



Xenos

Integrated Software Suite for X-ray Science Walkthrough Example

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Demonstration example – X-ray generation by a pulsed electron beam incident on a copper target

Although this calculation addresses a relatively simple geometry, it illustrates many advanced techniques for constructing **Xenos** runs. A pulsed electron beam with kinetic energy $T = 12.5$ MeV, current $I = 0.3$ A and envelope radius $r_0 = 0.5$ mm strikes a copper bremsstrahlung target. Reference to the NIST EStar site at

<http://www.physics.nist.gov/PhysRefData/Star/Text/ESTAR-t.html>

shows that the electron range at 12.5 MeV is about 8.2 mm. We pick a target thickness of 3.0 mm, about 37% of the range. To constrain the geometry, we assume that target is rigidly clamped to a water-cooled holder at a radius of 6.0 mm. We want to use **Xenos** to answer several questions:

- What is a conservative beam pulse length to avoid melting the target?
- What pulse separation is necessary to ensure that the target cools?
- What is the shape of the forward radiation cone?
- What is the forward dose at a distance of 1 m?

We shall make two-dimensional calculations with cylindrical symmetry that employ the codes **Trak**, **Mesh**, **GamBet**, **GBView2**, **TDiff** and **GenDist**.

The first task is to generate a file that contains parameters for a set of electrons to describe the incident beam. A quick approach is to use the *Circular beam generator* in the *Tools* menu of **Trak**. The utility creates a set electrons with uniform radial spacing with weighted current to approximate a uniform current density. Figure 1 shows the tool dialog with entries appropriate for the desired electron beam properties. Note that the program substitutes the electron mass in AMU if a zero appears in the *Mass* box. The choice of axial position (0.001 mm) ensures that the particles start just inside the upstream boundary of the target. In response to the *Write file* button, **Trak** creates the text file **BEAM300.PRT** containing 200 model electrons that will be used as input for **GamBet**.

The next step is to set up the primary **GamBet** calculation that generates two types of information: 1) deposited power density in the target that will be used for the thermal calculation and 2) the photon distribution in the forward direction to calculate the dose at 1 meter. File **COPPERTARGET.MIN** defines the geometry for both the **GamBet** and **TDiff** calculations. Region 1 (representing the copper block) has dimensions $0.0 \text{ mm} \leq z \leq 3.0 \text{ mm}$ and $0.0 \text{ mm} \leq r \leq 6.0 \text{ mm}$. In addition, there is an open region of nodes along the

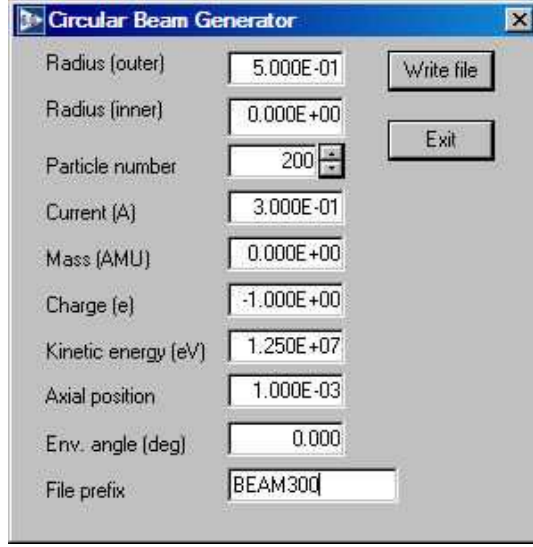


Figure 1: Dialog of the **Trak** *Circular beam generator* tool with parameters for the demonstration solution.

outer radial boundary. This region represent a fixed-temperature condition for the **TDiff** calculation, but plays no role in the **GamBet** calculation.

Table 1 shows the file `COPPERTARGET.GIN`. The *Geometry* section sets the spatial units to millimeters and loads the mesh file. The *Composition* section sets the first material to solid copper using the standard Penelope definition and associates the material with both regions. The *Source* section loads model electron parameters (including associated current values) from the file `BEAM300.PRT`. **GamBet** will create 100 showers for each primary electron (20,000 showers). In the *Process* section, the command

Force Brems 20.0

raises the probability of a bremsstrahlung interaction by a factor of 20.0 and adjusts output statistics accordingly. As a result, the run generates a large number of photons for the forward dose calculation. The **GamBet** run takes about 3 minutes. Of the incident power (3.75 MW), about 1.55 MW is deposited in the copper target, The remaining power is carried away by reduced-energy primary electrons and bremsstrahlung photons. Figure 1 shows the dose-rate distribution in the target plotted with **GBView2**. One cycle of smoothing was applied and result saved as `COPPERTARGETSMOOTH.G2D`.

