# Numerical Simulation of the Electric Field and the Study of the Electron Collection Efficiency in a Xe TPC

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# Abstract

The XENON Dark Matter Project uses a two-phase time projection chamber (TPC) with a liquid xenon target to detect weakly interacting massive particles (WIMPs). WIMP events are categorized by ionization and scintillation signals. The point of interaction of the WIMP with the xenon nucleus can be reconstructed in three dimensions with millimeter precision, when an appropriate fiducial volume cut is made. The electric field inside the TPC must be well understood in order to select the region where the electric field is adequately uniform and to reconstruct the interaction vertex with the desired resolution. In preparation for the final phase of the XENON experiments, the electric field and electron collection efficiency for the Demonstrator TPC and larger TPCs are studied and analyzed in this paper.

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# **1** COMSOL Multiphysics Software

COMSOL Multiphysics is a computational physics software which allows scientists to accurately simulate physical systems in 2D, or 3D, with many different physical properties. A single model can incorporate multiple physical properties of the system. COMSOL has a user-friendly interface, which allows for detailed simulation. The user creates the geometry of their system in COMSOL, selects materials for the objects, and applies the appropriate physics modules to their system. COMSOL meshes the geometry, meaning it creates a web of different points within the geometry, and then uses those points to calculate the physical results from the modules which the user has chosen. COMSOL allows for easy manipulations of systems, through user-defined variables and parameters.

In the study of the TPCs, the Electrostatics and Charged Particle Tracing modules, which are both part of the AC/DC module, were used.

# **1.1 Electrostatics**

The Electrostatics module allows for electric potentials, charges, and grounds to be applied to different geometrical objects. Charge conservation, Coulomb's Law, and classical electrostatics govern the physics in this module. With this module, electric fields and electric potential fields can be graphed and studied.

# **1.2 Charged Particle Tracing**

The Charged Particle Tracing module allows for particles to be released in the geometry of the system, and draws upon the results of the Electrostatics module to determine the paths of these particles. Either massless or Newtonian physics can be chosen, and the user must supply a particle mass, charge, and velocity. One or many particles can be studied simultaneously. The Coulomb Force governs the physics in this module (though this can be modified, see Section 3.1 and Appendix B for details). With this module, the paths of particles can be graphed and studied.

#### 1.3 Models

To aid in the R&D of XENON1T, three TPC models were created in COMSOL; one for the Demonstrator TPC, one for the 1m TPC, and one for the XENON1T TPC. Each was created according to certain specifications (see Appendix A for details).

#### 1.3.1 Demonstrator

The Demonstrator TPC is 30 cm tall, with an 8 cm diameter, 21 copper field shaping wires, and a cathode voltage of -15 kV.



Figure 1.1: 3D Model of the Demonstrator TPC.

#### 1.3.2 1m

The 1m TPC is 1 m tall, with a 7 cm diameter, 66 aluminum field shaping wires, and a cathode voltage of -100 kV, which creates a 1 kV/cm electric field inside the TPC.



Figure 1.2: 3D Model of the 1m TPC.

# 1.3.3 1T

The XENON1T TPC is 1 m tall, with a 1 m diameter.



Figure 1.3: 3D Model of the XENON1T TPC.

# 2 Electric Field Inside the TPC

For each model, appropriate electric potentials were applied to the geometrical objects, and the electric field was studied and analyzed. This allows for a better understanding of the uniformity and strength of the electric field in the TPC.

#### **2.1 Electrostatic Theory**

The AC/DC Electrostatics module is governed by charge conservation and classical electrostatics,

$$E = -\nabla V \tag{1}$$

$$\nabla \cdot D = \rho_f \tag{2}$$

where *E* is the electric field, *V* is the electric potential, *D* is the electric displacement field, and  $\rho_f$  is the free electric charge density.

#### 2.2 Demonstrator

The Demonstrator TPC exhibits a very uniform, vertical electric field. Any fluctuations from the cathode wires or field shapers diminish rapidly further inward of the TPC.

#### 2.2.1 Electric Potentials

The cathode is supplied with -15 kV, the bottom field shaper is supplied with -14.3189 kV, the next field shaper up is supplied with -13.6378 kV, and so on, so that each subsequent field shaper voltage is increased by 681.1 V, uniformly up to 0 V at the ground mesh (see section 2.2.4 to understand how this is implemented in the physical detector). This is done to create a uniform electric potential gradient, which will cause a uniform electric field inside the TPC.



Figure 2.1: The electric potential inside the Demonstrator TPC. The equipotential lines are very horizontal and uniformly spaced inside the TPC. The only disuniformities occur close to the mesh and field shaping wires (the effects of which are explored in sections 2.2.3 and 2.2.4). Dark blue marks -15 kV, the cathode voltage, progressing upwards to red, which marks 2.4 kV, the anode voltage. The equipotential lines progress similarly, going from dark red at the cathode voltage to white at the anode voltage.

# 2.2.2 Total Electric Field

The equal spacing of the field shapers and linear change in voltage creates a uniform electric field inside the TPC. The field is uniform and downwards, meaning electrons will travel upwards through the TPC. Note that  $1 \text{ kV/cm} = 10^5 \text{ V/m}$ .



Figure 2.2: The electric field inside the Demonstrator TPC. Inside the TPC, the electric field lines are very uniform and vertical, as desired. Fluctuations occur only close to the wires and outside of the TPC (explored in sections 2.2.3 and 2.2.4). The concentration of the lines is uneven in places because of the COMSOL mesh. The cathode ring causes the majority of disuniformities. The missing wire, towards the left side of the cathode, is apparent, because the field lines from the cathode escape through this enlarged gap. The blue represents a norm field value of 0.5 kV/cm.

# 2.2.3 Cathode Mesh

The cathode is a mesh of wires held at the same potential, -15 kV. Because the cathode is a mesh and not a solid plate, fluctuations are introduced into the field (see Figure 2.2). Furthermore, in the Demonstrator TPC, one cathode wire is missing, causing more fluctuations (see Figure 2.3). However, the field does become uniform after a height of just 0.917 cm above the cathode mesh, which is below the first field shaper (see Figure 2.4.a and Figure 2.4.b). This eventual uniformity allows for the simplification of the 3D geometry, where the cathode is not represented as a mesh of wires, but as a solid plate. In the physical TPC, the cathode must be a mesh, because it must allow light to pass through to the PMTs.



Figure 2.3: The electric field near the missing cathode wire in the Demonstrator TPC. The missing wire is indicated with a red arrow. This causes greater fluctuations in the electric field near the cathode than from the other cathode wires, because of the larger gap. Note that field lines were omitted from the left side of the field shaper and cathode, as to create a clearer picture. The blue represents a norm field value of 0.2 kV/cm.



