Report on JINST_002P_0122

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Title: Monte Carlo simulations of the electron - gas interactions in the KATRIN experiment

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I have three general comments:

The measurement of the neutrino mass in beta is very fundamental measurement. You should consider expanding on some of the details so that non-experts in this experiment can follow the Monte Carlo approach used to model the measured electron spectrum and the measurement at the endpoint.

Section 3 contains the heart of the modelling. Expanding some of the description should be considered to allow it to be more readily followed by non-expert readers.

The summary and discussion sections need expansion to explain how the conclusions are reached.

I noted quite a few English corrections. Please make another pass.

Line by line comments follow:

Abstract

Line 11: though "beta-spectrum of tritium" is understandable, I would refer to this as the beta-decay spectrum of tritium, as in line 49

Line 15,16: This electron spectrum plays a role in understanding electron energy loss processes, but also for the simulation of plasma processes. $->$ This sentence reads awkwardly. Perhaps rephrase along the line “In addition to providing data essential to the simulation of energy loss processes, the electron spectrum also provides information important in the simulation of plasma processes.

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"starting potential" only appears in the abstract and in the summary. What it is should be described in a sentence somewhere early in the paper.
Line 20: close to rear wall $->$ close to the rear wall
Line 21: unless there is a point to be made regarding tracking ions in the simulation, this sentence is lost in the abstract.

Page 2
Line 53: called Windowless $->$ called the Windowless
Line 61: but those with high energy $->$ except for those with high energy also can you provide a number?
Line 61: which are put on negative $->$ which are at negative
Line 61: The high energy fraction $->$ The high energy component
Line 61: Only a small portion $->$ However, only a small portion
Line 65-66: The description of the electron movement seems straightforward in first place, but the tritium gas is also a target for the primary electrons $->$ While the description of the electron movement seems straightforward, the tritium gas is also a target for the primary electrons from tritium beta decay,
Line 66-67: complication: Previous $->$ complication; previous
Line 72: answer some questions. Mainly, the $->$ answer some questions: the
Line 74: is undetermined by simulation $->$ I don't understand what is intended by this phrase. Is it because these currents can only be determined by simulation or because the prior simulations could not provide this information. I also believe that you are trying to state that these ion currents can only be determined at a few locations and that simulation must be used elsewhere. If so please consider reworking this paragraph (lines 71-80)

Page 3

Line 86: The code base for KARL was initiated in the Masters's Thesis of C. Reiling [5] $->$ The code base for KARL was initiated in the Masters's Thesis of C. Reiling [5], which provides the groundwork for the simulation of the relevant physical processes inside the source. then delete the sentence in lines 88-89.
Line 93: Tritium $->$ tritium
Line 93-94: The experiment takes data since 2018. $->$ The experiment has taken data since 2018.
Line 95: The target sensitivity $->$ please quote the number and perhaps also state how big an improvement this is over the previous best result

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Line 106-107: there is an incomplete sentence

Line 108-109: For an knowledgeable but not expert reviewer, it would be helpful to state why you need to remove the neutral tritium and by how much to reach the required sensitivity
Line 117: dipole electrodes of the DPS. The dipole electrodes are in the DPS installed to filter out the ions − > dipole electrodes of the DPS, which are installed in the DPS to filter out the ions

Page 5

Line 124-125: on the per-mille level stability [6] − > with a stability of 1 part in 1000 [6] I prefer not to use per-mille
Line 126-131: Please fix the text and remove "..." I think it is a cut and paste problem
Line 139-140: Delete "Therefore, the plasma has to be studied in the context of systematic effects." you stated it already on line 136

Page 7

Figure 3 caption: are added, when the particle − > are added when the particle
Equation 3.3: Do you need to use capital sigma for two different concepts – the macroscopic cross section and the mathematical symbol for performing a sum over all interaction channels. If the use of sigma is customary for the MCS, then use a larger symbol for the sum notation (as in equ. 3.4)
Line 195-196: In the context of this works, this state includes the final energy or the scattering angle of the particles. − > This sentence reads awkwardly. Are you trying to say that you can use either the energy of scattering angle to define the final state? Please rephrase.
Line 200: available from literature − > available from the literature

Page 11

Line 248: These interactions solely depend − > These interactions depend solely
Line 248: on primary particle − > on the primary particle
Line 249: enough, that it − > enough that it
Line 255: this is the first reference to an interaction partner. It is not clear

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what an interaction partner is (concept). Please clarify (perhaps referring to the paragraph starting at line 270).
Equation 3.16: Please define all parts of this equation. It looks as if n-alpha is a density (conventionally n is used for number and not density); and unless I missed it, t_i is not defined in the text near to the equation (I think it is the time in each iteration step), and I guess that the sum is over all particles of a specific species.
Line 264: please clarify the concept of simulated time (is it more appropriately termed time step?) Equ. 3.17 defines it but why is it termed "simulated time"?

