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A User's Guide to CEPXS/ONELD Version 1.1

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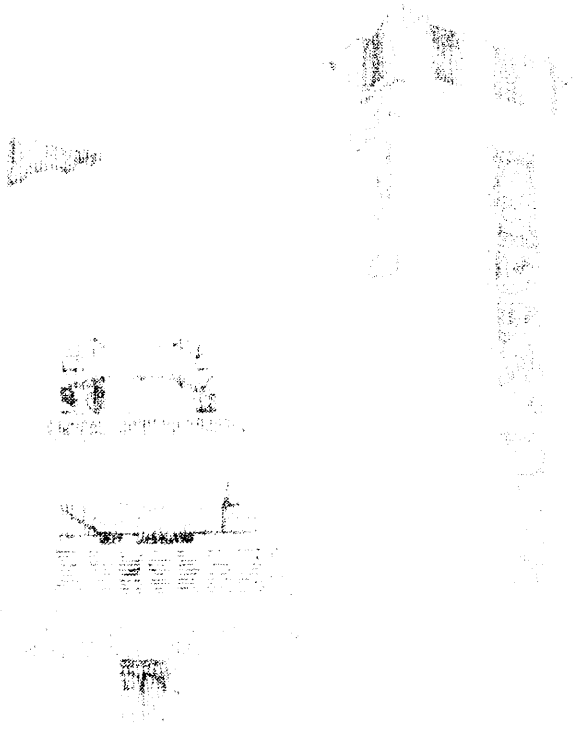

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A USER'S GUIDE TO CEPXS/ONELD VERSION 1.1

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ABSTRACT

This is the user's guide to CEPXS/ONELD Version 1.1, a code package for coupled electron-photon transport in one-dimensional slab geometry. The code package consists of the multigroup cross-section generating code, CEPXS; the preprocessor code, PRE1D; the discrete ordinates code, ONELD; and the postprocessor code, POST1D. In Version 1.1, new features have been implemented through several new keywords. Since Version 1.0 keywords are still applicable, this document should be considered as an addendum to the Version 1.0 User's Guide.

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I. NEW KEYWORDS

CEPXS/ONELD uses keyword input. The keywords for the original version of the code are described in the CEPXS/ONELD Version 1.0 User's Guide [LJLOREN1]. While Version 1.1 introduces several new keywords, earlier keywords are still applicable. Hence this document should be considered as an addendum to the Version 1.0 User's Guide. Another change in Version 1.1 is that a single output file (called "posto") is created rather than several output files as in Version 1.0. Further information on CEPXS/ONELD Version 1.0 is contained in the Physics Guide [LJLOREN2] and the Results Guide [LJLOREN3].

The new keywords that have been introduced in CEPXS/ONELD Version 1.1 are summarized below. Alphanumerical parameters are indicated by "p1, p2," etc. A string of numerical data separated by blanks is indicated by "(string)." A data string should be confined to a single line.

KEYWORD	DESCRIPTION
INTERNAL-SPECTRA p1 (string)	This keyword is used to obtain the electron and photon spectra differential in energy at interior positions. The mandatory parameter is the number of interior positions at which the internal spectra is desired. These positions appear in a data string on the subsequent line. Interior positions are measured in centimeters relative to the start of the first layer. For an internal spectrum to be obtained, the CURRE keyword must also be specified under OUTPUT.
MATERIAL **DETECTOR**	Any material may be designated as a detector material by the secondary keyword DETECTOR. A material may be a detector material and still be used in the transport calculation. The only effect of designating a material as a detector material is that, when the EQDEP option is used under OUTPUT, the kerma or equilibrium dose for all detector materials is obtained everywhere. This keyword is relevant only for photon sources. Kerma is obtained by folding the photon flux into the linear energy absorption coefficient of a detector material. Hence, the kerma profile for a detector material represents the dose that would be deposited in a layer of this material at each position provided that this

layer is thin to photons (so that the flux is unperturbed,) thick to electrons (so that the kerma can represent the dose,) and is surrounded by the materials that are actually used in the transport calculation.