Figure 2.4.a: Uniformity of the electric field at a height of just 0.917 cm above the cathode mesh. The disuniformities resulting from the mesh die out quickly inside the Demonstrator TPC, as desired. This is apparent from the graph, because the mesh wires are placed every 0.5 cm along the x-axis, and no fluctuations occur every 0.5 cm. An enlarged section of the graph from 7 cm to 8 cm is shown to confirm this fact. The fluctuations at the beginning and end of the x-axis are from the proximity to the edge of the TPC near the field shapers. The dip in the field value at 5.5 cm is due to the missing cathode wire.



Figure 2.4.b: The height at which the uniformities begin in the Demonstrator TPC, just 0.917 cm, or roughly two times the wires' pitch, above the cathode mesh. This is very close to the bottom of the TPC, below even the first field shaping ring, meaning that the large majority of the TPC experiences a uniform electric field.

# 2.2.4 Field Shapers

Similar to the fluctuations from the cathode wires, there are fluctuations in the electric field from the field shaping rings. The fluctuations decrease quickly further towards the center of the TPC (see Figure 2.5.a, 2.5.b, 2.6.a, and 2.6.b). However, unlike the cathode wires, the field shapers have a more substantial effect on the slight disuniformity of the electric field, and thus affect the path of electrons through the TPC (see section 3 for details). The field must be controlled by these field shaping rings, as opposed to a solid metal cylinder, because it is impossible to create a uniform electric field accurately enough with a metal cylinder of uniformly varying resistance. In the physical detector, the field shapers. This allows for the voltage to vary uniformly along the length of the TPC with great precision.



Figure 2.5.a: The location of the lines the electric field is examined along, on the left side of the Demonstrator TPC.



Figure 2.5.b: The fluctuations on the left side of the TPC are much smaller for lines positioned closer to the center of the Demonstrator TPC. This means the electric field is more uniform near the center of the TPC. The legend indicates which color corresponds to the distance in field shaper radii the line is away from the left array of field shapers. So line 6 (yellow) is 6 field shaper radii away from the left-side field shapers, and the electric field along this line fluctuates the least, as expected. The fluctuations of the electric field norm value along line 6 are only of 0.1 kV/cm.



Figure 2.6.a: The location of the lines the electric field is examined along, on the right side of the Demonstrator TPC.



Figure 2.6.b: The fluctuations on the right side of the TPC are much smaller for lines positioned closer to the center of the Demonstrator TPC. This means the electric field is more uniform near the center of the TPC. The legend indicates which color corresponds to the distance in field shaper radii the line is away from the right array of field shapers. So line 6 (yellow) is 6 field shaper radii away from the right-side field shapers, and the electric field along this line fluctuates the least, as expected. The fluctuations of the electric field norm value along line 6 are only of 0.1 kV/cm.

# 2.2.5 Guard Mesh

The guard mesh, below the cathode mesh, is held at a potential of 1.6 kV, to protect the PMTs from the strong electric field of the TPC. The highest electric field value the PMTs experience is a mere 0.28 kV/cm (see Figure 2.9).



Figure 2.7: Electric field norm value below the cathode in the Demonstrator TPC. The value directly below the cathode (from 5 cm to 10 cm is 7 kV/cm. The top right picture is included to show the line along which this is examined.



Figure 2.8: Electric field norm value below the guard mesh and above the PMTs in the Demonstrator TPC. The field reaches a value of nearly 0 kV/cm underneath the center of the guard mesh, as desired. The largest field values occur underneath the cathode ring, but are only 1 kV/cm. This shows the guard mesh is protecting the PMTs fairly well. The bottom right picture is included to show the line along which this is examined.



Figure 2.9: Electric field norm value inside the PMTs in the Demonstrator TPC. The field reaches a value of nearly 0 kV/cm underneath the center of the guard mesh, as desired. The largest field values occur underneath the cathode ring, but are only 0.28 kV/cm. This shows the guard mesh is protecting the PMTs very well. The bottom right picture is included to show the line along which this is examined.

# 2.3 1 m

The 1m TPC also exhibits a very uniform, vertical electric field. Any fluctuations from the cathode wires or field shapers diminish rapidly further inward of the TPC.

# 2.3.1 Electric Potentials

The cathode is supplied with -100 kV, the bottom field shaper is supplied with -98.5075 kV, the next field shaper up is supplied with -97.015 kV, and so on, so that each subsequent field shaper voltage is increased by 1492.5 V, uniformly up to 0 V at the ground mesh (see section 2.2.4 to understand how this is implemented in the physical detector). This is done to create a uniform electric potential gradient of 1 kV/cm, which will cause a uniform electric field inside the TPC.



Figure 2.10: The electric potential inside the 1m TPC. The equipotential lines are very horizontal and uniformly spaced inside the TPC. The only disuniformities occur close to the mesh and field shaping wires (the effects of which are explored in sections 2.3.4). Dark blue marks -100 kV, the cathode voltage, progressing upwards to red, which marks 0 V, the ground. The equipotential lines progress similarly, going from dark red at the cathode voltage to white at the ground.

# 2.3.2 Total Electric Field

The equal spacing of the field shapers and linear change in voltage creates a uniform electric field inside the TPC. The field is uniform and downwards, meaning electrons will travel upwards through the TPC.



Figure 2.11: The electric field inside the 1m TPC. Inside the TPC, the electric field lines are very uniform and vertical, as desired. There is just slight warping near the top ground mesh, the field shapers, and the cathode (explored in section 2.3.3). The blue represents a norm field value of 1 kV/cm.

# 2.3.3 Cathode Mesh

The cathode is a mesh of wires held at the same cathode potential, -100 kV. Because the cathode is a mesh and not a solid plate, fluctuations are introduced into the field (see Figure 2.11 and Figure 2.12). However, the field does become uniform after a height of just 0.52 cm above the cathode mesh, which is still within the cathode ring (see Figure 2.13.a and Figure 2.13.b). This eventual uniformity allows for the simplification of the 3D geometry, where the cathode is not represented as a mesh of wires, but as a solid plate. In the physical TPC, the cathode must be a mesh, because it has to allow light to pass through to the PMTs.



Figure 2.12: The electric field close to the cathode in the 1m TPC. Blue represents a norm field value of 1 kV/cm. The cathode ring has a strong effect, and some field lines even escape through the gaps in the cathode mesh. This has an effect on the path of the electrons which originate near the cathode (explored in section 3.3).



Figure 2.13.a: Uniformity of the electric field at a height of just 0.52 cm above the cathode mesh. The disuniformities resulting from the mesh die out quickly inside the 1m TPC, as desired. This is apparent from the graph, because the mesh wires are placed every 0.3 cm along the x-axis, and no fluctuations occur every 0.3 cm. The fluctuations at the beginning and end of the x-axis are from the proximity to the edge of the TPC near the field shapers, and the decrease towards the center is because this section is further from the large cathode ring.



