Phys. Med. Biol. 42 (1997) 1441–1449. Printed in the UK PII: S0031-9155(97)75589-1

Numerical calculation of energy deposition by high-energy electron beams: III-B. Improvements to the 6D phase space evolution model

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Received 7 June 1996, in final form 10 January 1997

Abstract. The phase space evolution model of Huizenga and Storchi, Morawska-Kaczyńska and Huizenga and Janssen *et al* has been modified to (i) allow application on currently available computer equipment with limited memory (128 Megabytes) and (ii) allow 3D dose calculations based on 3D computer tomographic patient data. This is a further development aimed at the use of the phase space evolution model in radiotherapy electron beam treatment planning. The first modification regards the application of *depth evolution* of the phase space state combined with an alternative method to transport back-scattered electrons. This depth evolution method requires of the order of 15 times less computer memory than the *energy evolution* method. Results of previous and new electron transport methods are compared and show that the new electron transport method for back-scattered electrons hardly affects the accuracy of the calculated dose distributions. The second modification regards the simulation of electron transport through tissues with varying densities by applying *distributed electron transport* through similarly composed media with a limited number of fixed densities. Results of non-distributed and distributed electron transport are compared and show that the distributed electron transport method hardly affects the accuracy of the calculated dose distributions. It is also shown that the results of the new dose distribution calculations are still in good agreement with and require significantly less computation time than results obtained with the EGS4 Monte Carlo method.

1. Introduction

The present work is a continuation of (i) 'Numerical calculation of energy deposition by broad high-energy electron beams' by Huizenga and Storchi (1989, paper I), (ii) 'Numerical calculation of energy deposition by broad high-energy electron beams: II. Multi-layered geometry' by Morawska-Kaczyńska and Huizenga (1992, paper II) and (iii) 'Numerical calculation of energy deposition by high-energy electron beams: III. Three-dimensional heterogeneous media' by Janssen *et al* (1994, paper III). In paper I the principles of the phase space time evolution model (PSTE model) for depth dose calculations for broad high-energy electron beams were presented as the extended version of the PSTE model by Cordaro and Zucker (1971). The model is based on the various interactions of electrons with matter resulting in electron energy loss, scattering and secondary-electron and bremsstrahlung production. Paper II describes the extension of the model to depth dose calculations in multi-layered geometries as well as a formal generalization of the theory. Paper III describes the extension of the model to a full three-dimensional model for dose calculations in arbitrarily

0031-9155/97/071441+09$19.50

composed heterogeneous media irradiated with arbitrary electron beams. The present work describes two modifications to the phase space evolution (PSE) model presented in paper III.

The first modification is the application of the depth evolution method, which in combination with an alternative model to transport back-scattered electrons results in a major reduction in required computer memory without loss of accuracy. This reduction in memory requirements is necessary because the memory required by the phase space energy evolution method, as described in paper III, exceeds the amount of available memory on most present-day workstations if clinical electron beam dose calculations are pursued. The phase space depth evolution method still requires a large amount of memory for clinical cases, but these memory requirements are within reasonable limits (128 Megabytes).

The PSE model as described in paper III can only perform dose calculations in 3D media composed of block heterogeneieties, where the materials are chosen from a limited set (e.g. water, water with density 0.5, aluminium, lead). The second modification is the simulation of electron transport through tissues with varying densities by distributed electron transport through similarly composed media with a limited number of fixed materials. This modification allows dose calculations in 3D patient geometries based on CT data without loss in accuracy.

2. Theory

The notion of some concepts introduced in paper III is required to understand the modifications presented in this paper. A concise notion of the required concepts is as follows. (i) The state of a patient or phantom with respect to irradiation is defined by the positions, the kinetic energies and the propagation directions of electrons with an energy above thermal in the phantom. (ii) The PSE model for electron beam dose calculations simulates the evolution of this state from an initial state via a sequence of non-empty states to a final or empty state. (iii) The initial state is defined by the positions, the energies and the directions of all high-energy electrons applied in the treatment, when entering the phantom or a predefined plane in front of the phantom. (iv) The final or empty state indicates the end of the evolution, when all high-energy electrons propagating through the phantom have lost their kinetic energy or have left the phantom. (v) Discretization of positions, energies and directions allows grouping of electrons which belong to the same position–energy–direction interval, thus allowing the implementation of the state with a 6D array with dimensions x, y, z, E, Θ and Φ identifying the positions, energies and directions of the electrons. (vi) Phasel is short for 'phase space element' or array element. Each phasel is associated with a mono-energetic and mono-directional electron pencil beam at a certain position. The content of a phasel (or array element) is the number of electrons in the corresponding position–energy–direction interval.