OUTPUT This keyword controls what output appears in the "posto" output file produced by the POST1D code.

CDEP The output file will contain the spatial profile of charged-particle deposition. If the keyword POSITRONS is absent, charged-particle deposition is the number of electrons and positrons deposited. If the keyword POSITRONS is used, charged-particle deposition is the number of electrons deposited less the number of positrons deposited.

CURRE The output file will contain the reverse and forward spectra differential in energy at the exterior interfaces for all particle species.

CURREA The output file will contain the spectra differential in both energy and angle at the exterior interfaces for all particle species.

CURRX The output file will contain the spatial profiles of the electron and photon number currents in both forward and reverse directions.

EDEP The output file will contain the spatial profile of the dose.

EQDEP The output file will contain the kerma or equilibrium dose profile for all detector materials. A kerma profile is also obtained for the material geometry specified. This keyword is relevant only for photon sources.

PEQE When this keyword is specified, pair secondaries are produced but positrons are not distinguished from electrons. This allows energy to be redistributed properly but distorts charge transfer. (This was the default in Version 1.0 of CEPXS/ONELD.)

If neither this keyword or the POSITRONS keyword is specified, the default is that pair secondaries are not produced. The default case allows allows charge transfer to be approximately correct but distorts energy transfer.

As in Version 1.0, the user can avoid energy and charge distortions by using the keyword POSITRONS. In this case, pair secondaries are produced and the positrons are tracked as separate particles. The only disadvantage of using the POSITRONS keyword is that significantly more memory may be required by CEPXS/ONELD which may be troublesome for users who do not have access to large mainframe computers.

II. KERMA

Kerma represents the dose that would be deposited locally if secondary electron transport is neglected [CHILTON]. In a kerma calculation, only energy in the form of photon radiation is allowed to escape from the site of the photon interaction. Since photon transport is allowed, this energy can be redistributed in the system. A fraction of the electron energy is also considered to be radiative. This is the energy that the electron radiates as bremsstrahlung in the course of slowing down. (For kerma, the secondary electrons are assumed to slow down without transport.)

In order to predict the kerma or equilibrium dose, CEPXS calculates the linear energy absorption coefficient, μ^{en}, for all materials. This coefficient is composed of contributions from incoherent, photoelectric and pair interactions:

$$\mu^{en} = \mu^{C} + \mu^{PE} + \mu^{PP}$$

The linear energy absorption coefficient due to incoherent interactions is:

$$\mu^{C}(E) = \sigma^{C}(E)\, E - \int dE'\, E'\, \sigma^{C}(E \to E') - \int d\epsilon\, \epsilon\, Y(\epsilon)\, \sigma^{C}(E \to \epsilon)$$

where:

σ^{C} = Total Incoherent Cross Section

E = Energy of the interacting photon

E' = Energy of the photon after incoherent scattering

ϵ = Electron energy

$Y(\epsilon)$ = Radiation Yield [ICRU] for an electron of energy ϵ

$$= \frac{1}{\epsilon} \int_0^{\epsilon} d\epsilon' \left[S_{col}(\epsilon') + S_{rad}(\epsilon') \right]^{-1} S_{rad}(\epsilon')$$

where S_{rad} is the radiative stopping power and

S_{col} is the collisional stopping power

The linear energy absorption coefficient due to photoelectric interactions is:

$$\mu^{PE}(E) = \sigma^{PE}(E)\ E - \sum_i \eta_i^f\ \sigma^{PE}\ E_i^{FL} - \sum_j \eta_j^e\ \sigma^{PE}\ \epsilon_j^A\ Y\left(\epsilon_j^A\right) - \sum_k \chi_k(E)\ \sigma^{PE}\ \epsilon_k^{PE}(E)\ Y\left(\epsilon_k^{PE}\right)$$

where:

σ^{PE} = Total Photoelectric Cross Section

η_i^f = Relaxation Efficiency for a fluorescence photon of type i

η_j^e = Relaxation Efficiency for an Auger electron of type j

E_i^{FL} = Energy of a fluorescence photon of type i

E_j^A = Energy of an Auger electron of type j

$\epsilon_k^{PE}(E)$ = Energy of a photoelectron from shell k produced by a photon of energy E

$\chi_k(E)$ = The probability that a photon of energy E ionizes shell k

The linear energy absorption coefficient due to pair interactions is:

$$\mu^{PP}(E) = \sigma^{PP}(E)\ E - 2\ \sigma^{PP}\ E^{AN} - \int d\epsilon\ \sigma^{PP}(E\rightarrow\epsilon)\ \epsilon\ Y(\epsilon)$$

where:

σ^{PP} = Total Pair Interaction Cross Section

E^{AN} = Energy of annihilation radiation (.511 MeV)

The kerma or equilibrium dose, κ, in units of MeV/g is:

$$\kappa = \int dE \quad \psi(E) \frac{\mu^{en}(E)}{\rho}$$

where:

μ^{en} = linear energy absorption coefficient (MeV/cm)

ρ = material density (g/cm^3)

ψ = photon flux ($photons/cm^2$)

The photon flux includes the source photons as well as secondary photons produced by bremsstrahlung and fluorescence interactions. The photon flux is obtained from a full transport calculation in which both photons and electrons are transported.

III. REFERENCES

[CHILTON] A. B. Chilton, J. K. Shultis, and R. E. Faw, Principles of Radiation Shielding, (1984).

[ICRU] Stopping Powers for Electrons and Positrons, ICRU Report 37 (1984).

[LJLOREN1] L. J. Lorence, Jr., J. E. Morel, and G. D. Valdez, "User's Guide to CEPXS/ONEDANT: A One-Dimensional Coupled Electron-Photon Discrete Ordinates Code Package Version 1.0," SAND89-1661 (1989).

[LJLOREN2] L. J. Lorence, Jr., J. E. Morel, and G. D. Valdez, "Physics Guide to CEPXS: A Multigroup Coupled Electron-Photon Cross Section Generating Code Version 1.0," SAND89-1685 (1989).

