is self-explanatory and sets the problems which have to be solved. For instance:

1) Should one use the Thomas-Fermi or Mott-Dirac cross section for elastic scattering regardless of the assumptions done for the equivalence between liquid, vapor and amorphous ice?

2) When different experimental data are available for the same event (e.g Danjo-Nishimura and Itikawa), is their link (overlap) adequate?

3) Should one use the Bethe or Gryzinski cross section for the K-shell ionization of oxygen? What is their accuracy?

These few questions are crucial since the liquid water is at the limit of our present knowledge of cross-sections; they show the usefulness of and the needs for further clarifications and guidelines.

Cross-sections used for liquid water

Institute	Energy range	Cross-sections used
KIPC *	<200 eV	experimental data of Danjo-Nishimura assuming liquid = vapor
	>200 eV	Thomas-Fermi
ORNL *	0 - 10 Ev	experimental data of Itikawa assuming liquid = 0.6*vapor
	<1000 eV	phase-shift Mott-Dirac formula
	>1000 eV	Thomas-Fermi
CPA *	0 - 8.4 eV	experimental data of Sanche-Michaud assuming liquid = ice
	up to 30 keV	phase-shift Mott-Dirac formula

Table 1 - Elastic cross-sections used in liquid water Monte Carlo codes.

Institute	Excitation state	Energy	Cross-sections used
KIPC ORNL CPA	A^1B_1 B^1A_1 Rydberg(A+B) Rydberg(C+D) Diffuse bands Collective	8.4 eV 10.1 eV 11.26 eV 11.93 eV 14.1 eV 21.4 eV	Integration of energy loss function within the limits of each peak width, using differential oscillator strengths determined with dielectric response function derived from experiments
ORNL	Subexcitation electrons	<8.4 eV	Stopping power calculated with optical data and Fermi age theory
CPA	Subexcitation electrons	<8.4 eV	Exper. cross sections of Sanche-Michaud, assuming liquid = ice

Table 2 - Excitation cross-sections used in liquid water Monte Carlo codes.

Institute	Ionization level	Cross-sections used
KIPC	Oxygen K shell	Asymptotic Bethe cross-section
	For outer shells: 8.76 - 25 eV >25 eV	Use of dielectric response function and Jain-Khare semi-empirical cross-sections
ORNL	Oxygen K and $1b_1$, $1b_2$, $2a_1$, $3a_1$ shells	Partitioning of the imaginary part of the dielectric function between the five levels with sum rules
CPA	Oxygen K shell For outer shells: $1b_1$, $1b_2$, $2a_1$, $3a_1$	Gryzinski cross-section Partitioning of the dielectric response function between the four levels

Table 3 - Ionization cross-sections used in liquid water Monte Carlo codes

*	KIPC	Karpov Institute for Physics and Chemistry, Russia
	ORNL	Oak Ridge National Laboratory, U.S.
	CPA	Centre de Physique Atomique Toulouse, France

3.3. Required Cross Section Data, their Accuracy and Format

In charged particle track structure calculations usually the Monte Carlo method has been selected to be able to take account of the stochastic variability in time and space of the ensemble of individual molecular changes making up the track left behind in the target material by a passing primary particle. In this type of computer calculations, a set of cross sections describing the likelihood and location of the interactions for the primary particle and its secondaries is needed. These cross sections may have different levels of accuracy depending, in general, on their relative importance for the radiobiological endpoint considered The types of cross sections and their required accuracy are specified in this section as well as the proposed database format in which such information should be made available to the scientific community working in this field.

Specification of cross sections needed in track structure calculations results from the needs to calculate

(a) the particle transport, and

(b) the locations and types of important chemical modifications, i.e the tracks left behind in matter.