Figure 2.13.b: The height at which the uniformities begin in the 1m TPC, just 0.52 cm, or about twice the wires' pitch, above the cathode mesh.. This is very close to the bottom of the TPC, still within the cathode ring, meaning that the large majority of the TPC experiences a uniform electric field.

# 2.3.4 Field Shapers

Similar to the fluctuations from the cathode wires, there are fluctuations in the electric field from the field shaping rings. The fluctuations decrease quickly further towards the center of the TPC (see Figure 2.14.a, 2.14.b, 2.15.a, and 2.15.b). However, unlike the cathode wires, the field shapers have a more substantial effect on the slight disuniformity of the electric field, and thus affect the path of electrons through the TPC (see section 3 for details). As explained in section 2.2.4, the field must be controlled by these field shaping rings, as opposed to a solid metal cylinder, because it is impossible to create a uniform electric field accurately enough with a metal cylinder of uniformly varying resistance.



Figure 2.14.a: The location of the lines the electric field is examined along, on the left side of the 1m TPC. The rectangular wire on the right side of the TPC is the voltage supply feed, explored in the next section, 2.3.5.



Figure 2.14.b: The fluctuations on the left side of the TPC are much smaller for lines positioned closer to the center of the 1m TPC. This means the electric field is more uniform near the center of the TPC. The legend indicates which color corresponds to the distance in half-field-shaper-widths the line is away from the left array of field shapers. So line 6 (yellow) is 3 field shaper widths away from the left-side field shapers, and the electric field along this line fluctuates the least, as expected. The fluctuations of the electric field norm value along line 6 are only of 0.002 kV/cm. This is a much smaller fluctuation than the 6<sup>th</sup> line of the Demonstrator TPC (Figure 2.5.b), because the 1m TPC has a smaller radius and larger field shapers, making this 6<sup>th</sup> line much closer to the center of the TPC.



Figure 2.15.a: The location of the lines the electric field is examined along, on the right side of the 1m TPC.



Figure 2.15.b: The fluctuations on the right side of the TPC are much smaller for lines positioned closer to the center of the 1m TPC. This means the electric field is more uniform near the center of the TPC. The legend indicates which color corresponds to the distance in half-field-shaper-widths the line is away from the right array of field shapers. So line 6 (yellow) is 3 field shaper widths away from the right-side field shapers, and the electric field along this line fluctuates the least, as expected. The fluctuations of the electric field norm value along line 6 are only of 0.003 kV/cm. This is a much smaller fluctuation than the  $6^{th}$  line of the Demonstrator TPC (Figure 2.6.b), because the 1m TPC has a smaller radius and larger field shapers, making this  $6^{th}$  line much closer to the center of the TPC. But this fluctuation is slightly larger than the left side of the 1m TPC (Figure 2.14.b), because of the influence of the voltage supply device (explored in section 2.3.5).

#### 2.3.5 Voltage Supply Device

The voltage is supplied to the cathode by a wire running down the side of the TPC. The top half of the wire is surrounded by a ground, but the bottom half is exposed. This slightly affects the electric field inside the TPC, and thus the path of the electrons, (see Figure 2.15 and section 3.3), but it is more important to see that the supply wire does not cause an overwhelming spike in the electric field value anywhere in the chamber, as to cause a spark (see Figures 2.16 and 2.17). A smaller wire reduces these possible spikes, (see Figures 2.16, 2.17, 2.18, 2.19).



Figure 2.16: The electric potential inside the 1m TPC with the voltage supply feed. The equipotential lines are very horizontal and uniformly spaced inside the TPC. The supply feed does not have a noticeable effect inside the TPC. Dark blue marks -100 kV, the cathode voltage, progressing upwards to red, which marks 0 V, the ground. The equipotential lines progress similarly, going from dark red at the cathode voltage to white at the ground.



Figure 2.17: The electric field inside the 1m TPC with the voltage supply feed. Inside the TPC, the electric field lines are very uniform and vertical, as desired. The field lines inside the TPC curve slightly away from the voltage supply feed on the right side (the effects are explored further in section 3.3). The blue represents a norm field value of 1 kV/cm.



Figure 2.18: The electric field between the field shapers and the voltage supply feed in the 1m TPC. The electric field in this gap reaches a maximum value of 35 kV/cm, which is not large enough to start an electron break-down.



Figure 2.19: The electric field between the voltage supply feed and the wall in the 1m TPC. The average value of the field here is 52.6 kV/cm with peaks in the norm field value at the top and bottom of the exposed wire, creating peaks of 54 kV/cm in the field value, which is not expected to start an electron break-down.



Figure 2.20: The electric field between the field shapers and the thick voltage supply feed in the 1m TPC. The electric field in this gap reaches a maximum value of 35 kV/cm, which is not large enough to do damage to the detector. This is the same as for the thinner voltage supply wire (Figure 2.16), because the distance between the field shapers and the voltage supply wire was kept the same.



Figure 2.21: The electric field between the thick voltage supply feed and the wall in the 1m TPC. The average value of the field here is 77 kV/cm with peaks in the norm field value at the top and bottom of the exposed wire, creating peaks of 85 kV/cm in the field value, which could start a discharge. So a thinner voltage supply wire is ideal. The electric field peaks are higher here because of the simple parallel plate approximation of the wall and the wire,

$$E = V/d \tag{6}$$

where E is the electric field, V is the voltage, and d is the distance between the wire and the wall. For the thicker wire, this distance is smaller, causing a larger and possibly harmful electric field magnitude.

# 2.4 1T

The 1T TPC has a fairly uniform and vertical electric field. Any fluctuations from the field shapers diminish rapidly further towards the center of the TPC.

# 2.4.1 Electric Potentials

The cathode is supplied with -100 kV, the bottom field shaper is supplied with -97.5 kV, the next field shaper up is supplied with -95 kV, and so on, so that each subsequent field shaper voltage is increased by 2500 V, uniformly up to 0 V at the ground mesh (see section 2.2.4 to understand how this is implemented in the physical detector). This is done to create a uniform electric potential gradient of 1 kV/cm, which will cause a uniform electric field inside the TPC.



Figure 2.22: Electric Potential in the 1T TPC. The equipotential lines are fairly horizontal and uniformly spaced inside the TPC. The only disuniformities occur close to the mesh and field shaping wires (the effects of which are explored in sections 2.4.3). Dark blue marks -100 kV, the cathode voltage, progressing upwards to red, which marks 0 V, the ground. The equipotential lines progress similarly, going from dark red at the cathode voltage to white at the ground.

# 2.4.2 Total Electric Field

The equal spacing of the field shapers and linear change in voltage creates a uniform electric field inside the TPC. The field is uniform and downwards, meaning electrons will travel upwards through the TPC



Figure 2.23: Electric Field in the 1T TPC. Inside the TPC, the electric field lines are fairly uniform and vertical. There is definite warping near the field shapers and the cathode. The blue represents a norm field value of 1 kV/cm. The sparse concentration of field lines in the left interior is a flaw of the COMSOL mesh.