The PSE model simulates the transport of electrons which belong to the same phasel by distributing the content of that phasel over all other phasels. The distribution of the contents of a number of phasels results in the evolution of the state to another state. Several 'phase space evolution methods' can be applied to control the evolution of the state. In order to evolve from one state to the next state in the sequence, the contents of a subset of the total set of phasels are distributed. Application of various PSE methods to distribute the contents of different subsets of phasels results in different sequences of states between the initial and the final empty state. Any choice of subset of non-empty phasels, of which the contents are to be distributed in order to evolve the state to the next state, is allowed. This freedom of choice is based on the independence of electron transport which can be stated

as follows: *The transport of electrons through a medium is independent of the transport of other electrons through that medium and independent of the moment in time at which they are transported.*

In paper III two methods are described which control the evolution of the state, (i) the phase space time evolution (PSTE) method, which results in a sequence of states representing the state of the phantom at distinct successive moments in time and (ii) the phase space energy evolution (PSEE) method, which results in a sequence of states representing the state of the phantom at distinct successive maximum energy levels. The dose distributions calculated with these methods are exactly the same, since both methods apply the same electron transport model. Since the PSEE method is faster, and requires less computer memory, this method is preferred over the PSTE method.

Although the PSEE method requires only half the amount of computer memory that the PSTE method does, it still requires too much memory for clinical application. As an example, consider (i) a phantom size of $20 \times 20 \times 15$ cm^3 (xyz) with a voxel size of $0.5 \times 0.5 \times 0.5$ cm^3, (ii) a maximum electron energy of 20 MeV with an energy interval size of 0.5 MeV and (iii) 80 directions formed by combining ten polar angles with eight azimuth angles. All possible phasel contents are administrated with a 6D array with dimensions x, y, z, E, Θ and Φ. This array contains $41 \times 41 \times 31 \times 40 \times 10 \times 8 = 167$ million real numbers which occupy 667 Megabytes computer memory (4 bytes/real). Most present workstations do not contain such large amounts of computer memory. The PSE method which we propose, which substantially reduces the amount of computer memory required, is the phase space depth evolution (PDSE) method.

2.1. The phase space depth evolution method

In the PSDE method proposed in this paper the subset of phasels corresponding to *one* depth layer in the phase space state is distributed to evolve the state to the next state. Here, a depth layer corresponds to a plane perpendicular to the beam axis. In the PSE model the z-axis coincides with the beam axis. This implies that obliquely incident electron beams are implemented by tilting the phantom with respect to the beam, instead of tilting the beam with respect to the phantom. The PSDE method will result in a sequence of states which describes electrons with distinct successive minimum penetration depths in the phantom if and only if two conditions are satisfied. These two conditions are (i) the initial state describes the electrons in the top layer of the phantom and (ii) all electrons in a state move downwards to greater depths in the phantom. The first condition is evidently satisfied since the initial state is defined by the positions, the energies and the directions of all electrons applied in the treatment, when entering the phantom or a predefined plane in front of the phantom. The second condition is not strictly satisfied. Most of the electrons move downward, but a small percentage of the electrons scatter backwards with respect to the beam axis towards the surface of the phantom.

The second condition can be satisfied if all back-scattered electrons are removed from all of the states (z-layers) before these states evolve into the next state. The backward moving electrons which are removed from a state cannot be neglected, since they will contribute to the dose distribution in the phantom, but they can be handled separately. The transport of the relatively small fraction of back-scattered electrons which is removed from the states is simulated with an alternative method based on average energy losses according to the product of total stopping power and average path length. Electrons moving backward with a polar angle between 90 and 180° deposit their energy according to this alternative method along the straight line given by their specific direction. There are two reasons why the

application of this alternative method to transport back-scattered electrons will only have minor effects on PSE calculated dose distributions.

(i) The fraction of back-scattered electrons is small in comparison with the total number of electrons contributing to energy deposition. Comparisons between full PSE calculations and PSE calculations in which back-scattered electrons are even completely removed from contributing to the dose distribution show differences in total deposited energy (MeV) of about 2%, resulting in local errors in dose (MeV g^{-1}) with a maximum of 3%. Therefore, the local errors in a dose distribution caused by the proposed alternative method to simulate the transport and energy deposition of back-scattered electrons is expected to be one order of magnitude less.