In the Monte Carlo track structure calculations, the distances between the successive events along the path of a particle are determined, in general, by the sum of the total inelastic cross sections, σ_{inel}, and the elastic scattering cross sections, σ_e, for a particle of energy T. The type of inelastic interaction in this context is selected on the basis of partial cross sections for

(a) the sum of all excitations $\sigma_{ex}(T,\varepsilon)$, since excitations appear to be of lesser importance here, where ε is the energy transferred from the projectile to the target;

(b) each dissociation $\sigma_{d,j}(T)$ separately (where the index j specifies the chemical consequences);

(c) each ionization $\sigma_{i,j}(T,\varepsilon)$ separately, including full information on the respective

(i) number of ejected electrons,
(ii) their double differential ejection cross sections $d^2\sigma_{i,j}/dEd\Omega(T,\varepsilon)$;

(iii) the molecular decay channels for each type of ionization into new chemical species of the target molecule/atom;

(d) the total stopping cross section σ_{st};

(e) if the projectile of atomic charge Z is "dressed" with N own electrons, additional cross sections are needed:

(i) the electron capture cross section $\sigma_c(T,Z-N)$;
(ii) the partial electron loss cross sections $\sigma_l(T,\varepsilon,Z-N)$ for loosing n electrons in a collision with energy transfer ε differential in the conditional energy and angular distributions for each of the n electrons.

In general it might be permissible for a calculation, or required by lack of knowledge, to sum up some of the partial cross sections for ionization or dissociation into one "gross"-cross section.

The accuracy of these data should be highest (better than 5%) for the total stopping and the total inelastic cross sections For the ionization cross sections of the target and the projectile (when applicable) an accuracy of about 10% might be acceptable. For the elastic and the energy differential electron ejection cross sections, an accuracy of 25% (and for its angular dependence even about 50%, or more) can be tolerated in this context. The cross section information on the production of new chemical species, however, must be as reliable as feasable, even despite the large gaps of knowledge there; a 10% accuracy is desirable regarding their yields and a few tenths of nanometers (typically 0.2nm) regarding the accuracy of their location.

The optimum format of the basic database of such cross sections is ALADDIN of the IAEA. This is, because ALADDIN is widely compatible with other software products consuming the data and is broadly accepted by other users of atomic and molecular data, it is accessible remotely by standard computer network systems, and permits data representation in analytical, graphical and tabular form, and allows for easy addition, modification etc. when new data sets become available.

3.4. Cross Sections, Targets and Projectiles of Importance for Track Structure Calculations

The structure of charged particle tracks is used to assess energy deposition patterns for a wide range of radiation types, from soft X-ray absorption to energy deposition by fast heavy ions used for radiation therapy. The spatial pattern of energy deposition is an important pattern in determining the biological effectiveness of different types of ionizing radiation. Because of the wide range of applications, the data needs cover an equally broad range of parametric space.

In this discussion we will limit the range of radiation types to those exposures commonly encountered in the nuclear fuel cycle, medical practices, and radiation therapy

using light ions. Interactions of importance include those involving electromagnetic radiation, from soft X-rays to ^{60}Co gamma rays (energies from a few keV to MeV), and charged particles ranging from electrons to protons, alpha particles and carbon ions. The energy range of heavy particles of interest is based on, at the low energies, neutron induced recoil ions in tissue and at the high energy, radiation therapy. Thus ion energies of concern range from about 1 keV/amu to 100 MeV/amu. Likewise, interactions of electrons with energies from 1 eV to 100 MeV result from the production of secondary electrons in interactions of X-rays and charged particles with the atomic and molecular constituents of the stopping (tissue) medium. In summary, data for the following particles and energy ranges are needed for charged particle track structure calculations:

- X-rays: 1 keV to 1 MeV
- electrons: 1 eV to 100 MeV
- protons: 1 keV to 100 MeV
- alpha particles/helium ions. 1 keV to 100 MeV/amu
- carbon ions: 1 keV to 100 MeV/amu

The lower energy cut-off in these requirements is based on the short range and decrease in ionization efficiency at lower energies of charged particles; thus a decreased biological effectiveness relative to higher energies.