# 2.4.3 Field Shapers

The field shaping rings create small fluctuations in the electric field along the edge of the TPC. The fluctuations decrease quickly further towards the center of the TPC (see Figure 2.24.a, 2.24.b, 2.25.a, and 2.25.b). The electric field disuniformites from the field shapers affect the path of electrons through the TPC (see section 3 for details). The field must be controlled by these field shaping rings, as opposed to a solid metal cylinder, because it is impossible to create a uniform electric field accurately enough with a metal cylinder of uniformly varying resistance. In the physical detector, the field shapers potentials are regulated by resistors connected between adjacent field shapers. This allows for the voltage to vary uniformly along the length of the TPC with great precision.



Figure 2.24.a: The location of the lines the electric field is examined along, on the left side of the 1T TPC.



Figure 2.24.b: The fluctuations on the left side of the TPC are much smaller for lines positioned closer to the center of the 1T TPC. This means the electric field is more uniform near the center of the TPC. The legend indicates which color corresponds to the distance in half-field-shaper-widths the line is away from the left array of field shapers. So line 6 (yellow) is 3 field shaper widths away from the left-side field shapers, and the electric field along this line fluctuates the least, as expected. The fluctuations of the electric field norm value along line 6 are only of 0.006 kV/cm.



Figure 2.25.a: The location of the lines the electric field is examined along, on the right side of the 1T TPC.



Figure 2.25.b: The fluctuations on the right side of the TPC are much smaller for lines positioned closer to the center of the 1T TPC. This means the electric field is more uniform near the center of the TPC. The legend indicates which color corresponds to the distance in half-field-shaper-widths the line is away from the right array of field shapers. So line 6 (yellow) is 3 field shaper widths away from the right-side field shapers, and the electric field along this line fluctuates the least, as expected. The fluctuations of the electric field norm value along line 6 are only of 0.006 kV/cm.

# **3** Electron Collection Efficiency of the TPC

Varying numbers of electrons were released in different locations in each model, and their paths were plotted and studied. This aids in deciding upon an appropriate fiducial volume cut.

#### **3.1 Electrodynamic Theory**

The AC/DC Charged Particle Tracing module calls upon the results of the electrostatics study to properly plot the particles' paths. The paths are governed by the Coulomb Force,

$$F = qE$$
 (3)  
where *F* is the force, *q* is the charge of the particle, and *E* is the value of the electric field at  
any given position along the particle's path. This, combined with Newton's Second Law,  
gives each particle an acceleration,

$$a = \frac{qE}{m} \tag{4}$$

where a is the acceleration, and m is the particle mass. The Charged Particle Tracing module allows the user to choose either the Newtonian formulation, where the mass of the particles must be provided, or a massless formulation. However, even in the massless formulation, if the paths are chosen to be dependent on the electric field, they are still governed by the Coulomb Force, thus experiencing an acceleration.

This acceleration does not accurately describe the path of the electrons in the TPC. Instead, the electrons are experiencing an average drift velocity upwards, proportional to the electric field, because of the random motion of the electrons travelling through the liquid and interacting with other particles,

 $v_d \alpha E$  (5)

where  $v_d$  is the drift velocity and *E* is the electric field (see Appendix B for details). To ensure the drift is modeled accurately, the massless formulation must be chosen in COMSOL, and the velocity of the particles can be made dependent on the electric field value (see Appendix A) by proportion of an appropriate constant (see Appendices B and C).

Ionization causes roughly 100 quanta/keV to be created in the TPC, so to properly and efficiently analyze the electron paths, anywhere between 40 and 1000 electrons were released into the model at a given time.

#### **3.2 Demonstrator**

The Demonstrator TPC has a 50.3% electron collection efficiency when the electrons are released from a circular disk the full radius of the TPC (see Figure 3.4) and an average focusing of 0.33 cm transverse to the drift direction. It has a 100% collection efficiency for electrons released within a circle of radius 3.35 cm, which is 83% of the total radius (see Figure 3.5).

#### 3.2.1 Electron Paths

The electrons travel fairly uniformly upwards in the Demonstrator TPC (see Figure 3.1). Their paths are slightly skewed from the missing wire (see Figure 3.1), but they successfully travel upwards to the gas-liquid interface (see Figure 3.3).



Figure 3.1: Electron paths in the Demonstrator TPC. The electrons are released just above the height of uniform field (as explained in section 2.2.3). Their paths are slightly focused inward, due to the strong electric field near the field shaping wires, and the effect of the missing wire on the left side is noticeable. The color denotes time, with the particles released at time 0, so the uniform gradation of color confirms the constant drift velocity.



Figure 3.2: The bottom section of the electron paths in the Demonstrator TPC. The paths are skewed inwards, from the non-vertical electric field near the field shapers, and the effect of the missing cathode wire on the left is apparent, by skewing the paths further. Color represents time.



Figure 3.3: The top section of the electron paths in the Demonstrator TPC. The electrons arrive at the top of the TPC slightly focused from their starting points, but all successfully evade the ground mesh and arrive at the gas-liquid interface, so that they can be pulled into the gaseous xenon region and create the S2 signal.

# 3.2.2 Radius of 100% Efficiency

All electrons released within a radius of 3.35 cm from the center of the TPC will reach the liquid-gas interface. Beyond this, electrons will either escape through the gaps between the field shapers or get captured into the field shapers. The electrons within this radius experience a slight inward focusing of 0.33 cm transverse to their vertical drift direction.



Figure 3.4: Electron paths in the Demonstrator TPC. The electrons are released above the height of uniform field (explored in section 2.2.3), 1 cm above the cathode plate. Many electrons are lost in the first gap between the field shapers, and more towards the edge of the TPC are captured by the field shapers. 50.3% of the initial electrons arrive at the liquid-gas interface.



Figure 3.5: Distance electrons travel in the Demonstrator TPC. The colors indicate the release height in cm where 8 cm is the height of the cathode. Electrons were not released below a height of 9.5 cm, because cathode field disuniformities caused many of the electrons to travel to or through the cathode. A y-value of 1.0 means the electrons in this section reached the liquid-gas interface. An x-value of 7.5 cm corresponds to the center of the TPC, 3.487 cm is the left side, 11.513 cm is the right side. 100% efficiency is between 4.10 cm and 10.85 cm, corresponding to a radius of 3.35 cm.

# 3.3 1m

The 1m TPC has an 80.1% electron collection efficiency (section 6.5 explores why this is larger than for the Demonstrator) when the electrons are released from a circular disk the full radius of the TPC (see Figure 3.9) and an average focusing of 0.41 cm transverse to the drift direction. Including the influence of the voltage source wire, the 1m TPC has a 100% collection efficiency for electrons released within a circle of radius 2.9 cm, which is 83% of the total radius (see Figure 3.11).

