Considerations for Modeling Electron Drift in Argon and Helium

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Introduction

Reuter-Stokes has been a leading supplier of gas filled neutron and gamma detectors since 1956. In all cases the incident radiation generates electrons, either directly or indirectly, which are directed to an anode by the application of an electric field. Since the amount of charge initially produced is small the charges are amplified using a technique often referred to as *gas gain*. The principle is that electrons gain enough energy in the electric field to ionize gas atoms which then ionize others in a cascade resulting in a signal to noise ratio that is high enough to yield a measurable pulse. The objective of the work described in this paper was to better understand how electrons interact with the gas by way of electron to atomic collisions. These collisions are of various types and their combined effect determines velocity and the gas ionization as a function of gas mix and electric field. Since there are too many detector configurations to model in one study a small number of cases were chosen with the hope that if results could be obtained that reasonably agreed with published data, we could be confident that more complex cases could be modeled.

Cases Chosen for Study

One of the primary causes for complexity in modeling electron transport is the electric field within the detector. Typically, the geometries are cylindrical where a small diameter anode lies at the center of the tube. This yields a non-linear electric field as opposed to a parallel plate geometry where the field is constant. Since data is available in the literature for the constant field case, all the simulations described in this paper use a 3D parallel plate geometry. The assumption is if these models agree with existing data, we can have a level of confidence that models with more complex geometry will yield useful solutions. An additional variable is the gas used as the detection medium, and the two most common species are Ar with CH_4 and ^{3}He with Ar. Since data for Ar/CH_4 and He/Ar are readily available it is these two mixtures which will be modeled, and in all cases the pressure will be 760 torr.

Drift Velocity Model

The first step was applying COMSOL charged particle tracing id to determine the drift velocity of electrons in the selected gas mixes. Collisions that require inclusion in the simulation are elastic, excitation and ionization. For each gas species collision cross section data is required as a function of electron energy. An open-access database named LXCat[1] is available and was used as the source of these cross sections. As an example, the following plot shows the cross section of Argon for these three collision types. Note that there are three different excitation cross sections having different excitation energies.

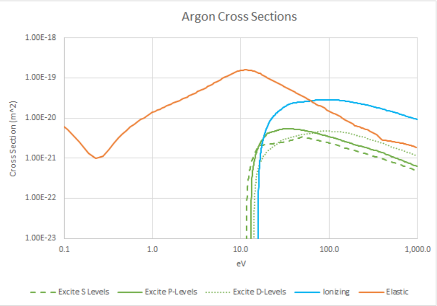


Figure 1. Argon Cross Sections

Once cross sections are established the next parameter is the time step. What was not initially understood was the difference between the model and the solver time step. The former is used to stipulate how often a result is saved, while the later determines how often a collision step is solved for. As a rule of thumb the COMSOL designers have recommended a solver time step 10x the average collision interval and it is this relationship that was evaluated in the first phase of the study. Since we had no data at the beginning to determine the proper solver time step the collisions per second can be estimated from the cross section and is displayed in Figure 2.

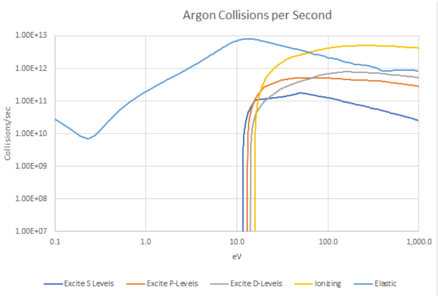


Figure 2. Argon Collision Rate

Based on this data the maximum collision frequency is 10^{13} collisions/sec it was determined to run the simulation with solver time steps of 10^{-12},10^{-13} and 10^{-14} seconds to study how this parameter affects the outcome.

Results as a Function of Solver Time Step

The gas combination studied for this analysis was Ar/CH_4 (90%/10%). To perform the particle tracing simulation electrons are released into the gas under the condition of a constant electric field. Figure 3 shows a typical particle trajectory for a field of 5 kV/cm and a total time of $4e^{-8}$ seconds.