Target atoms, molecules, and materials of interest to track structure calculations reflect the importance of simulating interactions in tissue, and at the same time being practical from a data gathering point of view. Traditionally, track structure calculations have focussed on water as a primary constituent of tissue and therefore the medium in which energy is predominantly deposited. In addition, condensed phase experiments to determine basic interaction cross sections are inherently difficult, leading to a major part of the data available being obtained from gas phase material. Often one must combine information from gas and condensed phase measurements, employing a theoretical knowledge of the energy deposition process, to obtain data for use in track structure calculations. To fulfill the needs of track structure computations, at least in the present state of development, cross sections for interaction of X-rays and charged particles in water vapor are used extensively. For interactions involving energy losses greater than a few 10s of eV, water vapor provides a reasonable approximation to the primary interactions in tissue and vapor lends itself to a wide range of measurement techniques not possible in condensed phase. For energy losses less than a few 10s of eV, the molecular and condensed phase effects of the target become increasingly important and interaction cross sections based on properties of liquid water are used. In order to test electron transport codes in condensed phase, data from foils, in particular carbon foils, are used. Thus, data for electron emission from carbon foil, differential in electron emission energy and angle are needed. As calculations become more sophisticated in detail, it is important to have interaction cross sections for constituents of mammalian cells other than water. Therefore data for energy deposition and transport in DNA and associated proteins become very important. These are critical data for Monte Carlo codes aimed at describing DNA damage and subsequent cellular repair and/or mutation induction. In summary, data of importance to track structure calculations include interactions in the following materials:

- water vapor
- liquid water
- carbon foils
- DNA and proteins.

The cross sections of importance to any charged particle track structure calculation must begin with the production of seconday electrons and address the fate of the target molecule. Secondary electrons transport the deposited energy via subsequent interactions that define the spatial coordinates of the "track" and provide the basis for subsequent chemical reactions. For heavy charged particles, the cross sections for production of secondary electrons become the source terms for track structure calculations. The mean free path between interactions is determined by the total ionization cross sections, the energy lost in each interaction is provided by the single differential cross section, $\sigma(\varepsilon)$ or $d\sigma/dQ$ (where ε is the ejected electron energy and Q is the energy loss given by $Q=\varepsilon+B$ with B equal to the electrons initial binding energy), and information required for the spatial characteristics of the track is contained in the doubly differential cross section, $\sigma(\varepsilon,\theta)$ or $d^2\sigma/dQd\Omega$ In addition, for heavy charged particles one needs to know the charge transfer cross sections, σ_{if}, in which the projectile changes from charge state i to f This is particularly important for ions with energy less than a few hundred keV per atomic mass unit where electron capture and loss become important processes affecting the energy loss.

For heavy charged particles, there is an increasing probability with particle charge that more than one electron may be ejected in a single interaction. This process produces multiple ionization/electron tracks that are correlated in time and may have special contributions to the subsequent chemical reactions and, thereby, to the biological damage. There is considerable data available, especially for gas phase targets, that contribute to our ability to develop accurate models of the structure of charged particle tracks. Combined with appropriate collision theory and a theoretical understanding of the effects of target structure, one can develop an extensive database of cross sections for track structure calculations. In particular one requires data for the range of projectiles and targets discussed above for the following cross sections

- Total ionization cross section σ_T
- Singly differential ionizations cross sections $\sigma(\varepsilon)$; $d\sigma/dE$
- Doubly differential ionization cross sections $\sigma(\varepsilon,\theta)$, $d^2\sigma/dQd\Omega$
- Charge transfer cross sections: σ_{if}
- Multiple ionization cross sections; σ^{if}
- Dissociation cross sections for molecular target

In principle, one would like information of the doubly differential, and singly differential, cross sections for emission of all electrons in multiple ionization and molecular dissociation processes. Also, information on photoionization and photoabsorption processes are required to provide initial photoelectron production cross sections for track structure calculations as well as to provide information on the oscillator strength of materials that contribute information on energy loss processes in condensed materials.

The needs for data for charged particle track structure simulation are extensive. A large database exists and additional data are being added from ongoing studies It is the recommendation of this Consultants' Group that the existing database for the particles, targets, and interactions indicated above be assembled, appropriately up-dated and when necessary extended, and made available in a "user friendly" manner to all Monte Carlo track structure applications

3.5. Data Availability

The cross section data are available from experiment and theory at widely different levels of precision and reliability, depending upon (1) the kinds of incident particles, (2) the materials, and (3) the kinds of cross sections Table 1a presents a summary of the data situation for electron impact To give an idea of the data quality, the following symbols are used: (a), meaning that the data are well established to the level of a few percent, (b), meaning that the data are based on incomplete information but are estimated with a reasonable level of confidence, (c), meaning that the data must be estimated from fragmentary information or incomplete theory, and (d), meaning that an estimation is highly tentative.