# 3.3.1 Electron Paths

The electrons travel fairly uniformly upwards in the 1m TPC (see Figure 3.6). Their paths are influenced by the voltage source wire (see Figure 3.7), and they do experience some transverse focusing (see Figure 3.8).



Figure 3.6: Electron paths in the 1m TPC. The electrons are released above the height of uniform field (as explained in section 2.3.3). Their paths are slightly focused inward, due to the strong electric field near the field shaping wires, and they are also shifted leftward, due to the effect of the voltage supply device. The color denotes time, with the particles released at time 0, so the uniform gradation of color confirms the constant drift velocity.



Figure 3.7: Electrons are lost to the field shapers on the left side of the 1m TPC, because of the voltage supply wire on the right side. Color denotes time.



Figure 3.8: The bottom section of the electron paths in the 1m TPC. The paths are skewed inwards, from the non-vertical electric field near the field shapers. The effect of the voltage supply wire is barely noticeable, by the slight leftward skew of the paths. Color represents time.

# 3.3.2 Radius of 100% Efficiency

All electrons released within a radius of 2.9 cm from the center of the TPC will reach the liquid-gas interface. This radius is limited by the slight push from the voltage source wire. Beyond this radius, electrons will either escape through the gaps between the field shapers or get captured into the field shapers. The electrons within this radius experience a slight inward focusing of 0.41 cm transverse to their vertical drift direction.



Figure 3.9: Electron paths in the 1m TPC. The electrons are released above the height of uniform field (explored in section 2.3.3), 1 cm above the cathode plate. Only a few electrons are lost in the first gap between the field shapers (apparent in Figure 3.10), and more towards the edge of the TPC are captured by the field shapers. 80.1% of the initial electrons arrive at the liquid-gas interface.



Figure 3.10: Initial electron loss in the 1m TPC. Some electrons are lost to the first few field shapers (many less are lost in the 1m TPC than in the Demonstrator, this is explored in section 3.5).



Figure 3.11: Distance electrons travel in the 1m TPC. The colors indicate the release height in cm where 10 cm is the height of the cathode. Electrons were not released below a height of 13.5 cm, because cathode field disuniformities caused many of the electrons to travel to or through the cathode. A y-value of 1.0 means the electrons in this section reached the liquid-gas interface. An x-value of 7.5 cm corresponds to the center of the TPC, 4.03 cm is the left side, 10.97 cm is the right side. 100% efficiency is between 4.60 cm and 10.55 cm, corresponding to a radius of 2.90 cm.

# 3.4 1T

The 1T TPC has a 98.9% electron collection efficiency (section 3.5 explores why this is the largest of all of the TPC models) when the electrons are released from a circular disk the full radius of the TPC (see Figure 3.14) and an average focusing of 2.52 cm transverse to the drift direction. The 1T TPC has a 100% collection efficiency for electrons released within a circle of radius 48.95 cm, which is 97.9% of the total radius (see Figure 3.16).

# 3.4.1 Electron Paths

The electrons travel fairly uniformly upwards in the 1T TPC (see Figure 3.12). Their paths experience transverse focusing (see Figure 3.13).



Figure 3.12: Electron paths in the 1T TPC. The electrons are released at a height so that none escape down through the cathode mesh. Their paths are focused inward, due to the strong electric field near the field shaping wires. The color denotes time, with the particles released at time 0, so the uniform gradation of color confirms the constant drift velocity.



Figure 3.13: Bottom portion of the electron paths in the 1T TPC. The inward focusing is quite dramatic, with only a few electrons escaping to the field shapers. Color denotes time.

# 3.4.2 Radius of 100% Efficiency

All electrons released within a radius of 48.95 cm from the center of the TPC will reach the liquid-gas interface. Beyond this radius, electrons will either escape through the gaps between the field shapers or get captured into the field shapers. The electrons within this radius experience an inward focusing of 2.52 cm transverse to their vertical drift direction.



Figure 3.14: Electron paths in the 1T TPC. The electrons are released 1 cm above the cathode plate. Only a few electrons are to the first gap between the field shapers (apparent in Figure 3.15). 98.9% of the initial electrons arrive at the liquid-gas interface.



Figure 3.15: Initial electron loss in the 1T TPC. Some electrons are lost to the first few field shapers (many less are lost in the 1T TPC than in the other TPCs, this is explored in section 3.5).



Figure 3.16: Distance electrons travel in the 1T TPC. The colors indicate the release height in cm where 8 cm is the height of the cathode. Electrons were not released below a height of 12 cm, because cathode field disuniformities caused many of the electrons to travel to or through the cathode. A y-value of 1.0 means the electrons in this section reached the liquid-gas interface. An x-value of 55 cm corresponds to the center of the TPC, 5.5 cm is the left side, 104.5 cm is the right side. 100% efficiency is between 6.05 cm and 103.95 cm, corresponding to a radius of 48.95 cm.

#### 3.5 Comparison

The most electrons were lost in the Demonstrator TPC, less in the 1m TPC, and even less in the 1T TPC. Following this same trend, the electron paths were slightly focused in the Demonstrator TPC, more so in the 1m TPC, and very much so in the 1T TPC. Both of these trends are due to the release sites, geometry, and electric potentials of the TPCs.

In each TPC, the electrons were released 1 cm above the cathode (refer to the 3D Figures 3.4, 3.9, and 3.14). For the Demonstrator and 1m TPCs, this is within the first gap between the cathode ring and the first field shaper. This gap is larger in the Demonstrator TPC (0.7815 cm) compared to the gap in the 1m TPC (0.375 cm), so there is an increased chance of escape in the Demonstrator TPC. In the 1T TPC, this release height is within the cathode ring, so the electrons experience an immediate inward push, causing less to be lost to the first field shapers.

The electron paths are more focused in the 1m TPC than in the Demonstrator TPC, because of the larger cathode voltage and field shaper voltages, which cause a strong inward push. The electron paths are most focused in the 1T TPC, because of the larger size of the TPC and the large cathode voltage. Compared to the radius of the TPC, the Demonstrator TPC maximum focus distance is 8.2% of its radius, the 1m TPC maximum focus distance is 11.8% of its radius, and the 1T TPC maximum focus distance is 5% of its radius. The percentage for the 1m TPC is largest because of its small radius and large cathode voltage. This focusing effect is only dramatic for the electrons close to the edge of the TPC, so an appropriate fiducial cut would minimize the corrections needed to compensate for this focusing.

#### 4 Summary

The XENON Dark Matter Project is using LXe TPCs to detect WIMPs. The XENON100 detector has produced the most stringent limits on WIMP interactions to date. The project is now moving into its final phase, XENON1T. This detector will host a 1000 kg fiducial volume of LXe.

In preparation for the final stage of the project, multiple TPCs were created and simulated. A detailed analysis of the electric field and electron collection efficiency of the simulated TPCs was completed. The Demonstrator TPC has been built, tested, simulated, and deconstructed. The 1m TPC is being built, and the 1T TPC is just a simulated prototype.