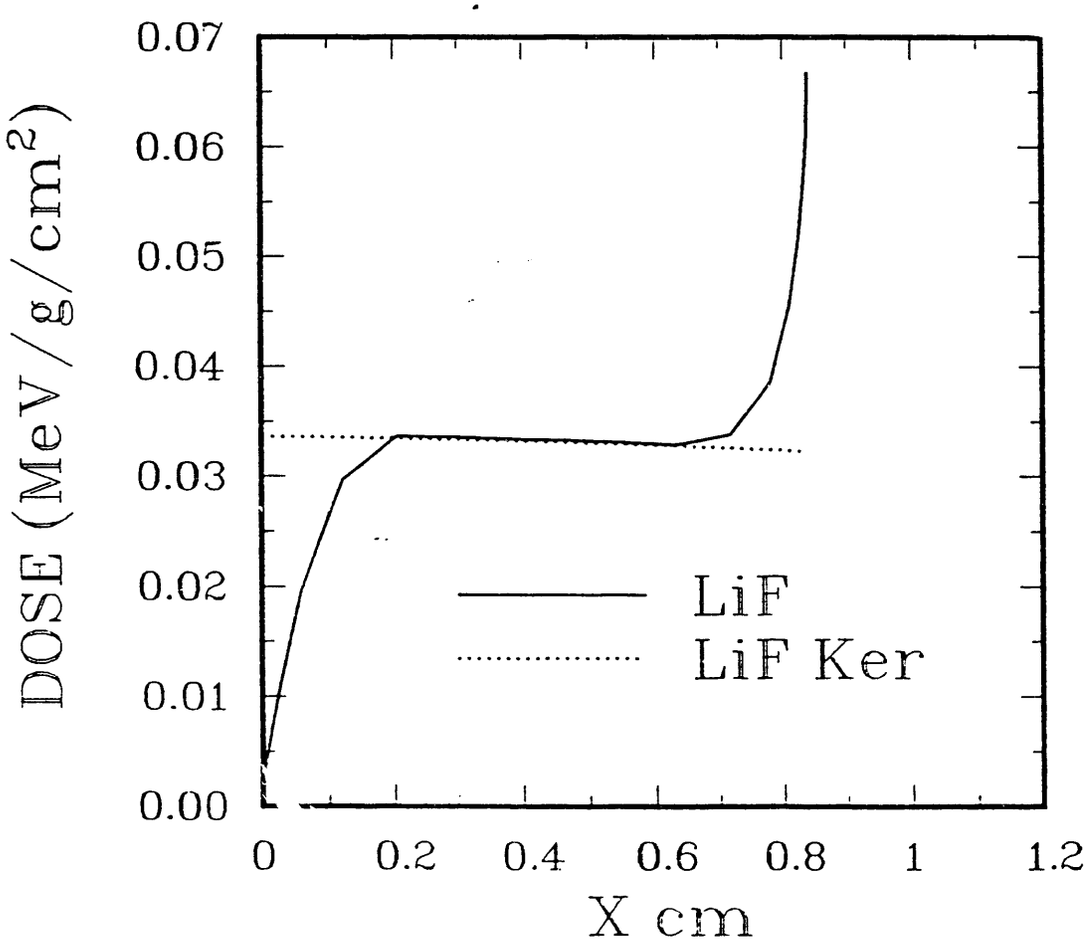
[LJLOREN3] L. J. Lorence, Jr., J. E. Morel, and G. D. Valdez, "Results Guide to CEPXS/ONELD: A One-Dimensional Coupled Electron-Photon Discrete Ordinates Code Package Version 1.0," SAND89-2211 (1990).

```
TITLE
Example #2A
MATERIAL LI .2675 F .7325
 DENSITY 2.635
MATERIAL PB
 DETECTOR
ENERGY 1.33
CUTOFF .01
PHOTON-SOURCE
 FULL-COUPLING
LEGENDRE 15
GEOMETRY 1
 1 10 1.0 10
ELECTRONS
 LINEAR 50
PHOTONS
 LINEAR 30
DIRECTION
 NORMAL
OUTPUT
 EDEP
 EQDEP
```

