EGS4 Artifacts in the Production of Čerenkov Radiation
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EGS4 contains a number of non-physical parameters introduced to allow the modelling of various physical processes; the most usually discussed are ESTEPE, the parameter that controls the maximum allowable step length, and AE, the parameter that defines the calculational boundary between discrete interactions and continuous energy loss for electrons. In this case, a discrete interaction is one in which a secondary particle is created and placed on the stack to be subsequently followed.

The fact that these (non-physical) parameters can produce 'artifacts'[1] is well documented [1, 2]. However, this document sets out to explore a specific form of artifact; the artifacts in the angular distribution of Čerenkov photon, which have been the subject of recent discussion.

1 The problem...

The problem is that multiple scattering of the electron is applied at the end of any one step - during the step, the electron is assumed to be moving in a straight line; thus all the Čerenkov photons come out at the Čerenkov angle with respect to the electron's initial direction. This may be important for pattern recognition software, as this feature will presumably give more of a pattern than should be there.

For high energy electrons, this feature is not so much of problem. Using the formulae given in [3], an infinite volume of water and assuming a step length of 1% gives a multiple scattering angle of $\sim 1°$ per step for a 50 MeV electron, $\sim 3°$ for a 5 MeV electron, $\sim 7°$ for a 1 MeV electron. It should be noted however, that the approximations made in deriving the multiple scattering angle formula given in [3] are only valid for step lengths of larger than $\sim 0.01\%$ of the material's radiation length (36 cm in the case of water) and that the estimates given above for low energy electrons are operating on the limit of the approximations. Nevertheless, they do demonstrate that whilst a 50 MeV electron is essentially undeviated on any one step, a low energy electron ends a step with an obviously different direction than it had at the start of the step. Assuming that all the Čerenkov radiation is emitted at the Čerenkov angle with respect to the direction of the electron at start of the step will unrealistically clump the photons. More importantly, the level of this clumping will be a function of how often the direction of the electron is updated - ie a function of the step length.

The presence of the an artifact is easy to demonstrate; Table 1 shows assorted parameters describing the Čerenkov angular distribution for different values of AE and ESTEPE. The simulation assumes 5 MeV electrons stopping in an infinite volume of heavy water. The

[1] In this case, an artifact is defined as a feature of the calculation that varies with the non-physical parameters.

AE = 10 KeV									
ESTEPE	Frac-1	Frac-2	0-30	30-60	60-90	90-120	120-150	150-180	$\bar{\theta}$
0.1%	0.025	0.112	0.155	0.504	0.223	0.082	0.030	0.007	55.2
1.0%	0.034	0.117	0.152	0.506	0.218	0.084	0.031	0.008	55.6
3.0%	0.049	0.130	0.150	0.513	0.218	0.083	0.030	0.007	55.2
5.0%	0.059	0.141	0.148	0.517	0.215	0.082	0.029	0.007	55.1
0.01%	0.029	0.134	0.183	0.598	0.186	0.029	0.003	0.000	47.0
Default	0.193	0.256	0.142	0.603	0.181	0.055	0.016	0.003	53.4
AE = 100 keV									
ESTEPE	Frac-1	Frac-2	0-30	30-60	60-90	90-120	120-150	150-180	$\bar{\theta}$
0.1%	0.025	0.113	0.156	0.507	0.222	0.080	0.028	0.007	55.0
1.0%	0.034	0.118	0.153	0.507	0.222	0.081	0.029	0.007	54.9
3.0%	0.057	0.135	0.152	0.521	0.213	0.079	0.028	0.007	55.1
5.0%	0.079	0.153	0.151	0.531	0.211	0.075	0.026	0.006	55.0
0.01%	0.032	0.149	0.183	0.640	0.159	0.015	0.002	0.000	45.0
Default	0.188	0.253	0.143	0.592	0.188	0.057	0.017	0.003	50.8