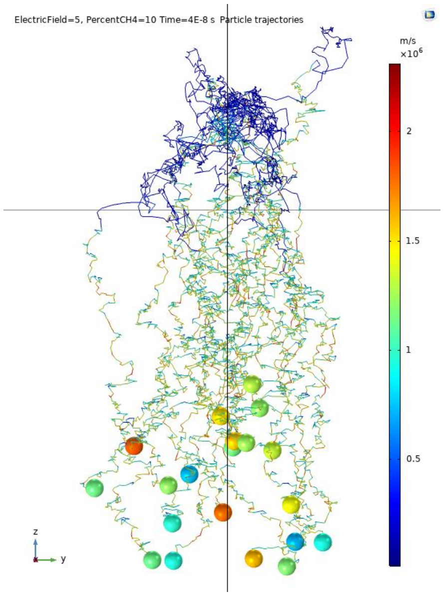
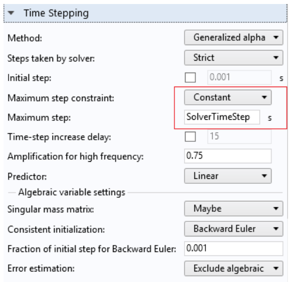


Figure 3. Particle Trajectories

To control the solver time steps the time-dependent solver must be constrained by fixing the maximum step size. The following screen-shot shows the settings for the time stepping portion of the solver configuration. The highlighted area shows the parameters that are used for this purpose.


Time Stepping

Method: Generalized alpha
Steps taken by solver: Strict
Initial step: ☐ 0.001 s
Maximum step constraint: Constant
Maximum step: SolverTimeStep s
Time-step increase delay: ☐ 15
Amplification for high frequency: 0.75
Predictor: Linear
Algebraic variable settings
Singular mass matrix: Maybe
Consistent initialization: Backward Euler
Fraction of initial step for Backward Euler: 0.001
Error estimation: Exclude algebraic

Figure 4. Time Dependent Solver Configuration

To illustrate how the time step affects the result the drift velocities are plotted for 3 solver time steps, 10^{-12}, 10^{-13} and 10^{-14} seconds.

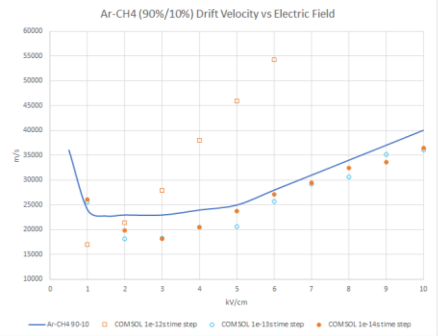


Figure 5. Drift Velocity vs Electric Field

The solid line was taken from research being done at CERN[2,3], and the marker values were computed by COMSOL for the 3 different solver time steps. The results show significant deviation from the expect values for a step of 10^{-12} s. Once the step is reduced to 10^{-13} s further reductions have a minimal effect on the outcome. This result is in line with the guidance to use a step size 0.1 times the collision interval, which would suggest a step of 10^{-14} s.

Commented [SAI(1]: Is this true? I thought in this case the collision interval was 10e-13 sec, which means 10e-14 is 1/10X the collision interval not 10X

Drift Velocity Results

The results for the four Argon and Helium cases are plotted in the following figures. A 10^{-14} second time step was used in generating these plots.

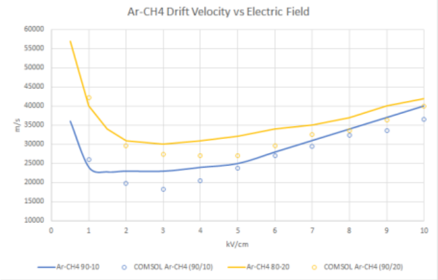


Figure 6. Ar-CH4 Drift Results vs Published Data

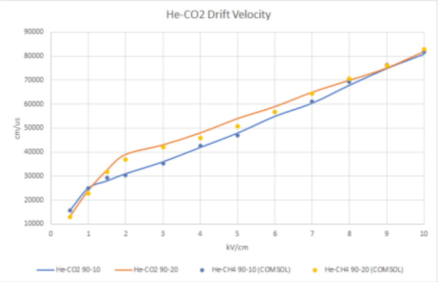


Figure 7. He-CO2 Drift Results vs Published Data

Drift Velocity Transient Behavior

Electrons released into the gas do not necessarily reach their steady state velocity immediately. When electrons are released with a Maxwellian energy distribution in thermal equilibrium the electrons take time to reach their steady-state drift velocity. This time depends on the electric field but typically is on the order of 10^{-8} s. Since the total simulation time was typically 10^{-6} to 10^{-7} seconds the initial transient period needed to be excluded before calculating the average velocity.