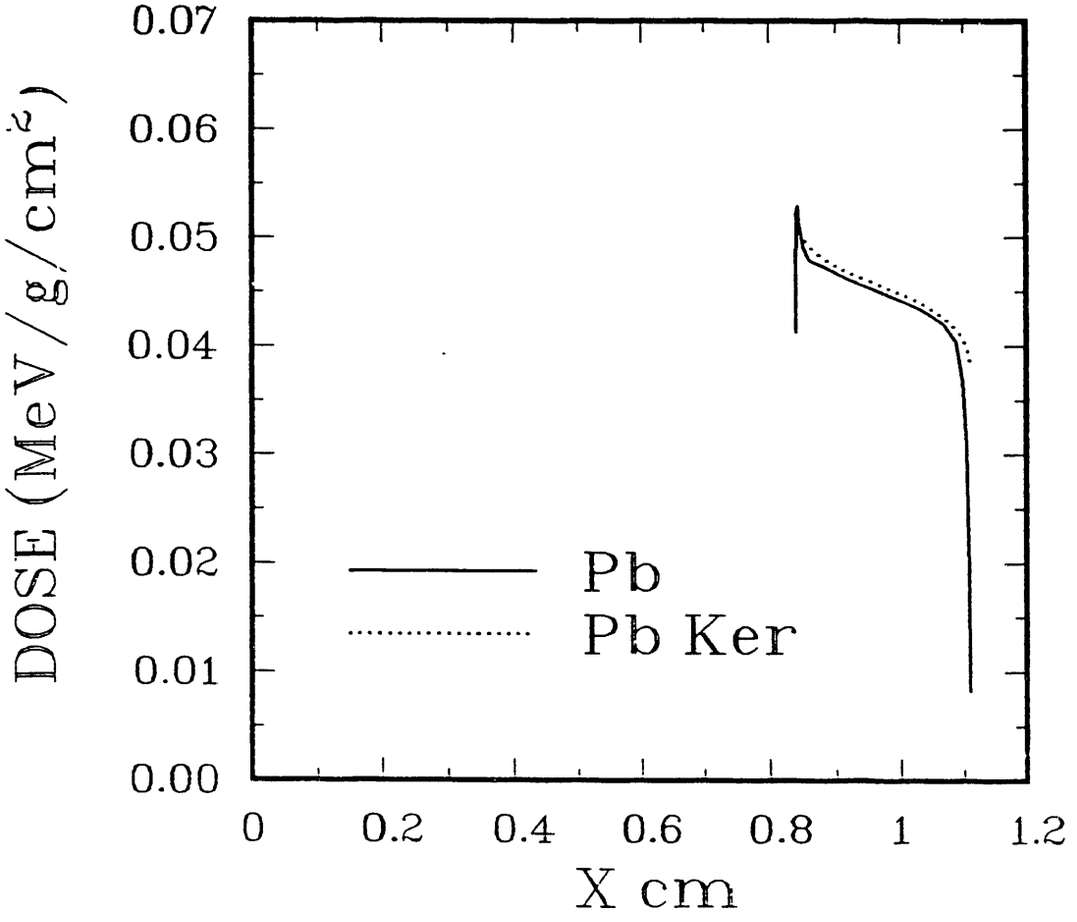
```
TITLE
Example #2B
MATERIAL LI .2675 F .7325
 DENSITY 2.635
MATERIAL PB
ENERGY 1.33
CUTOFF .01
PHOTON-SOURCE
 FULL-COUPLING
LEGENDRE 15
GEOMETRY 3
 1 10 .49
 2 10 .02
 1 10 .49
ELECTRONS
 LINEAR 50
PHOTONS
 LINEAR 30
DIRECTION
 NORMAL
OUTPUT
 EQDEP
```

COMMENTS: In Example Problem #2, the only material that is used in the transport calculation is LiF since it appears in the actual geometry. Lead is specified as a detector material. The detector kerma profile in the figure represents the kerma that would be deposited in a layer of lead at each position provided that this layer is thin to photons, thick to electrons, and is surrounded by LiF. This is seen by a comparison of the detector kerma profile with the kerma profile for the material configuration (Example Problem #2A) in which a lead layer that is thin to photons is sandwiched between two LiF layers. The kerma in the sandwiched lead layer of Problem #2A matches the detector kerma profile at the proper position.

```
TITLE
Example #1
MATERIAL LI .2675 F .7325
 DENSITY 2.635
MATERIAL PB
ENERGY 1.33
CUTOFF .01
PHOTON-SOURCE
 FULL-COUPLING
LEGENDRE 15
GEOMETRY 2
 1 10 .84 10
 2 10 .27 10
ELECTRONS
 LINEAR 50
PHOTONS
 LINEAR 30
DIRECTION
 NORMAL
OUTPUT
 EDEP
 EQDEP
```