Table 1: Parameters describing the angular distribution of Čerenkov light from 5 MeV electrons in heavy water. Frac-1 is the fraction of light within $\pm 0.5°$ of the Čerenkov angle. Frac-2 is the fraction of light within $\pm 2°$. $\bar{\theta}$ is the average angle of emission. The remaining columns show the fraction of light in certain angular ranges. Expected statistical errors are of the order of $\pm 1\%$ of any value. The default is the EGS4 default, not the SNOMAN default.

axis of coordinates is taken to be the electron's initial direction. The number of photons at the Čerenkov angle is clearly a function of both parameters, as is the overall shape of the distribution. The number of photons at the Čerenkov angle doubles as the step size is increased from 1% to 5% and is clearly an artifact. The default step length is included as a cautionary reminder of what happens when the EGS4 default is used at low energies.

It is interesting to note that whilst the angular distribution varies considerably as a function of the step length, the average angle of emission, $\bar{\theta}$, does not. This implies that fitters which use this parameter, or other associated parameters, will not be effected by the artifact. Conversely, fitters looking for correlations (pattern recognition fitters looking for rings for example) will be strongly effected.

The step length dependance is expected, the dependance on the energy cutoff may be understood by remembering that lowering the cutoff makes a discrete interaction more likely, and so a full length step is far less likely. This then is a different way of shortening the average step. The ESTEPE of 0.01% is included to demonstrate the 'switching off' of multiple scattering at small step lengths (q.v.).

2 The Solution....

The first thing to define is what solution to look for. For the purposes of this work, an effective solution is one that removes the ESTEPE and AE dependance from the problem. This is not the same as having the *correct* solution, which would be the one that actually matches the experimental Čerenkov distribution.

Several ideas were tried and immediately discarded. The obvious solution of reducing the

AE = 10 keV								
ESTEPE	Frac-1	Frac-2	0-30	30-60	60-90	90-120	120-150	150-180
0.1%	0.024	0.112	0.153	0.503	0.220	0.084	0.032	0.009
1.0%	0.026	0.114	0.155	0.505	0.221	0.083	0.030	0.007
3.0%	0.027	0.118	0.154	0.509	0.222	0.080	0.028	0.007
5.0%	0.028	0.118	0.154	0.509	0.220	0.081	0.029	0.007
AE = 100 keV								
ESTEPE	Frac-1	Frac-2	0-30	30-60	60-90	90-120	120-150	150-180
0.1%	0.024	0.110	0.153	0.502	0.221	0.086	0.030	0.008
1.0%	0.027	0.116	0.154	0.512	0.218	0.080	0.029	0.007
3.0%	0.028	0.118	0.154	0.508	0.221	0.082	0.029	0.007
5.0%	0.030	0.123	0.152	0.515	0.217	0.081	0.029	0.007

Table 2: Parameters describing the angular distribution of Čerenkov light from 5 MeV electrons in heavy water. The photons are emitted with respect to an interpolated direction. Frac-1 is the fraction of light within $\pm 0.5°$ of the Čerenkov angle. Frac-2 is the fraction of light within $\pm 2°$. The remaining columns show the fraction of light in certain angular ranges. The expected statistical error is $\sim 1\%$ of any value.

step length is a non starter for several reasons. Neglecting the problem of which step length to select (which angular distribution would you like?), there are two main problems. Firstly, as the step length is reduced below a certain point, multiple scattering becomes 'switched off' which exacerbates the problem. This can be seen in the change between a step length of 0.1% and 0.01% in Table 1. Secondly, other work [2] has shown that how well EGS4 can simulate the results of multiple scattering and back scattering experiments depends on the step length chosen. Arbitrarily choosing the step length will ensure that EGS4 does not agree with the experiments, and if we have not got the electron transport correct, then whether there is an artifact in the Čerenkov angular distribution becomes a moot point!

Applying a Gaussian 'fuzz' to the direction of the photons, with a width equal to the multiple scattering angle for that step, had little effect. The artifact was somewhat broadened by the procedure, but still present.