In general, the stopping cross section is best known, or can be estimated better than other cross sections. The stopping cross section is also the most decisive for analysis of the particle transport, and has been the subject of other tabulations (e.g. ICRU reports). The total (elastic plus inelastic scattering) cross section can be determined from measurements of beam attenuation, which have been carried out for H_2O vapor. The total elastic cross section and the total inelastic-scattering cross section are derivable from theory with fair accuracy. The differential elastic-scattering cross section has been measured for H_2O vapor, and has been also evaluated theoretically.

The differential cross section for ionization and excitation, as a function of energy loss of a particle, is called the energy-loss spectrum and has been measured for many materials at least for small scattering angles. Together with the photoabsorption cross section (which is closely related to the energy-loss spectrum for a fast charged particle), the energy-loss spectrum constitutes the most important and general source of data

The singly differential ionization cross section describes the energy distribution of secondary electrons resulting from an ionizing collision. A considerable volume of data is available for H_2O and basic organic molecules, from which data on DNA and proteins may be inferred. The singly differential ionization may be further classified into the partial cross sections, each of which corresponds to a particular electron shell or subshell that is ionized in a collision. Finally, the doubly differential ionization cross section characterizes an ionization process in full detail including the angle of electron ejection.

The multiple ionization cross section can be also characterized into higher levels of details, in terms of the number, kinetic energies, angles of ejection of secondary electrons, as well as of the quantum states of ions left behind In general, the data availability is less for cross sections of higher levels of details.

Table 1b shows a summary of the situation for protons, and Table 1c for heavier particles. Compared to electrons, the data are more incomplete for protons, and even more scarce for heavier particles

Some remarks are in order on the four materials listed. The meaning of the "H_2O vapor" is simplest; however, even here a qualification is necessary. We consider isolated H_2O molecules in the ground electronic state, but with rotational and vibrational energies corresponding to room temperature The "H_2O liquid" means water at room temperature and hence accomplished by rotational, vibrational, and librational energies as well as by intermolecular hydrogen bonds By "carbon" we mean here amorphous or microcrystalline carbon, prepared by evaporation and condensation on a solid surface. By "DNA" we mean here a mean chemical structure without precise specific actions of the base sequence and of conformation By "protein" we also mean a mean over many different chemical species.

Table 1a - Data availability for electrons

Kinds of cross sections / Materials	H_2O vapor	H_2O liquid	Carbon	DNA	Protein
Stopping	a	a	a	a	a
Total (elastic plus inelastic)	a	b	b	c	c
Total elastic	a	b	b	c	c
Differential elastic	a	c	b	c	c
Total inelastic	b	c	c	c	c
Total ionization	b	c	c	d	d
Differential in energy loss	a	b	a	b	b
Differential ionization	a	c	c	d	d
Partial ionization	a	c	d	d	d
Doubly differential ionization	b	d	d	d	d
Multiple ionization	b	c	d	d	d
Total excitation	b	c	d	d	d
Individual excitation (dissociation, etc.)	b	d	d	d	d

Table 1b - Data availability for protons

Kinds of cross sections / Materials	H_2O vapor	H_2O liquid	Carbon	DNA	Protein
Stopping	a	a	a	a	a
Total (elastic plus inelastic)	a	b	b	c	c
Total inelastic	b	c	c	c	c
Differential in energy loss	b	c	d	d	d
Total ionization	b	c	c	d	d
Differential ionization	b	c	c	d	d
Partial ionization	b	c	d	d	d
Doubly differential ionization	b	d	d	d	d
Multiple ionization	b	d	d	d	d
Total excitation	c	d	d	d	d
Individual excitation (dissociation, etc.)	d	d	d	d	d