(ii) The proposed alternative method to handle back-scattered electrons is almost the same as the method already applied by the PSE model to transport very low phasel contents. Normally, in the PSE model, electrons are distributed according to the combination of three distribution functions describing motion, energy loss and scattering, but in order to restrict the computation time required by the PSE model scattering is switched off if the fractions of electrons to be distributed are relatively small. This means that in the PSEE (and PSTE) method small fractions of forward travelling or back-scattered electrons are distributed according to the combination of two distribution functions describing motion and energy loss without any change in transport direction. In the PSDE method small fractions of forward travelling electrons are still distributed according to the combination of the two distribution functions describing motion and energy loss without any change in transport direction. Furthermore, in the PSDE method all fractions of back-scattered electrons are distributed according to the aforementioned alternative method. This means that in the PSDE method all fractions of back-scattered electrons are distributed according to the combination of two distribution functions describing motion and average energy loss without any change in transport direction. In the PSDE method the difference between distributing small fractions of forward travelling electrons and distributing all fractions of back-scattered electrons is the applied distribution function for energy loss. For distributing small fractions of forward travelling electrons the energy distribution function is applied, which accurately describes the associated distribution over the full energy range (Huizenga and Storchi 1989, Korevaar *et al* 1996). When distributing all fractions of back-scattered electrons, the electron energy decreases by the product of path length and total stopping power. For the relatively small fractions of back-scattered electrons this difference is not expected to affect the calculated dose distribution significantly.

The PSE model would lose an advantage over Fermi–Eyges based models if the errors introduced by the application of the alternative method to transport back-scattered electrons were too large. One obvious problem for electron beam models based on the (small-angle) Fermi–Eyges multiple-scattering theory is that they are oblivious to back-scattering of electrons (Jette 1995 and references therein). In principle, the PSE model does not ignore back-scattered electrons: it treats back-scattered and forward (small- and large-angle) electrons in a similar way. The PSE model could therefore, in principle, yield more accurate dose distributions than Fermi–Eyges based models. With this in mind, it seems illogical to pursue a method which interferes with the handling of back-scattered electrons in the PSE model. However, there is one major advantage of the PSDE method in comparison with the PSTE and PSEE methods if the errors introduced by the application of the alternative method to transport back-scattered electrons are negligible. The advantage of the PSDE method with respect to the PSEE and PSTE method is that it requires substantially less computer memory. To perform the evolution of the state, the PSDE method requires two

5D phase space arrays with dimensions x, y, E, Θ and Φ. One of these arrays is required to keep the initial state representing electrons in one z-layer, the other 5D array is required to gather the result of the distribution into the next state (z-layer). The implementation of two of these 5D phase space arrays requires only 43 Megabytes for the example given above instead of the 667 Megabytes required by the PSEE method to implement one 6D phase space array.

2.2. Electron transport through tissues with varying densities

The PSE model simulates the transport of electrons which belong to the same phasel by distributing the content of that phasel over all other phasels. The distribution functions which control this process differ for each combination of initial electron energy, propagation direction and voxel material. Distribution functions are calculated based on data associated with a specific voxel material. These data consist of the density ρ, effective atomic number $\langle Z \rangle$, effective atomic mass $\langle A \rangle$, effective $\langle Z/A \rangle$, mass absorption coefficient μ_{en}/ρ and mass collisional and radiative stopping powers S_{col}/ρ and S_{rad}/ρ of the voxel material (Huizenga and Storchi 1989). Densities of tissues in the human body are in the range from $\rho = 0$ g cm^{-3} to $\rho = 2$ g cm^{-3}: air, $\rho = 0.0012$ g cm^{-3}; lung, $\rho = 0.3$ g cm^{-3}; water, $\rho = 1.0$ g cm^{-3}; cortical bone, $\rho = 1.92$ g cm^{-3} (ICRU 1984, 1989). Tissues with densities in the range $0.25 \leqslant \rho \leqslant 1.1$ (g cm^{-3}) are generally considered to be water equivalent. The data of water equivalent material are identical to the data of water ($\rho = 1.0$ g cm^{-3}) with an adjusted density. It is assumed that tissues with densities in the range $1.1 < \rho \leqslant 1.92$ (g cm^{-3}) are well simulated with mixtures of cortical bone and water. This assumption is supported by comparing theoretically the stopping and scattering powers of human bones with bone–water mixtures with equal density. Except for the dependence on electron energy the collisional stopping powers and scattering powers of a material depend primarily upon $\langle Z/A \rangle$ and $\langle Z^2/A \rangle$ respectively (Klevenhagen 1993). For example, the stopping and scattering powers of a bone–water mixture with a density of 1.5 g cm^{-3} are 1.1% higher and 3.3% lower respectively than those for a human bone with the same density (humerus shaft; White *et al* 1987). If, on the other hand, humerus shaft is simulated by a material with the same properties as cortical bone with an adjusted density (1.5 g cm^{-3}), the stopping and scattering powers become 2.3% too low and 15% too high respectively. The errors introduced by simulating human bone with a mixture of cortical bone and water are considered to be acceptable or in any case preferable to the errors introduced by simulating human bone with cortical bone with an adjusted density. The data of a bone–water mixture are determined from the published data of cortical bone ($\rho = 1.92$ g cm^{-3}) and water ($\rho = 1.0$ g cm^{-3}) according to the ratio of water and cortical bone required to obtain the density of the mixture.