TDiff can be used to determine an acceptable beam pulse length and the time between pulses to allow target cooling. To start, we can estimate the maximum heating time. At ambient temperature, copper has following thermal properties: melting point $T_m = 1084$ °C, density $\rho = 8960$ kg/m³, thermal conductivity $k = 385$ W/(m·°C) and specific heat 387 J/(kg·°C).

Table 1: Contents of the file COPPERTARGET.GIN

```
GEOMETRY
  DUnit = 1.0000E+03
  GFile2D = CopperTarget.MOU (Cylin)
END
COMPOSITION
  Material = 29
  Region( 1) = 1
  Region( 2) = 1
END
SOURCE
  PFile = BEAM300
  NPMult = 100
END
PROCESS
  EMax = 1.5000E+07
  EAbs(Electron) = 5.0000E+04
  EAbs(Photon) = 5.0000E+04
  EAbs(Positron) = 5.0000E+04
  DsMax = 1.0000E-01
  StepMax = 500000
  Time = 86400
  Force Brems 20.0
END
ENDFILE
```

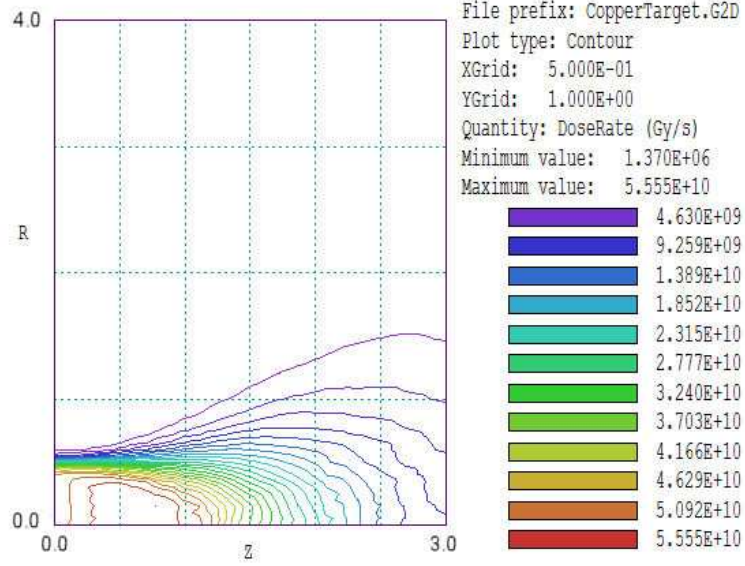


Figure 2: Smoothed dose-rate distribution, electron beam with kinetic energy 12.5 MeV, radius 0.5 mm and current 0.3 A incident on a copper target of thickness 3.0 mm.

The beam irradiates an approximately cylindrical volume with radius 5×10^{-4} m and length 3×10^{-3} m. The volume is about 2.36×10^{-9} m³ and the irradiated mass is $M = 2.11 \times 10^{-5}$ kg. The deposited beam power is about

$$P \cong 3.75 \frac{3.0}{8.2} = 1.37 \text{ MW}. \quad (1)$$

Ignoring thermal conductivity, the time rate of change of temperature is

$$MC_p \frac{\Delta T}{\Delta t} \cong P. \quad (2)$$

Solving Eq. 2 for Δt and taking $\Delta T \cong T_m$, the beam pulse length should be $\Delta t \leq 6.4 \mu\text{s}$. To be conservative, we shall use $\Delta t = 5.0 \mu\text{s}$ in the thermal calculation.

Table 2 shows the control file for the **TDiff** calculation with several interesting features. Here, Region 1 has the thermal properties of copper, while the boundary region at $r = 6.0$ mm has the fixed temperature 37 °C. The file **COPPERTARGETSMOOTH.G2D** defines a spatially-dependent thermal source. In the **TDiff** calculation, quantities recorded in the **GamBet** output file are interpreted as power density rather than dose. The source is active for 5.0 μs pulse – the simulation continues for 5 ms to study cooling by conduction. The file **PULSE5US.MOD** defines the source modulation function. The function has the value 1.0 for $t \leq 5.0 \mu\text{s}$ and 0.0 thereafter. Note that the *Linear*