In the electrostatic simulations, each TPC has a uniform, vertical electric field, as desired. There is some field line disuniformity near the cathode wires and field shapers in each TPC, but these fluctuations die off quickly toward the center of the TPC. The fluctuations from the cathode wires subside after 0.917 cm above the cathode in the Demonstrator TPC, and 0.52 cm above the cathode in the 1m TPC, so the electric fields are uniform throughout the majority of both TPCs. Also, the guard mesh in both TPCs achieves its purpose of effectively shielding the lower PMTs from the strong electric field.

In the electrodynamic simulations, each TPC successfully ushers electrons upwards to the xenon liquid-gas interface. Only some of the outer electrons escape through the sides of the TPC. The Demonstrator TPC has an overall electron collection efficiency of 50.3%, with 100% efficiency inside a radius 83% the size of the total radius. The 1m TPC has an overall electron collection efficiency of 80.1%, with 100% efficiency inside a radius 83% the size of the total radius. And the 1T TPC has an overall electron collection efficiency of 98.9%, with 100% efficiency inside a radius 97.9% the size of the total radius. As the electrons travel upwards through the TPCs, they also experience some transverse inward focusing of their paths. In the Demonstrator TPC, this focusing is 8.2% the length of the total radius. In the 1m TPC, it is 11.8% the length of the total radius. And in the 1T TPC it is 5% the length of the total radius.

With an appropriate fiducial cut, based on these results, the WIMP interaction vertex can be reconstructed with very high precision.

# Appendices

# **Appendix A: Methods**

This appendix provides step-by-step instructions for creating and studying the TPC models in COMSOL 4.2/4.2a.

- 1. Create 2D and 3D Models of the TPC, using the COMSOL Multiphysics Software Package.
  - a. Base models on the given specifications of the TPC.

Specifications	Demonstrator TPC	1m TPC**	1T TPC**	Notes
TPC height	30.013 cm	1 m	1 m	
Inner Radius	4.013 cm	3.47 cm	0.5 m	Radius to innermost edge of Field Shapers
Total Radius	7.5 cm	7.5 cm	-	Just needs to be large enough to contain Field Shapers entirely
Cathode Voltage	-15 kV	-100 kV	-100 kV	
Anode Voltage	2.4 kV	-	-	Because of the shielding from the ground mesh (see Geometry), this can be ignored in the model
Number of Field Shapers	21	66	39	
Voltage Drop Between Field Shapers	681.1 V	1492.5 V	2500 V	Calculated so that the drop is 1[kV/cm] from the cathode to the ground
Field Shaper Spacing	1.4 cm	1.5 cm	2.5 cm	Center-to-center
Field Shaper Width	0.3 cm	0.66 cm	1 cm	
Field Shaper Height	0.3 cm	1 cm	2 cm	
Cathode, Field Shaper, Mesh shape	-	-	-	See Geometry (1.c.)
Number of Mesh Wires	14	11	-	2D only(Demonstrator missing one)
Mesh Wire Radius	0.007 cm	0.01 cm	-	
Materials	-	-	-	See Materials (1.d.)
Space from Bottom of TPC to lowest Field Shaper/ from highest Field Shaper to Top of TPC	-	-	-	Even spacing on top and bottom
Space Between Anode and Ground Mesh	0.5 cm	0.5 cm	-	
Space Between Cathode and Protective Meshes	2 cm	2 cm	-	2D only, because of shielding, can be ignored
Protective Mesh Voltage	1600 V	1700 V	-	

Table A.1: Model Specifications\*

\*Anything left unspecified does not have a significant impact on the model. For example, the height of the liquid xenon layer does not matter as long as it falls in between the ground mesh and cathode.

\*\*Note that the 1m TPC and 1T TPC are still test models, while the Demonstrator TPC has actually been built. Many of the values for these TPCs have been left blank, because they are not yet specified. In the case where they are not specified, the Demonstrator values were used.

# b. Define global parameters in order to easily adapt models to differently sized TPCs.

Name	Expression*	Value**	Description
UniverseLength	D+BottomSpace+gasD+0.25 cm	0.39963 m	total height
UniverseWidth	15 cm	0.15 m	total width
BottomSpace	8 cm	0.08 m	space underneath cathode
gasD	1.7 cm	0.017 m	height of gas at top of TPC
radius	0.15 cm	0.0015 m	radius of field shaper coil
length	8.026 cm	0.08026 m	diameter of TPC
D	30.013 cm	0.30013 m	height of TPC
d	0.5 cm	0.005 m	distance between mesh wires
dMin	1.4 cm	0.014 m	minimum distance between center of field shaping coils
dd	2 cm	0.02 m	distance between cathode and guard mesh
ddMin	(D-3*radius-20*dMin)/2	0.007815 m	distance between cathode and first field shaper, last field shaper and ground mesh
radiusWire	0.007 cm	7e-5 m	radius of mesh wires
Vc	-15 kV	-15000 V	cathode voltage
Va	2.4 kV	2400 V	anode voltage
Vmesh	1.6 kV	1600 V	guard mesh voltage
deltaV	Vc/22	-681.82 V	difference in voltage between each ring
mu	-0.000002 m^2*V^-1*s^-1	$-2e-6 \text{ m}^2/(\text{Vs})$	electron mobility xenon

\* Note that these are the values given for the 2D Demonstrator TPC model. Values will change for each model, according to Table 1.

\*\* COMSOL automatically calculates the Value from the Expression. The Value column is included here for completeness.

#### Table A.3: 3D Model Parameters

Name	Expression*	Value**	Description
TotalR	7.5 cm	0.075 m	total radius
TotalL	TPCh+BottomSpace+2*TopSpace	1.06 m	total height
BottomSpace	4 cm	0.04 m	space underneath cathode
TopSpace	1 cm	0.01 m	space above anode
gasD	1.6 cm	0.016 m	height of gas at top of TPC
TPCr	3.8 cm	0.038 m	TPC radius
TPCh	1 m	1 m	TPC height
CuR	0.25 cm	0.0025 m	radius of field shaper coil
d	1.5 cm	0.015 m	distance between field shaper centers
dMin	(TPCh-65*d-4*CuR-3*CuR)/2	0.00375 m	minimum distance between center of field shaping coils
Vc	-100 kV	-1e5 V	cathode voltage
Va	2.4 kV	2400 V	anode voltage
deltaV	Vc/67	-1492.5 V	difference in voltage between each ring
mu	-0.000002 m^2*V^-1*s^-1	$-2e-6 \text{ m}^{2}/(\text{Vs})$	electron mobility xenon

\* Note that these are the values given for the 3D 1m TPC model. Values will change for each model, according to Table 1. \*\* COMSOL automatically calculates the Value from the Expression. The Value column is included here for completeness. c. Create geometry of the TPC.