Table 1c - Data availability for heavier ions

Kinds of cross sections / Materials	H_2O vapor	H_2O liquid	Carbon	DNA	Protein
Stopping	b	b	b	b	b
Total (elastic plus inelastic)	b	b	b	c	c
Total elastic	b	b	b	c	c
Differential elastic	c	c	c	c	c
Total inelastic	c	d	d	d	d
Differential in energy loss	b	c	d	d	d
Total ionization	c	d	d	d	d
Differential ionization	c	d	d	d	d
Partial ionization	c	d	d	d	d
Doubly differential ionization	c	d	d	d	d
Multiple ionization	c	d	d	d	d
Total excitation	d	d	d	d	d
Individual excitation (dissociation, etc.)	d	d	d	d	d

4. ESTABLISHMENT OF AN INTERNATIONAL REFERENCE A+M DATABASE FOR THE MONTE CARLO CODES: NEED, SCOPE AND OBJECTIVES OF AN IAEA CRP

The analysis performed by the participants of the present Meeting regarding the current status of the A+M data required in the Monte Carlo codes for track structure calculations have revealed existence of large discrepancies, uncertainties and gaps in the databases currently used in these codes. This state of the input information has significant impact on the accuracy of the results obtained by the codes On the other hand, there is a growing interest for an accurate description of the radiation induced subcellular damage (on the level of DNA, or its basic components) which can be best achieved by detailed Monte Carlo track structure calculations. This interest is strongly motivated by the needs for further development of our knowledge on the onset of biological effects of ionizing radiation, in particular for clarification and the study of some critical aspects of the radiation carcinogenesis.

In order to increase the reliability of Monte Carlo track structure calculations and enhance their relevance to radiobiological research, significant improvements must be introduced in the underlying physics of corresponding computational codes. These improvements are related, in the first place, to the completeness and accuracy of the A+M data for the most important physical processes, particularly the data information determining the spatial patterns of energy deposition in relevant target materials The amount of required data information to be compiled, critically assessed or generated for establishment of a complete and reliable A+M database of specified accuracy for the Monte Carlo computational codes is such that a concerted and well organized international effort is necessary for achieving this goal in a timely and cost efficient manner. The already available data information, accumulated expertise and developed data generation capabilities, make the feasibility of this task realistic on a timescale of three to five years. The IAEA A+M Data Unit, through its established co-operation links with the atomic physics community, elaborated data compilation and evaluation methodologies and the available data storage, processing and exchange/dissemination facilities (ALADDIN), its close co-operation with the international A+M Data Centre Network (comprising about 15 national data centres), seems to be in an extremely appropriate position to undertake the co-ordinating role in the implementation of this task Therefore, it would be highly beneficial for the advancement of radiobiological research if the Agency initiates in 1994 a Co-ordinated Research Programme (CRP) on the establishment of an "Atomic and Molecular Database for Radiation Induced Damage in Sub-Cellular Structures", with an initial duration of three years and anticipated extension for additional two years The scope of this CRP should include the processes and interacting species discussed in section 3 of the present report, and should concentrate on generating the currently missing data for the processes listed in the tables of section 3.5 The proposed CRP should also provide improved sets of data for those processes in section 3.5 for which the current data information is of inacceptably low accuracy. The CRP should also provide the necessary information on the condensed phase effects in the collected data.

The principal objectives of the proposed CRP are, therefore, to

(i) establish a complete, sufficiently accurate A+M database for the Monte Carlo codes which would make their predictive power compatible with the requirement in the current radiobiological research;

(ii) organize and present the reference database into a format which would allow easy implementation in the Monte Carlo codes;

(iii) develop a detailed understanding of all physical processes involved in the formation of various track structure patterns; and

(iv) develop a standard computational tool for description and analysis of radiation induced track structures on a subcellular level.

The structure of the institutions which should be invited to participate in the proposed CRP should reflect the following requirements for successful accomplishment of the CRP objectives:

- institutions with data collecting, evaluating and formatting potential (the IAEA A+M Data Unit, selected members of the international A+M Data Centre Network, other groups)

- institutions (or research groups) having experimental or theoretical capabilities for generating the required (missing, or of low accuracy) A+M data (atomic, molecular and radiation physics communities)

- institutions (or research groups) possessing operational Monte Carlo codes for track structure calculations (radiobiological community)

It is estimated that a number of 12 to 15 carefully selected collaborating institutions would be sufficient for accomplishment of the CRP objectives.