The distribution functions describe point kernels which are the result of transporting (a unit number of) electrons from a particular phasel to surrounding phasels. The calculation of the distribution functions is rather time consuming. To relieve the PSE program from these calculations a separate program PRECAL was developed to calculate the distribution functions in advance and to store them on disk for further use by the PSE program. The distribution functions were pre-calculated for a limited number of materials (e.g. air, water, water with density 0.5, cortical bone, bone with density 1.5). However, the materials of voxels defined by a patient geometry based on CT data are not restricted to the limited set of pre-calculated materials. Therefore, not all the required distribution functions are pre-calculated. The PSE model has been modified to simulate electron transport through tissues with varying densities applying the pre-calculated distribution functions for a limited number

of materials only. The transport of a fraction of electrons f through a voxel containing a material with arbitrary density ρ is simulated by a *distributed electron transport method* which is described as follows.

(i) Two materials are chosen from the set of materials for which pre-calculated distribution functions exist. The choice of the two materials depends on their respective densities ρ_l and ρ_h which have to be as close to ρ as possible such that $\rho_l \leqslant \rho \leqslant \rho_h$

(ii) The fraction of electrons f which has to be transported through the voxel is divided into two fractions $w_l f$ and $w_h f$ such that $\rho = w_l \rho_l + w_h \rho_h$. With $w_l + w_h = 1$ this results in $w_l = (\rho_h - \rho)/(\rho_h - \rho_l)$ and $w_h = (\rho - \rho_l)/(\rho_h - \rho_l)$.

(iii) The transport of the electron fraction f through the voxel containing the material with density ρ is simulated by the transport of electron fractions $w_l f$ and $w_h f$ according to the pre-calculated distribution functions specific for voxels containing materials with densities ρ_l and ρ_h respectively.

The intended effect of this distributed electron transport method is to simulate the transport of electrons as if pre-calculated distribution functions for a voxel material with density ρ were available. If the spacing between the material densities for which pre-calculated distribution functions are available is small, the effect of this method is certainly close to the intended effect, but a relatively small spacing between material densities requires (i) a larger amount of hard-disk space to store all pre-calculated distribution functions and (ii) a larger amount of computer memory for the PSE program to handle all pre-calculated distribution functions. The pre-calculated distribution functions for one specific material occupies about 0.1 Megabytes hard-disk space. Within the PSE program these pre-calculated distribution functions are expanded and occupy about 0.5 Megabytes of computer memory. The results in the next section will show that pre-calculated distribution functions for 13 different materials are sufficient for adequate simulation of electron transport through geometries based on CT data.

3. Results

The PSE model has been applied to examine the effect of the proposed modelling of the transport of back-scattered electrons and the proposed distributed electron transport method to simulate electron transport through tissues with varying densities.

Table 1. Maximum local errors (%) in dose relative to dose maximum, introduced by alternative methods to transport back-scattered electrons in different geometries.