	Shape	Location	Size	Action*
1.	Total Rectangle	Corner: (0, 0)	X: UniverseWidth Y: UniverseLength	
2.	Rectangle Gas	Corner: (0, UniverseLength-gasD)	X: UniverseWidth Y: gasD)	
3.	Cathode Mesh Circle	Center: ((UniverseWidth-length)/2+d, BottomSpace)	Radius: radiusWire	Array: x:15or11, y:1 Displacement: x:d, y:0
4.	Protective Mesh Circle	Center: ((UniverseWidth-length)/2, BottomSpace-dd)	Radius: radiusWire	Array: x:17, y:2 Displacement: x:d, y:-d
5.	Ground Mesh Circle	Center: ((UniverseWidth-length)/2, BottomSpace+D+radiusWire)	Radius: radiusWire	Array: x:17, y:1 Displacement: x:d, y:0
6.	Anode Mesh Circle	Center: ((UniverseWidth- length)/2+d/2, BottomSpace+D+d+2*radiusWire)	Radius: radiusWire	Array: x:16, y:1 Displacement: x:d, y:0
7.	Cathode Bottom Rectangle	Corner: ((UniverseWidth-length)/2- radius, BottomSpace-5*radius)	X: 4*radius Y: 5*radius	Fillet: (bottom 2 corners) 2*radius Array: x:2, y:1 Displacement: x:length- 2*radius, y:0
8.	Cathode Top Rectangle	Corner: ((UniverseWidth-length)/2- radius, BottomSpace)	X: 2*radius Y: 3*radius	Fillet: (top 2 corners) radius Array: x:2, y:1 Displacement: x:length, y:0
9.	Field Shaper Rectangle	Center: ((UniverseWidth-length)/2, BottomSpace+ddMin+3*radius)	X: 2*radius Y: 2*radius or 4*radius	Fillet: (all corners) radius Array: x:2, y:21or66 Displacement: x:length, y:dMin

Table A.4: 2D Model Geometry Steps

\* Demonstrator TPC directions listed first, 1m TPC after the "or."



Figure A.1: Finished 2D Geometries (Demonstrator left, 1m center, 1T right).

Table A.5:	3D Model	Geometry Steps
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	Shape	Location	Size	Action
1.	Total Cylinder	(0, 0, 0)	Radius: TotalR Height: TotalL	
2.	Cylinder Gas	(0, 0, TotalL-gasD)	Radius: TotalR Height: gasD	
3.	Cathode Plate Work Plane (xy- plane, z-coordinate: BottomSpace) Geometry: Circle	Center: (0, 0)	Radius: TPCr	
4.	Ground Work Plane (xy-plane, z- coordinate: BottomSpace+TPCh) Geometry: Circle	Center: (0, 0)	Radius: TPCr	
5.	Anode Work Plane (xy-plane, z- coordinate: TotalL-TopSpace) Geometry: Cirlce	Center: (0, 0)	Radius: TPCr	
7.	Field Shaper Work Plane (yz-plane, x-coordinate: 0) Geometry: Rectangle	Center: (TPCr, BottomSpace+dMin+3*CuR+2*CuR)	X: 2*CuR Y: 2*CuR or 4*CuR	Fillet: (all corners) CuR Array: x:1, y:21or66 Displacement: x:0, y:d Revolve: point: (0, 0), revolution axis: (0,1) Convert to Solid
8.	Cathode Ring Work Plane (yz- plane, x-coordinate: 0) Geometry: 2 Rectangles	1. Corner: (TPCr-CuR, BottomSpace) 2. Corner: (TPCr-3*CuR, BottomSpace-5*CuR)	1. X: 2*CuR Y: 3*CuR 2. X: 4*CuR Y: 5*CuR	<ol> <li>Fillet (top 2 corners) CuR</li> <li>Fillet (bottom 2 corners) 2*CuR</li> <li>Revolve: point: (0,0), revolution axis: (0,1)</li> <li>Convert to Solid</li> </ol>



Figure A.2: Finished 3D Geometries (Demonstrator left, 1m center, 1T right).

- d. Select materials and modify accordingly.
  - i. Blue: largest domain liquid xenon (start with liquid water from material library, change relative permittivity to 1.9)
  - ii. Orange: coils copper (from material library) for Demonstrator, aluminum (from material library) for 1m
  - iii. White: mesh, cathode, anode, ground stainless steel (from material library)
  - iv. Gray: top domain xenon gas (start with air from material library, change relative permittivity to 1.0)



Figure A.3: Materials of the 2D and 3D models.

- e. Mesh the geometry.
  - i. Mesh with the smallest size possible, which still allows COMSOL to run in a reasonable amount of time. The 2D models should pose no problem, but the 3D models may be more time-consuming.
  - ii. 2D mesh element count should be  $10^5$ , 3D mesh count should be  $10^6$  (exact count: 2D 921440 elements, 3D 4098929 elements).
  - iii. Tips:
    - 1. Make sure that the minimum element size is smaller than the diameter of the mesh wires (0.007 cm) in the 2D models.
    - 2. For the 3D models, start with a "Normal" sized mesh, then save, then try a smaller element size ("Fine" is small enough to get reasonable results).



Figure A.4: Meshed Geometry.

# Perform an Electrostatics Study using the AC/DC Module. a. Apply electric potentials to geometric objects.



Figure A.5: Electric potentials schematic diagram with instructions.

- b. Perform a stationary study.
  - i. Check that the study is only dependent on the Geometry, Mesh, and Electrostatics.
- c. Acquire appropriate graphs.
  - i. Electric potential (choose the Multislice option, which includes 2D cross sections in the result)
  - ii. Electric field (in various locations: close to field shapers, close to cathode mesh, etc.) (choose the Streamline with Color Expression option to show the total electric field)
- 3. Study Charged Particle Tracing, using the AC/DC Module.
  - a. Choose massless formulation.
  - b. Apply study dependencies.
    - i. Check that the study is only dependent on the Geometry, Mesh, and Charged Particle Tracing. Electrostatics should not be selected at this time. In order to use the results from the Electrostatics study (which is necessary, as Charged Particle Tracing will need to draw upon the stationary study results), select "Values of variables not solved for" under "Values of Dependent Variables," and choose "Method: Solution," "Study: Study1, Stationary," "Stationary: Automatic."