It is desirable that the proposed CRP be initiated as soon as possible. In view of the limited Agency resources to support this programme in its full extent, the Agency is encouraged to approach the Governments of the participating institutions, or other intergovernmental organizations, requesting extrabudgetary support to this CRP.

5. CONCLUSIONS AND RECOMMENDATIONS

Summarizing their work, the Meeting participants formulated the following conclusions and recommendations:

1) The Monte Carlo track structure computation codes are presently the only tool by which the radiation induced effects in biological substances can be studied on a sub-cellular level, essential for understanding the underlying mechanisms of biological effects of ionizing radiation.

2) The formation of track structure patterns, described by the Monte Carlo codes, critically depends on the atomic and molecular processes induced by the primary and secondary particles in the target material during the energy deposition process. (On sub-nanometer and nanometer levels, the form of track patterns can be closely related to the type of radiation induced damage of sub-cellular structures and correlated with the biological consequences)

3) Despite the large amount of collected atomic and molecular data information already introduced in the codes, there are still significant gaps in the required atomic and molecular database for realistic predictions and analysis of track structure patterns in substances of radiobiological interest The present atomic and molecular data content of Monte Carlo codes is also characterized by significant uncertainties with serious consequences on the reliability of obtained computational results

4) There is a strong need for establishing a comprehensive international reference database for the atomic and molecular processes involved in the physical problem considered and included in the structure of Monte Carlo codes The completeness and accuracy of this database should be on the level which would guarantee highly reliable code results for radiobiologically relevant target materials (such as DNA, in particular)

5) For establishing such a reference A+M database in a time scale compatible with the growing needs of radiobiological research (e g in radiation induced carcinogenesis), a concerted and well co-ordinated international effort has to be initiated as soon as possible Because of its already developed methodological and technical capabilities in the area of A+M data compilation, evaluation and generation, its close relations with the atomic physics community and co-ordinating role in the international A+M Data Centre Network, the International Atomic Energy Agency is best suited to undertake the co-ordination of this international effort

6) It is hereby strongly recommended that the IAEA initiate a five year Co-ordinated Research Programme on the establishment of a reference "Atomic and Molecular Database for Radiation Induced Damage in Sub-Cellular Structures" already in 1994. The scope and objectives of this CRP are outlined in the previous section of this report

7) Because of its high relevance to the current radiobiological research, and in particular to the radiation induced carcinogenesis, and in view of the size of the effort and limited Agency resources, the IAEA is encouraged to approach certain of its Member States (potential participants in this CRP) and request additional extrabudgetary support for this programme

Appendix 1

IAEA Consultants' Meeting on
Atomic and Molecular Data Needs for Monte Carlo Track Structure Calculations of Radiation Induced Damage in Biological Substances

IAEA Headquarter, Vienna, 11-12 November 1993
Meeting Room C04-51

MEETING AGENDA

Thursday, November 11

09.30 - 09:45 - Opening
- Adoption of Agenda

09:45 - 12:00 *) Analysis of atomic physics content of presen Monte Carlo codes for track structure calculations

12:00 - 14:00 **Lunch**

14:00 - 18:00 *) Required improvements in atomic physics database of Monte Carlo codes for enhancing their reliability and predictive power

Friday, November 12

09:00 - 12:00 *) Formulation of detailed atomic and molecular data requirements for improved Monte Carlo track structure calculations in specific biological substances (including requirements on the data format)

12:00 - 14:00 **Lunch**

14:00 - 17:30 *) Formulation of the scope and objectives of an IAEA CRP on this subject (to be initiated in 1994) including suggestions regarding CRP participants

*) 15 minutes coffee break is envisaged.

Appendix 2

IAEA Consultants' Meeting on
Atomic and Molecular Data Needs for Monte Carlo Track Structure Calculations of Radiation Induced Damage in Biological Substances

IAEA Headquarter, Vienna, 11-12 November 1993
Meeting Room C04-51

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