	Pure water	Aluminium slab	Air slab
Back-scattered electrons ignored/removed	3.0	2.5	1.8
Back-scattered electrons with alternative method	< 0.1	< 0.1	< 0.1

3.1. The transport of back-scattered electrons

The dose distribution resulting from a 20 MeV parallel 5 × 5 cm^2 electron beam has been calculated for three different geometries, (i) a pure water phantom, (ii) a water phantom containing a half-slab aluminium of thickness 1.5 cm located between 2 and 3.5 cm depth and (iii) a water phantom containing a half-slab of air of thickness 1.5 cm located between 2

and 3.5 cm depth. The PSE model has been applied to calculate the dose distributions for all three geometries incorporating three different methods to transport back-scattered electrons (i) ignoring/removing all back-scattered electrons, (ii) with the alternative method as applied in the PSDE method and (iii) with the original full distribution of back-scattered electrons as applied in the PSEE and PSTE methods. Table 1 shows maximum local errors in dose (MeV g^{-1}) caused by the alternative methods (i) and (ii) in comparison with method (iii). The results show that (i) back-scattered electrons cannot be neglected in accurate electron beam dose calculation models and (ii) the errors introduced by the alternative method to transport back-scattered electrons are negligible. Therefore, there is no objection to apply the PSDE method in combination with the alternative method to transport back-scattered electrons in the PSE model.

3.2. The distributed electron transport method

The dose distribution resulting from a 20 MeV parallel 5×5 cm^2 electron beam has been calculated for several water phantoms containing a half-slab of thickness 1.5 cm located between 2 and 3.5 cm depth of a material with a density between 0.25 and 1.92 g cm^{-3}. Tissues with a density between 0.25 and 1.1 g cm^{-3} are considered to be water equivalent material. Tissues with a density between 1.1 and 1.92 g cm^{-3} are considered to be a mixture of water and cortical bone as described above. The PSE model has been applied to calculate the dose distributions for the geometries incorporating two different methods to simulate the electron transport through the voxels which belong to the slab, (i) applying distribution functions especially pre-calculated for electron transport through materials with that arbitrary density and (ii) applying the distributed electron transport method for simulating electron transport through tissues with varying densities and using only already available pre-calculated distribution functions. A comparison between the two methods show that maximum errors in dose (MeV g^{-1}) introduced by the second method are smaller than 0.2% if pre-calculated distribution functions are available for (i) water equivalent materials with densities of 0.25, 0.30, 0.40, 0.50, 0.60, 0.80, 1.00 and 1.10 g cm^{-3}, (ii) water–cortical bone mixtures with densities of 1.10, 1.30, 1.60 and 1.92 g cm^{-3} and (iii) air. These results show that the PSE model can simulate the transport of electrons through tissues with varying densities with only a minor loss in accuracy if pre-calculated distribution functions are available for the 13 materials mentioned.

The results shown so far are obtained by comparing PSE calculations based on different electron transport methods with each other. There is also a good agreement between PSE and Monte Carlo results. Figure 1 shows a comparison between dose distributions calculated by the PSE program XYZET incorporating the two modifications mentioned and the EGS4 Monte Carlo program (Nelson *et al* 1985). The EGS4 dose calculations are performed with the EGS4 code called XYZDOS (Bielajew and Rogers 1992) with two million histories, using ESTEPE = 0.04, ECUT = 0.7 MeV, PCUT = 0.01 MeV and the PRESTA algorithm (Bielajew and Rogers 1987). The resolution for both PSE and MC calculations of the dose distribution is $0.5 \times 0.5 \times 0.5$ cm^3. The standard errors of the EGS4 calculations are between 1 and 2% of dose maximum. The differences between XYZET and EGS4 in dose values or isodose lines are typically less than 1% or 1 mm respectively. XYZET requires ten times less computation time than EGS4 for the calculation shown.

For clinical electron beam dose calculations the PSE model requires an initial phase space as input. This initial phase space is the description of a clinical electron beam in terms of energy and angular distribution in a plane perpendicular to the beam axis between applicator and patient. Both dose distributions shown in figure 1 are based on the same