- c. Define particle type.
  - i. For electrons, enter velocities dependent on the electric field (explained in section 3.1 and Appendix B):
    - $v_x = mod1.es.Ex*mu$
    - $v_y = mod1.es.Ey*mu$
    - $v_z = mod1.es.Ez*mu$
- d. Define wall properties.
  - i. Choose the "bounce" option for the liquid-gas interface (when the particles hit this wall they will bounce off with a reflected angle equal to the incident angle). This accurately describes what happens in the chamber, because if an electron escapes and hits this liquid-gas interface without passing through the ground mesh, it will not likely have enough energy to bridge the gap into the xenon gas. Choose "freeze" for the field shapers (when the particles hit this section they will stick there), as well as for the outer walls and ground mesh. This is accurate, because if an electron follows the electric field lines and hits a field shaper, it will be absorbed.
- e. Define particle inlet
  - i. For the 2D models: Define a Release from Grid, with the release time at 0, initial coordinates in a horizontal line inside the TPC, and initial velocity in the y direction. For these models, initial x range from 4 to 10 with 40 values, initial y value of 10 works well.
  - ii. For the 3D models: Under Geometry, define a Work Plane Inlet. The plane should be an xy-plane, positioned just above the cathode. Its geometric objects can vary depending on what needs to be studied. In general, a z-coordinate of "BottomSpace+TPCh/150" and circle with radius "TPCr-CuR" works well (for more advanced studies, inlet rings can easily be created). Define a Release, select the inlet just created as the domain, with release time 0, number of particles per release 1000, and density proportional to 1.
- f. Set appropriate time duration.
  - i. This is dependent on the initial velocity, electric field, and height of the TPC. So for these models, 10 s with 100 values works well.
- g. Perform a time dependent study.
  - i. Check that the dependencies are correct (3.b. and 3.f.). Also, for faster results (especially for the 3D models), select "Generate default plots" only, not "Generate convergence plots."
- h. Acquire appropriate graphs.
  - i. particle trajectories
  - ii. cross-sections of particle trajectories (Poincaré Map of Cut Plane, Color Expression showing either Particle velocity or Particle index is useful for analysis)
- i. Create animation of particle trajectories.
  - i. Under Export, create an Animation from Particle Trajectories (cpt), output type movie (AVI works best), quality between 0 and 1, 4 frames per second works well, and use all output times. The animation file saves to the location where the model is saved.
- 4. Perform Data Analysis.
  - a. Check uniformity of electric field.

- i. In Streamline plots of the 2D and 3D models, the field lines should be uniform and vertical. Likewise, Contour lines of the electric potential should be uniform and horizontal. Any fluctuations due to the field shapers or cathode mesh should disappear towards the center and further up the TPC.
- b. Analyze the particle attenuation throughout length of TPC and the particle collection efficiency at top of TPC.
  - i. Feed screen shots (taken with Microsoft's Snipping Tool) of Poincaré Maps of different horizontal cut planes into DotCount (v1.2, March 2012, Dr. Martin Reuter) [1], and count the number of particles, with appropriate settings.



Figure A.6: Dot Count Program.

- ii. Tips:
  - Create Cut Planes under Data Sets, choosing the Cut Plane Data set to be "Particle 1." Make 20 Cut planes (xy-planes with z-coordinates "BottomSpace+TPCh/20," "BottomSpace+2\*TPCh/20," etc.).
  - 2. In COMSOL, set particle radius to 0.02 with scale factor 1. In DotCount, choose minimum size 4, maximum size 16.
  - 3. For 2D models, merely looking at the trajectories and counting by hand should work.
- c. Analyze particle paths, to understand corrections needed to determine interaction vertex coordinates.
  - i. For example, if particles spread out as they travel upwards, take this extra horizontal movement into account when calculating the origin of the particle.

#### **Appendix B: Electron Drift**

Section 3.1 explained that COMSOL uses the Coulomb Force equation to calculate charged particle trajectories, but does not take into account inter-particle interactions. In reality, the electrons in the TPC will not simply accelerate upwards in the TPC, but instead have an average drift velocity which is proportional to the electric field. This is because the energy gained from the acceleration due to the electric field is canceled out by the energy lost from collisions with atoms, resulting in a constant drift velocity. As mentioned in section 3.1, it is possible to change the relationships in COMSOL so that the particles do in fact experience this drift velocity. The challenging part is defining the proportionality constant.

In theory, the drift velocity should depend on the electron mobility,  $\mu$ , in the substance,

$$\overline{v_d} = \mu \vec{E} \tag{6}$$

where  $v_d$  is the drift velocity, and *E* is the electric field [2]. However, for the conditions of the LXe in the TPCs, the mobility is not always the same value. See Appendix C for further discussion on determining the value of the electron mobility in LXe.

More precisely, the drift velocity can be expressed,

$$\overline{v_d} = \frac{2}{3} \frac{q\vec{E}}{m} \frac{\lambda_e}{u} \tag{7}$$

where q is the charge of the electron,  $\lambda_e$  is the mean free path of the electron, m is the mass of the electron, and u is the initial velocity of the electron, usually taken to be the thermal velocity [2]. The mean free path takes into account the effects of particle collisions.

If a Maxwellian velocity distribution is assumed for the electrons, the velocity can be approximated,

$$v_d \sim (\sqrt{\frac{\Delta\varepsilon}{2}} \frac{qE}{m} \lambda_e)^{1/2} \tag{8}$$

where  $\Delta \varepsilon$  is the fraction of energy  $\varepsilon$  lost in one collision [2]. The energy term further accounts for the effect of the particle collisions.

If the energy dependence is approximated by power laws,

$$\Delta \varepsilon \sim \varepsilon^m \tag{9}$$

$$\lambda_e \sim \varepsilon^{-n} \tag{10}$$

then the drift velocity can be approximated,

$$v_d \sim E^{(m+1)/(m+2n+1)} \tag{11}$$

where *E* is the electric field [2].

In this study of the electric field inside the TPC, it suffices to use a reasonable proportionality constant to relate the drift velocity to the electric field. So using the massless formulation in COMSOL, the particle velocity will be denoted,

$$v_x = mod1.es.Ex^*constant$$
  
 $v_y = mod1.es.Ey^*constant$  (12)  
 $v_z = mod1.es.Ez^*constant$ 

which uses the COMSOL syntax to call upon the calculated electric field components to create the user-defined velocity. The constant value is discussed in Appendix C.

# **Appendix C: Electron Mobility in Liquid Xenon**

The electron mobility,  $\mu$ , of LXe varies with temperature, pressure, density, and electric field. The theory behind the electron mobility of LXe is not well understood, so most values are found experimentally.



Figure C.1: "In liquid xenon, there is a dramatic drop in the mobility approaching the critical temperature and the number of energy levels in an average size fluctuation goes up at the same time." [3]

Figure C.1 would suggest that LXe mobility values could range from 0.00027  $m^2/Vs$  to 0.0054  $m^2/Vs$ . If these values are used in the simulation, the electron paths are far too linear. The electrons reach the edges of the TPC before they have a chance to truly follow the electric field lines.

Working backwards, the drift velocity should be 2 mm/ $\mu$ s [4], and the electric field is 1 kV/cm, which would give a mobility of 0.02 m<sup>2</sup>/Vs,

$$\mu = \frac{v_d}{E} \tag{13}$$

which is still far too large for the simulation. Instead, a value of  $2 \times 10^{-6}$  m<sup>2</sup>/Vs was used, giving reasonable paths.

# References

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