The most successful solution was, in retrospect, the most obvious; for each photon generate a random number and use this to linearly interpolate between the initial and final direction of the electron. The photon is then emitted at the Čerenkov angle with respect to this interpolated direction. When this is done, the angular distribution is far less sensitive to either step length or cutoff energy - see Table 2. The variation in the peak at the Čerenkov angle has been reduced to $\sim 0.1\%$ of the total number of photons, which, although outside the expected statistical fluctuations, is a significant improvement over the original case. The other parts of the distribution are also in far better agreement, and mostly appear to fluctuate within the expected bounds. Reducing the value of AE has the effect, as noted before, of further reducing the significance of any artifacts. Although not a perfect solution, the method described above has reduced any artifacts down to the level where it is unlikely to be a problem; the difference between 2.4% and 2.8% of the light going into the Čerenkov angle is a difference of 0.2 of a photon for a 5 MeV electron.

3 Possible Effects on Fitters

The effect of the artifacts and the proposed solution can be tested on two simple hit pattern characteristics: the so called mean $\cos\theta$ and spread in $\cos\theta$. These are calculated by taking a hit pattern and moving the coordinate origin to the true vertex position. The mean hit direction is then calculated as a simple unit vector sum of each hit direction. The scalar products between this unit mean direction and each unit hit direction are then calculated. The mean $\cos\theta$ statistic is the mean of these scalar products and the spread in $\cos\theta$ is their standard deviation. These statistics will be familiar to people trying to distinguish neutral and charged current hit patterns.

Neglecting the clearly unphysical values of ESTEPE (the default and 0.01%) then runs of 10^4 5 MeV electrons with each of the parameter settings of Tables 1 and 2 produce two sets of histograms; one set of mean $\cos\theta$ and one of the spread in $\cos\theta$. Despite varying ESTEPE and AE, and regardless of whether the solution described above was implemented, no mean $\cos\theta$ histogram can be distinguished from any other and likewise for the spread in $\cos\theta$. These results can be inferred from the last column of Table 1, which implies that the average angle of emission is not a function of ESTEPE or AE. However, no such tests have been made with fitters that actually look for patterns, and would presumably be vulnerable to this artifact.

4 Conclusions

The artifacts in the angular distribution of Čerenkov light associated with the EGS4 parameters can be removed by continuously altering the electron's effective direction throughout any step. This will be implemented in SNOMAN as of version 2_08. However, this only solves the problem of a computational artifact; whilst the results of the calculation can be made artifact free, this does not necessarily mean that our calculation is correct! Further work might be useful here.

Another point that cannot currently be addressed is what the effect of these artifacts might have had on a pattern recognition fitter. There are no pattern recognition algorithms currently installed in SNOMAN (as of version 2_07), and it may be that there is something to be learned by seeing what effect a known artifact has on such a fitter. Fitters relying on average parameters such as $\bar{\theta}$ or similar quantities would appear to be unaffected by the artifact.

References

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1. 15 litres of 0.1M NaOH is mixed in the recirculation reservoir.

2. The solution is recirculated at high flow (up to 100 l/min) in the flow pattern shown in Figure C, with Permtop open to begin with. This should produce about 10 psi backpressure and will cause the outer casing of the cartridges to fill with alkali (hence the need for 15 litres of alkali). When the casing is full, Permtop is closed and the solution is recirculated for about one hour.

3. The recirculation pump is stopped and the rig is drained. This is done by opening valves Permbot, Drain, Gasperm and Gasconc.

4. The procedure is repeated so that the membrane is washed again with fresh alkali flowing in the downward direction (Figure D).

5. Steps 2-4 are repeated twice with water to wash out the alkali from the membrane in order to bring the pH back down to 10-11 (it will further reduce during HTiO priming and deuteration and will approach pH 7 by the time the membrane is ready for D_2O filtration).