Table 2: Contents of the file COPPERTARGET.TIN

```
* ---- CONTROL ----
Mesh = CopperTarget
Mode = TVar
Geometry = Cylin
DUnit = 1.0000E+03
TMax = 5100.0E-6
DtMin = 5.0E-9
Interp = Linear
SourceFile = CopperTargetSmooth.G2D
SourceMod = Pulse5us.MOD
TStepMod = CTargTStep.MOD
* ---- REGIONS ----
* Region 1: COPPER
Cond(1) = 3.8500E+02
Cp(1) = 3.8700E+02
Dens(1) = 8.9600E+03
Init(1) = 3.7000E+01
* Region 2: OUTERBOUND
Fixed(2) = 3.7000E+01
* ---- DIAGNOSTICS ----
SetTime = 5.0000E-06
SetTime = 5000.0000E-06
History = 0.700 0.133
EndFile
```

option is used for interpolations because of the discontinuous nature of the function.

The challenge of the calculation is the large difference in time scales for heating and cooling. The automatic time-step routines of **TDiff** would be inefficient if adjusted to ensure good accuracy during the short heating time. Instead, we actively set the integration time to follow the source variations. The command

```
TStepMod = CTargTStep.MOD
```

signals that **TDiff** should set the integration time step equal to the product of the modulation function contained in the file **CTARGETSTEP.MOD** and the value of *DtMin* (5.0 ns). Table 3 shows the contents of the modulation file. The time step is 5 ns during the heating phase, then rises to 5 μ s over the interval $5.0 \mu\text{s} \leq t \leq 20.0 \mu\text{s}$. Figure 3 shows the temperature distribution at times 5.0 μ s and 5.0 ms. The initial distribution closely tracks the power

Table 3: Contents of the file CTARGETSTEP.MOD

```

0.0E-6      1.0
5.0E-6      1.0
20.0E-6     1000.0
100.0E-6    1000.0
10000.0E-6  1000.0
ENDFILE

```

density profile, indicating that thermal conductivity is negligible the heating pulse. The maximum temperature of 750 °C is well below the melting point. After a 5.0 ms interval, the peak temperature drops to about 113 °C. With more complex forms for the files PULSE5US.MOD and CTARGETSTEP.MOD, we could investigate the equilibrium peak temperature from a train of pulses.

To conclude, we consider the photon dose in the forward direction at a distance of 1 meter. The **GamBet** run controlled by COPPERTARGET.GIN produces a record of all electrons, photons and positrons lost from the solution volume in the file COPPERTARGETESC.SRC. This information can be used for the dose calculation if electrons, positrons and backscattered photons are removed. The filter capability of **GenDist** is useful for this operation. When the raw escape file is loaded, **GenDist** reports that it contains 21,048 electrons, 506,139 photons and 399 positrons. In response to the command *Analysis/Apply filter*, the program displays the dialog of Fig. 4. The filter parameters shown limit particles to photons that have reached the downstream boundary of the target at $z = 3.0$ mm. The command *Write PRT/SRC file* is used to create the file FILTERFORWARD.SRC that contains 429,865 forward-directed photons. **GenDist** can also create graphs of the filtered distribution. For example, Fig. 5 shows the angular distribution of photons. From an inspection of slope, the energy flux density peaks in the forward direction and falls off at about 4°. At 1 meter, the angle corresponds to radial spread of about 7 cm.

For the second **GamBet** calculation, the file FORWARDDOSE.MIN defines a solution volume of radius 10.0 cm that contains two regions: a void of axial length 100 cm and an aluminum target with axial length 5.0 cm. The element resolution in the void region is coarse because it is not necessary to resolve deposited dose. The element size in the target is about 0.5 cm in both the axial and radial directions. Table 4 shows the contents of the file FORWARDDOSE.GIN. There are several interesting features:

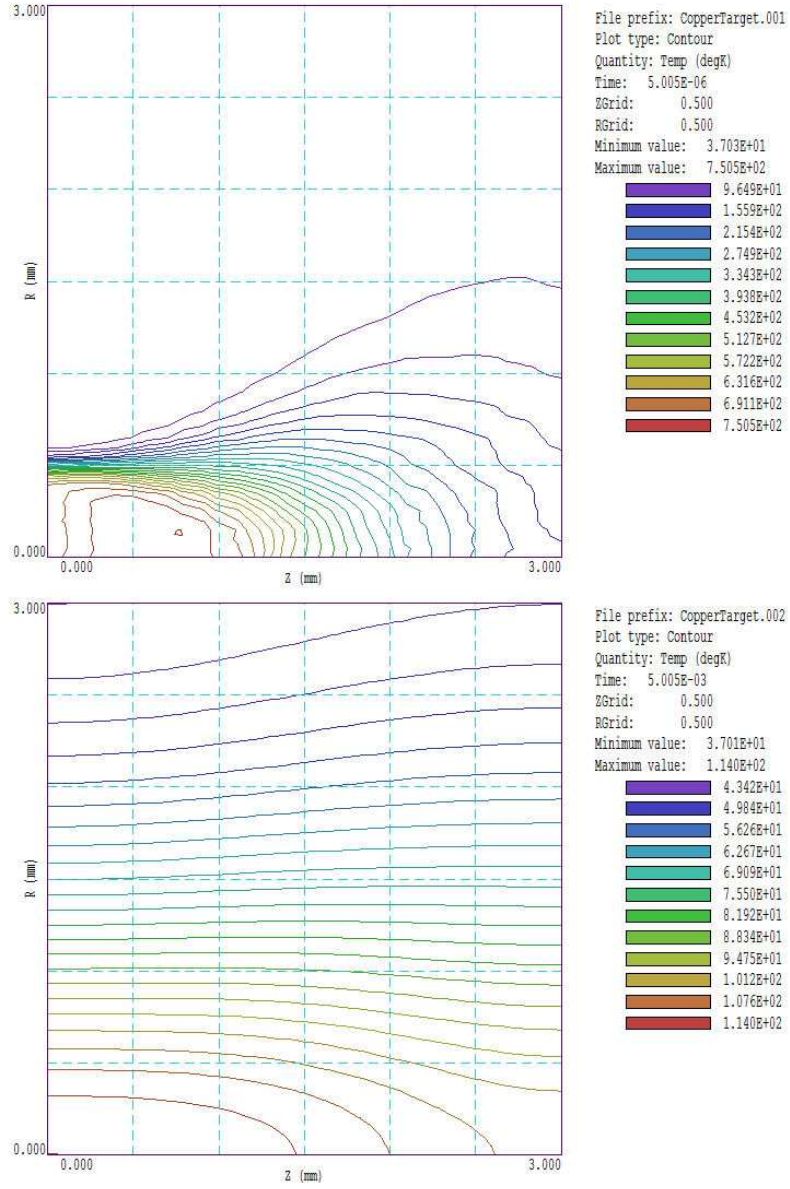


Figure 3: Thermal solution using a **GamBet** source. Top: $5.0 \mu\text{s}$. Bottom: 5.0 ms .

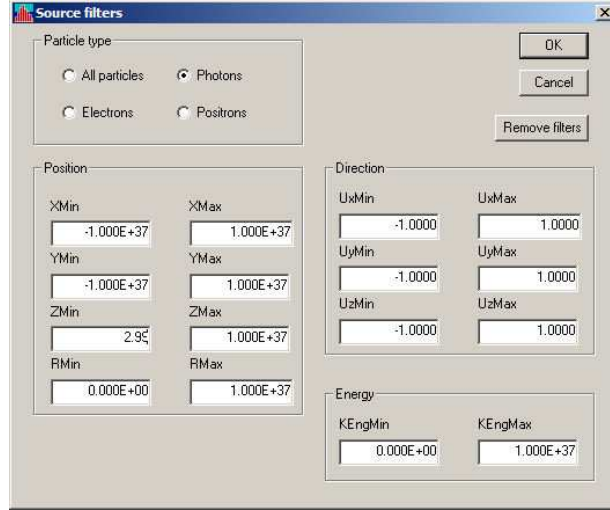


Figure 4: Dialog to set particle filter in **GenDist**.

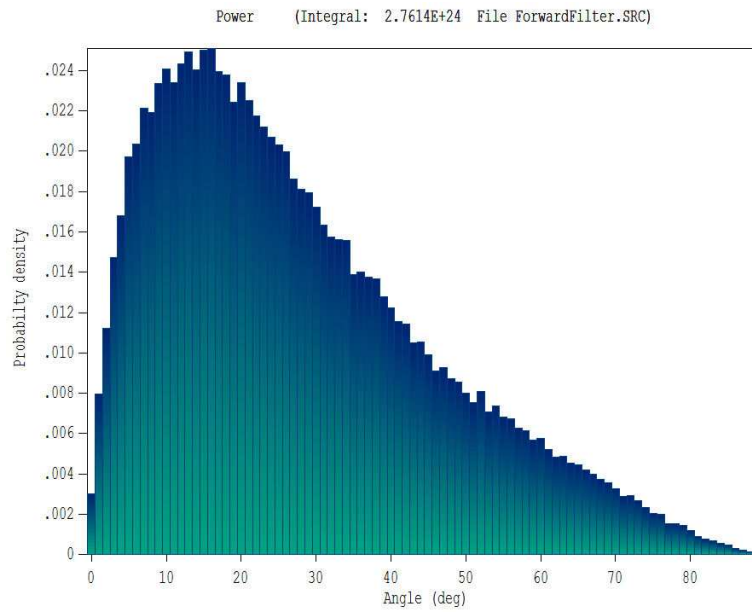


Figure 5: Energy-weighted distribution of photons in angle relative to the z axis.