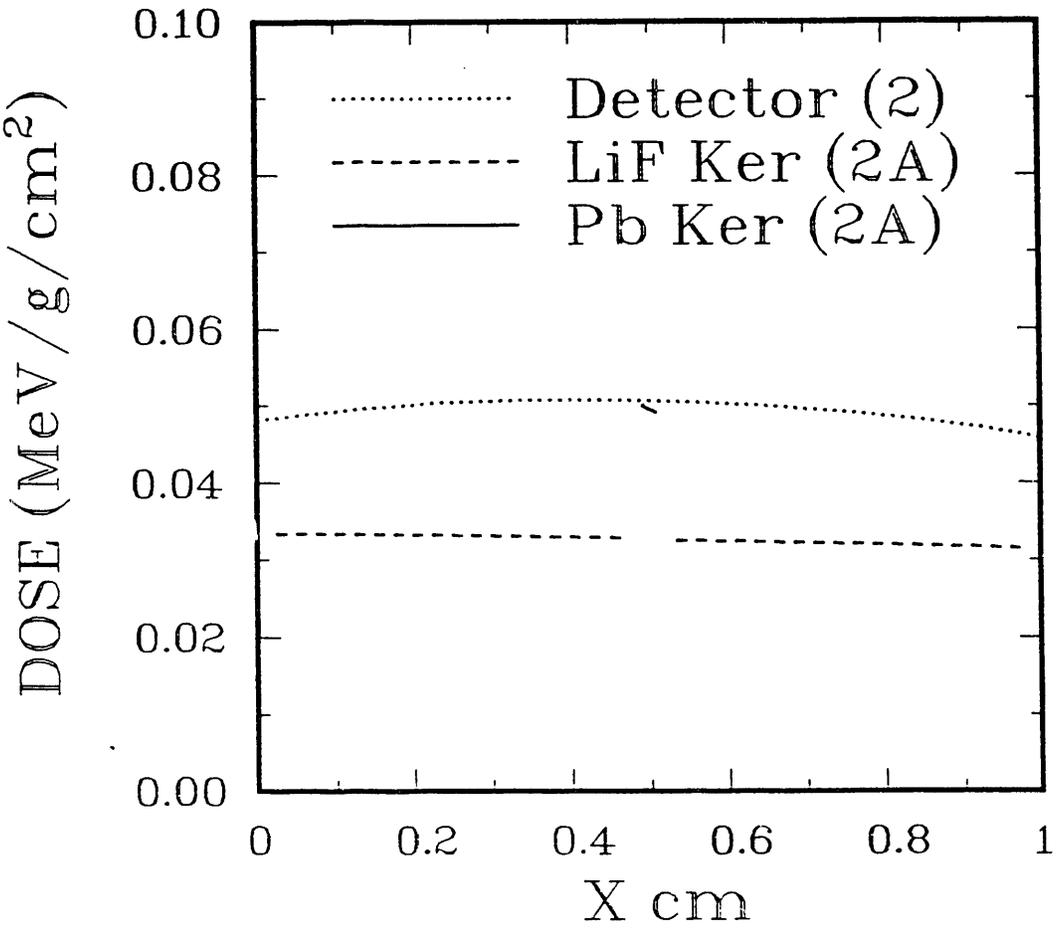


Example #1 (cont.)