Townsend Coefficient and Gas Gain

The Townsend coefficient (α) in units of cm^{-1} is the number of ionization collisions per unit length and can be used to calculate the gas gain over a distance. The value of the gain is expressed by the following equation where d is the distance (d) the electrons travel.

$$gain = e^{\alpha d}$$

This relationship will only apply for uniform electric fields. For gain determination in more complex fields, secondary electrons will need to be generated and tracked as they follow the electric field and will again release further electrons as they gain energy. Since in this paper we are assuming a parallel plate geometry, secondary electrons are not necessary since we can determine gain by the Townsend coefficient alone.

As with the drift study, Townsend coefficients are available as a function of electric field and those used in this paper are from the CERN publication[2] shown in the references. To compute the values from the model the number of ionization collisions is used along with the distance traveled in the direction of the electric field as follows.

$$\alpha = \frac{\textit{Number of Ionization Collisions}}{\textit{Distance Traveled}}$$

Results from the ArCO2 gas mixes are below. What is noteworthy in the results is that in determining ionization a smaller time-step is needed vs. calculating the drift velocity.

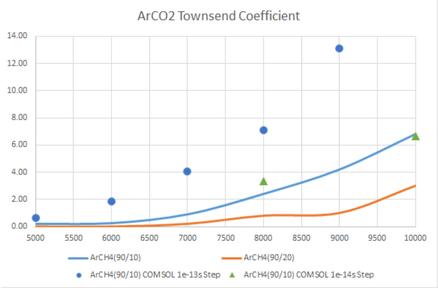


Figure 8. Townsend Coefficients for Ar/CH4

Un-Accounted for Gain Phenomenon

There are two mechanisms identified that generate ionizations in the gas that are not being modeled in COMSOL and may generate incorrect values since their effects are not included in the Townsend coefficient. The first is the release of electrons by the *photoelectric effect*. This occurs when the gas atom's

Commented [SAI(3]: Uniform? Constant implies a time element.

Commented [SAI(2]: Any hypothesis around why the He-CO2 results are better than Ar-CH4? Is this related to molecular structure?

excited electrons return to their ground state and emit a UV photon. These photons are then absorbed by another atom thereby ejecting an electron into the gas. Typically, in radiation detectors a “quench” gas such as CH_4 is used to absorb these photons and prevent photoelectric emission. The second phenomenon is referred to as the *Penning effect*. This occurs when the excitation state of the gas is higher than the ionization energy of an additive gas component. A collision between an excited atom and another at its ground state can transfer energy to the additive gas component thereby producing an electron. In typical cases where the gas gain is required this effect can by significant.

Commented [SAI(4]: These two sections should probably be moved before the Conclusions. As it stands, it does not flow very well.

Conclusions

The simulated results reasonably match with expectations, but the exercise has demonstrated the importance of the time steps. One of these limitations is simply the time to execute the simulation, especially where the electron path lengths are long. Utilizing a batch sweep can greatly reduce the modelling time for multiple parametric cases but there are limitations to how much parallelism can be applied to a single particle tracing model. This time issue is particularly problematic for determination of gas gain where a very small step is required. In real world cases the distance electron travel is on the order of centimeters and this severely limits the usefulness of particle tracing for these cases.

References

1. LXCat is a component of the open source data base Plasma Data Exchange Project.
https://fr.lxcat.net/home/

2. Transport Properties of Operational Gas Mixtures used at LHC. Y.Assran* Suez Canal University and A.Sharma CERN CH1211 Geneva, Switzerland
https://arxiv.org/ftp/arxiv/papers/1110/1110.6761.pdf

3. Drift and Diffusion of Electrons in Gases.
Anna Peisert and Fabio Sauli
https://inis.iaea.org/collection/NCLCollectionStore/_Public/15/073/15073101.pdf?r=1&r=1

Acknowledgements

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