HTiO Priming:

This operation is very similar to the standard acid elution method:

1. An HTiO solution is introduced into the recirculation reservoir. It is expected that 0.5 g Ti/m^2 will be required on the membrane so that 5g of Ti (in HTiO form) are required for the H53P30-20 cartridges (10 m^2 total) and 2.5g for the H26MP01-43 (5 m^2 total).

2. The solution is recirculated through the rig, as shown in Figure B (Drawing N2-93-98), with the pump and throttle valve adjusted so that Flowconc = Flowperm = 20-40 l/min and the transmembrane pressure is in the range 5-10 psi. Recirculate for one hour.

3. The pump is then switched off, and the valves Gasconc, Gasperm and Drain are opened.

4. Gasperm, Gasconc and the drain are then closed.

Deuteration:

After the above HTiO priming operation there will be about 800 ml of H_2O in the walls of the membrane. This amount has to be reduced to 10 ml, the acceptable downgrade per SUF run. The simplest method of deuteration, from an operational point of view, is repeated rinsing of the membrane with pure D_2O. In theory only two 16 litre rinses (using the standard acid elution recirculation method) are required before the 10 ml target is reached, however it seems prudent to have three such rinses. Also to reduce the cost of this process it is best to use already downgraded D_2O for the first rinse, e.g. 95-99% D_2O would be adequate. The question arises as to how many different grades of D_2O one is willing to keep track of? An alternative

deuteration technique has been proposed, using warm gas to dry off the 800 ml of H_2OHowever no tests have been performed so far, and there is a risk that some of the HTiO could be converted to TiO_2 (which is totally insoluble in mild acids) in this drying step. A more feasible method is to perform the drying stage before HTiO priming, which would then be replaced by DTiO priming. Clearly these different deuteration techniques require careful study from which a decision choice must be made which will largely be based on cost, and security of the D_2O.

Membrane Maintenance:

It is important that the integrity of the UF membranes are periodically checked, perhaps monthly, to assure that the fibres are undamaged. The results of a fibre breaking are that the efficiency of the SUF system will drop slightly but much more importantly there is a chance that a small quantity (mg) of HTiO will escape into the permeate. Integrity testing may be performed as follows:

1. Water is introduced into the reservoir and used to slightly over half fill the permeate side of the membrane, with Permbot closed and Permtop open.

2. With the upper concentrate side of the membrane shut, 2psi N^2 gas pressure is applied through Gasconc. Steady bubbling on the permeate side of the membrane indicates a broken fibre.

3. Reverse membrane and repeat the procedure.

The principle governing the success of this technique is surface tension. If the membrane fibres are intact then, at the applied low pressure, N_2cannot percolate through the membrane walls because the surface tension of the water contained in the pores (0.1μ) is too great. The surface tension of breaks in the fibre are, of course, much lower and N_2 can bubble through.

Additionally, it is well documented and has been found in lab-scale tests that the filtration rate of ultrafiltration membranes drops with use. This may be partially restored by backflushing the membrane with 0.1M NaOH or HCl through the fibre walls via a filtrate port (Figure E). Backflushing should not be confused with the alkali washing (forward and reverse) detailed earlier. Only backflushing can significantly improve the flow rate of a membrane. It should be done cautiously as the internal structure of the membrane is principally designed to withstand high inlet pressure. High pressure from the outlet side may collapse the fibres. So, whilst this procedure may be done automatically, it might be prudent if this operation is overseen. Backflushing may be done as follows:

1. 15 litres of cleaning solution is introduced into the reservoir.

2. The solution is pumped at 5-10psi through Permbot, with Permtop initially open and the concentrate side open to the covergas (Figure E). When the permeate side of the membrane is full Permtop is shut.

3. When the reservoir is empty the pump is switched off. The rig is then drained by opening valves Gasperm, Permbot and Drain.

4. Repeat the procedure twice with 15 litres of water.

5. When finished, rinse the membranes three times with 15 litres of water.

References

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