- The mesh was constructed in units of centimeters, so the command `DUnit = 100` should precede the *GFile2D* command.
- The file `FORWARDFILTER.SRC` defines the primary photons. Because the dimensions in this file are in millimeters, the command `DUnit = 1000` must appear before the *SFile* command.
- The program creates four showers for each primary photon for good resolution of the deposited dose in the target.
- Units are reset to centimeters in the *Process* section.
- It is a good practice to include the *StepLimit* command in any simulation involving photon transport through multiple regions. Individual values of the step size are assigned to the two regions. The large step size (25.0 cm) in the void is sufficient to ensure that photons have at least one virtual interaction. The virtual interaction allows **GamBet** to determine when photons cross the boundary between the void and the target. The step size in the aluminum target has the conventional value 0.25 cm.

The plotting capability of **GBView2** is useful to understand the dose-rate distribution in the target. Figure 6 shows the result (with three cycles of smoothing applied). It is apparent that we must take care defining the forward photon dose-rate, which depends on both radial position and depth in the target. The value is small on the front face and increases with depth because of the buildup of the secondary electron density. For an aluminum target and a bremsstrahlung spectrum with a 12.5 MeV endpoint, the dose reaches its maximum value at a depth of about 1.8 cm. At this position, the dose-rate on axis is about 2.5×10^3 Gy/s. The accumulated dose for the 5 μ s pulse is 0.0125 Gy or 1.25 R.

Table 4: Contents of the file FORWARDDOSE.GIN

```
GEOMETRY
  DUnit = 100.0
  GFile2D = ForwardDose.MOU (Cylin)
END
COMPOSITION
  Material = 13
  Region( 1) = Void
  Region( 2) = 1
END
SOURCE
  DUnit = 1000.0
  SFile = ForwardFilter
  NPMult = 4
END
PROCESS
  DUnit = 100.0
  StepLimit
  DsMax(1) = 25.0
  DsMax(2) = 0.25
  EMax = 1.5000E+07
  EAbs(Electron) = 5.0000E+04
  EAbs(Photon) = 5.0000E+04
  EAbs(Positron) = 5.0000E+04
  StepMax = 500000
  Time = 86400
END
ENDFILE
```

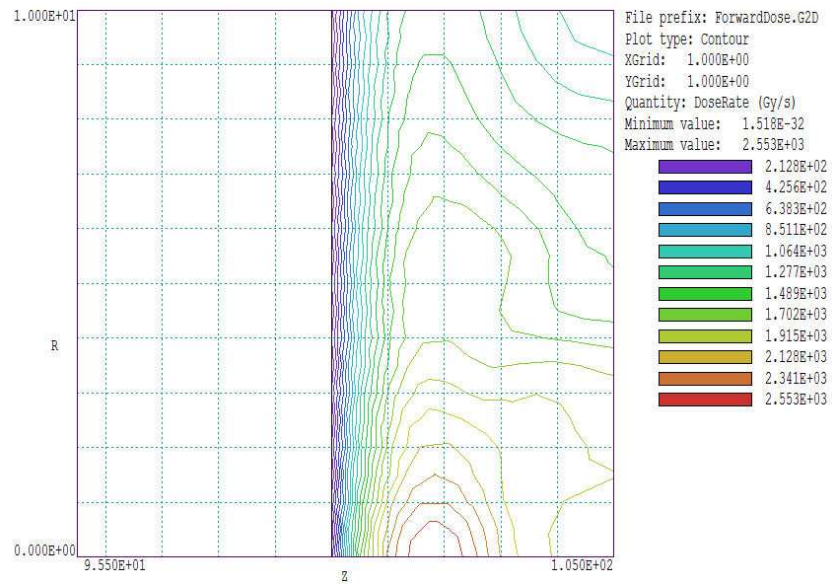


Figure 6: Dose-rate in an aluminum block a distance 1.0 m from the copper bremsstrahlung target. Three cycles of smoothing have been applied.