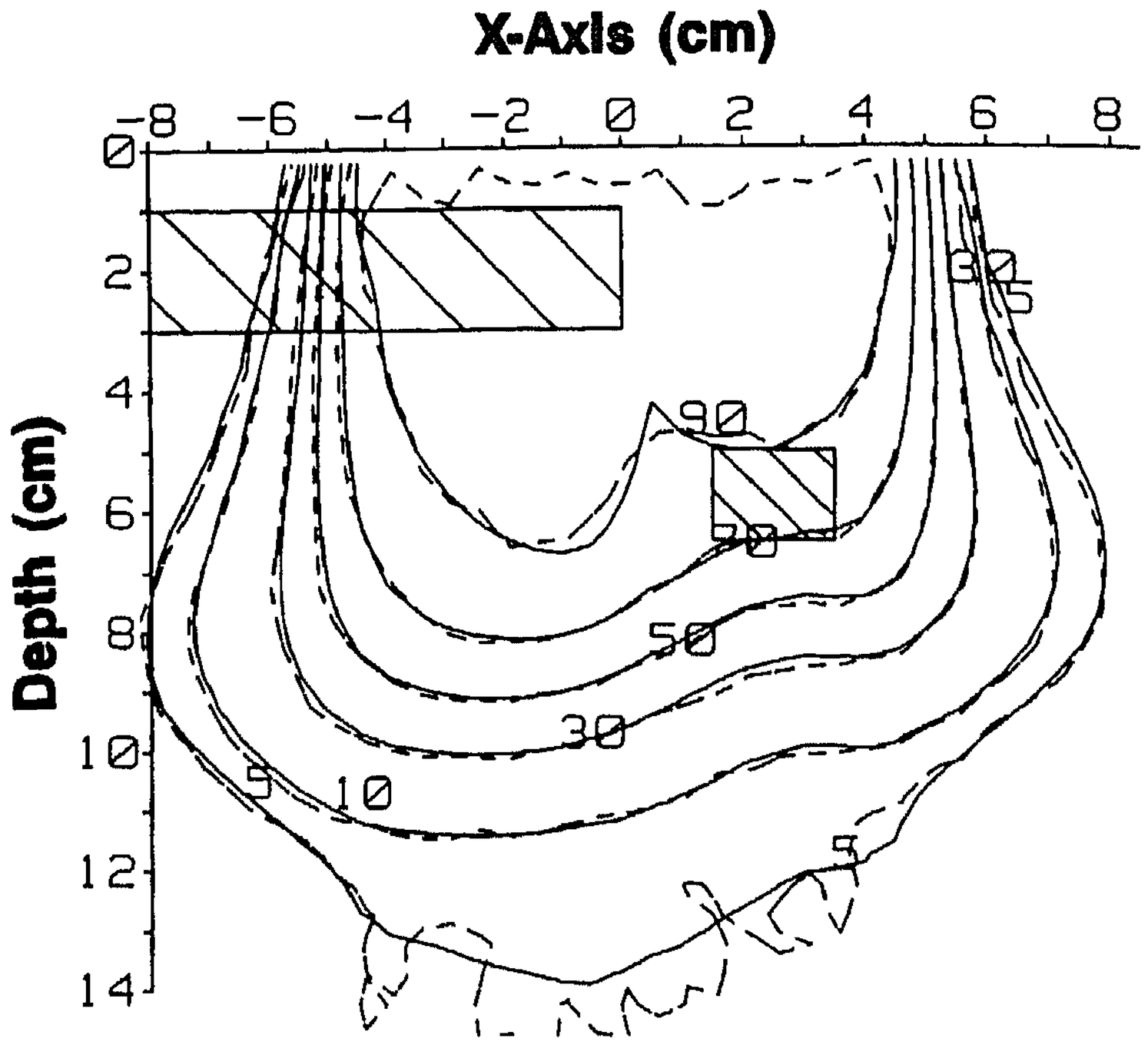

Figure 1. The dose distribution of a 21 MeV 10 × 10 cm^2 Siemens KD2 electron beam in a water phantom containing two water equivalent heterogeneities of 0.4 g cm^{-3} and 1.5 g cm^{-3}: solid lines, XYZET; dashed lines, EGS4.

initial phase space of a clinical electron beam. Research is on-going to determine the initial phase space of a clinical electron beam from a measured depth dose curve and a set of measured profiles (Korevaar *et al* 1995).

4. Conclusions

Dose distributions calculated with the PSE model utilizing the PSDE method and applying the alternative method to simulate back-scattered electron transport show negligible errors in comparison with dose distributions calculated with the PSEE (or PSTE) method. Since the PSDE method requires substantially less computer memory, without loss in accuracy or requiring more computation time, this method is to be preferred over the PSTE and PSEE methods. The application of the distributed electron transport method to simulate electron transport through tissues with varying densities shows only a minor loss in accuracy. The PSE model incorporating the mentioned modifications allows full 3D electron beam dose calculations based on 3D computer tomographic patient data on computers with a memory of 128 Megabytes.

Acknowledgments

The authors thank Professor A Hermans (Delft University of Technology) for stimulating discussions. Two of the authors (JJJ and EWK) acknowledge a grant (NKB 92-94) from the Dutch Cancer Society.

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