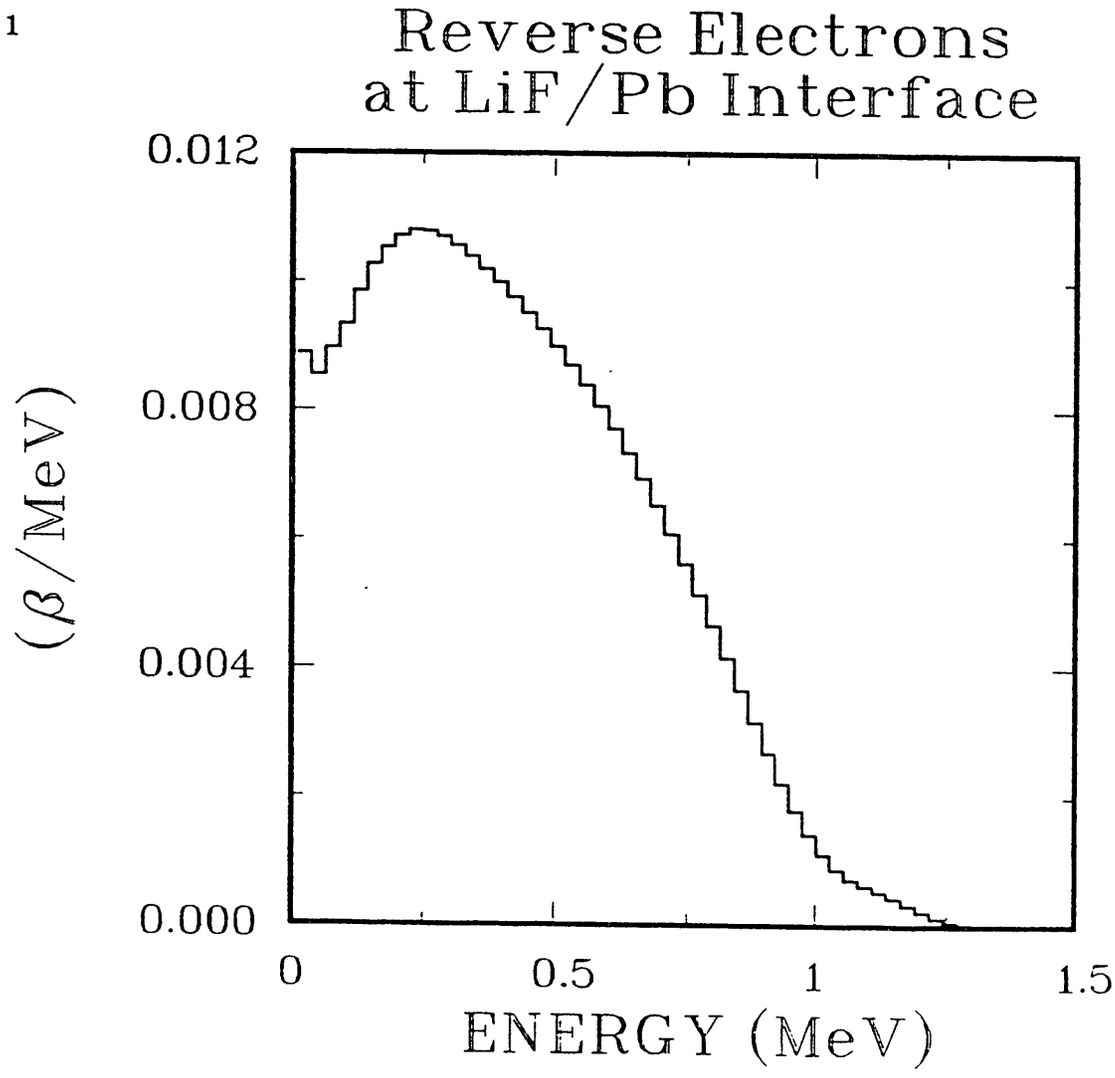


COMMENTS: Note that, as expected, the kerma or equilibrium dose (obtained with the keyword EQDEP) is the same as the dose (obtained with the keyword EDEP) only in the interior of the two layers. In the figures, the dose is denoted by the bold plot and the kerma is denoted by the dashed plot.

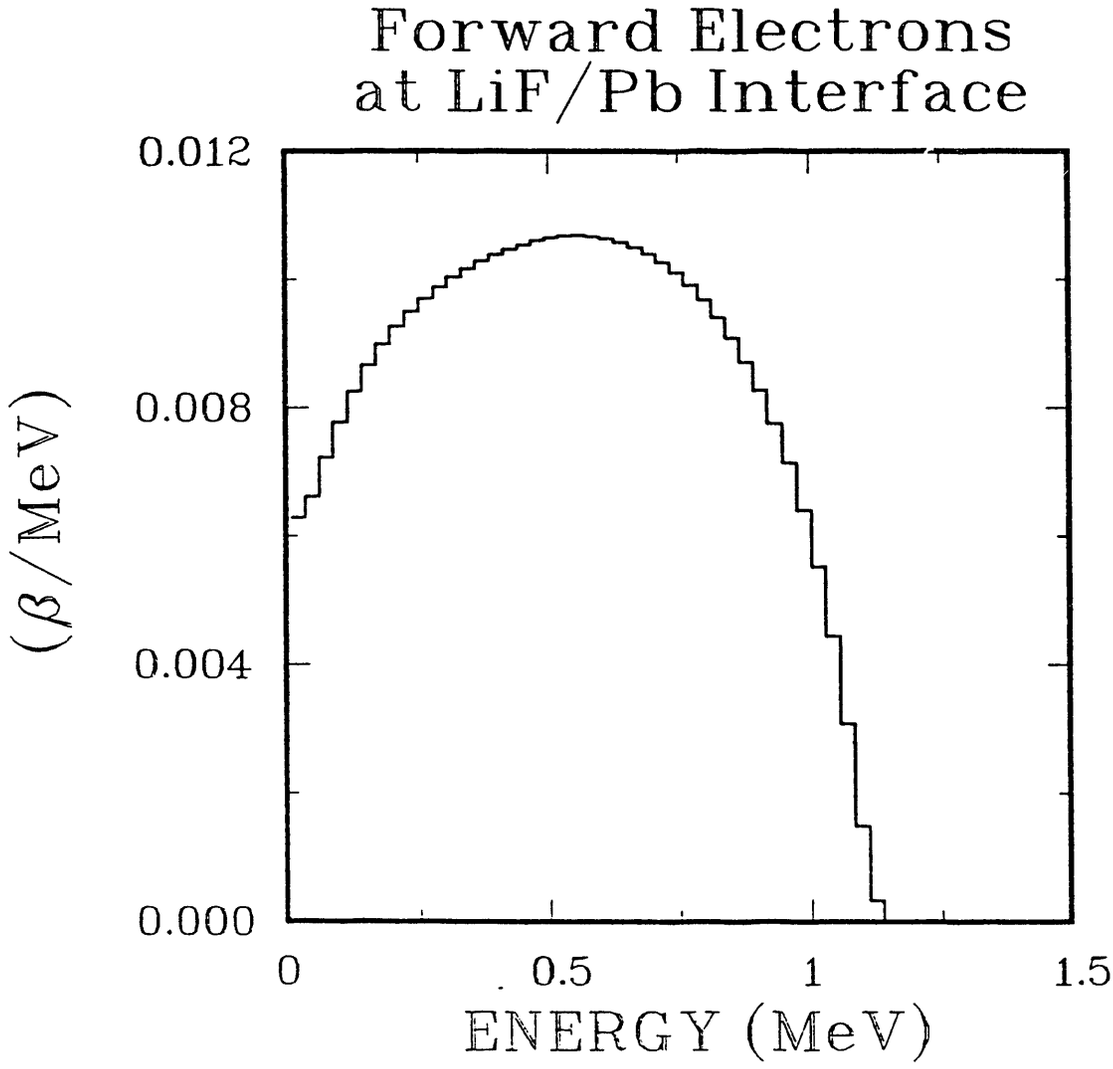
Example #2 (cont.)



```
TITLE
Example #3
MATERIAL LI .2675 F .7325
 DENSITY 2.635
MATERIAL PB
ENERGY 1.33
CUTOFF .01
PHOTON-SOURCE
 FULL-COUPLING
LEGENDRE 15
GEOMETRY 2
 1 10 .84 10
 2 10 .27 10
ELECTRONS
 LINEAR 50
PHOTONS
 LINEAR 30
DIRECTION
 NORMAL
OUTPUT
 CURRE
INTERNAL-SPECTRA 1
 .84
```



Example #3 (cont.)



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