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Line 280: the statement concerning density fields is too obscure. I presume the intention is to refer to the particle species density n-alpha. Please clarify the text.
Line 290: the concept of virtual barriers should better explained. I believe they refer to the planes within the source at which the particle currents are calculated using Equ. 3.18. On line 292 there is a statement that these virtual barriers have a segmentation similar to the density fields but unless I missed it there is no explicit description of the algorithm used in either case.
Page 13

Line 312: from literature $->$ from the literature
Line 312: comprised $->$ compiled
Line 313-314: I am not sure I agree with this statement. In my experience to establish an uncertainty in a Monte Carlo model you would run the model many times, varying the parameters in the model about some suitably motivated central value and range. What is stated would be appropriate if you had two different physical models. Is this the case?

Page 14

Line 325: A recoil of the $->$ The recoil of the

Page 17

Line 362: The shift is applied in random x-y-direction.$->$ I think you mean "The shift is applied randomly in the x and y directions." ? Please rephrase.
Line 365: mostly depend on state $->$ mostly depend on the state

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Line 367: in ground state − > in the ground state
Line 368: It is odd to refer to the first excited state as the maximal state, since the transition is only from the ground state to the first excited state. Please reword.
Line 374: In the dissociative ionization − > In dissociative ionization

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Line 389: is in ground state, prior − > is in the ground state prior
Line 391: electric excitation − > electronic excitation also please check elsewhere in the paper

Page 19

Line 399: looses − > loses
Line 414: I think you mean cm**-3 or 10**6/cm**3

Page 20
Figure 8 caption: Cross sections for T+2 and T + 3 of dissociative recombination from [22] − > Cross sections for T +2 and T + 3 dissociative recombination from [22] also following sentence in caption. Please check elsewhere in the text.
Line 428: which is significantly larger as the extent of the experiment − > What is meant by the extent of the experiment? Please rephrase.
Line 430: show, that most − > show that most

Page 21

Line 453: the T +2 also adopt − > T +2 also adopts
Line 454: implemented as a − > implemented as an
Line 456: kinematic − > kinematics appears twice on this line
Line 458: distributed, due − > distributed due
Line 460-461: In the charge exchange process, a new ion is created from the velocity distribution of the neutral gas.− > Perhaps you mean created with the velocity distribution? Please rephrase.

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Line 464: shows, that − > shows that
Line 468: In the ternary association − > In the ternary association clustering process

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Line 470: the sentence is singular – does it refer to both clustering processes? Please correct.
Line 479: scenarios, where $->$ scenarios where
Line 485: tests show, that $->$ tests show that

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Line 491: in the limits $->$ within the limits
Line 497: electrons loose energy $->$ electrons lose energy
Line 502: field in $->$ field in the
Line 502: there exist no dependence $->$ there is no dependence
Line 510-511: Additionally, it was collected how many simulated electrons and ions recombine in the simulation. $->$ This is awkward English. Please rephrase.
Line 511: In the case, where $->$ In the case where

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Line 521: pumping probability $->$ probability can't be the correct term - do you mean pumping rate?
Line 522: at design conditions $->$ at the design conditions
Line 539: velocity in longitudinal $->$ velocity in the longitudinal

Page 25

Line 548-549: by a multitude of super conducting magnets $->$ by xxx superconducting where xxx is the number of magnets

Page 26

Lines 566-568: Is there a reason why you chose not to use the actual length and injection point in the simulation? Figure 10 caption: rear wall $->$ Rearwall {to be the same as on the figure
Figure 10: Please add vertical lines showing the boundaries of the three regions discussed in the text Line 563-564: Three distinct positions are compared here: a segment, which is directly connected to the tritium inlet, a segment, which is next to the rear wall and a segment, which is connected to the DPS. $->$ Three distinct positions are compared here: a segment which is directly connected to the tritium inlet; a segment which is next to the rear wall; and a segment, which is connected to the DPS.

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Line 570: Thus $->$ Therefore
Line 570: loose $->$ lose
Line 571: Nevertheless, there $->$ There in any event, Nevertheless is not the adverb to use
Line 576: at this energy range $->$ in this energy range
Line 580: shows, that $->$ shows that
Line 585: can you show the power law on the figure and a suitably normalized Maxwell-Boltzmann distribution difficult to visualize given that the figure is log-log scale
Line 590: end of the power law $->$ end of the region described by the power law
Line 597: in first order $->$ to first order

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Line 619: effects as of $->$ effects as for
Lines 625-633: This paragraph should be reworked to expose the logical connections more clearly, and in particular should clarify the impact of the tritium density along the DPS, which varies by a factor of 12 from 4 to 12m (Figure 9).
Line 634: in longitudinal direction $->$ spaced longitudinally
Line 638: refers implicitly back to lines 241-244. It may be obvious but, it would help the reader if the reflection mechanism could be presented explicitly.

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Figure 12: Rather than just the end points, could the regions of flat current (0-2m, 12-16m) be discussed. Is there potential barrier of some sort at 4 and 12m?
Figure 12 caption: injected at 8m away $->$ injected at a point 8m away
Line 654: "Therefore, more collisions occur, which shift the guiding center" $->$ This may be obvious to a plasma physicist. However, could this be explained (and/or referenced) so that a non-expert reader can understand why more ion collisions compared to electron collisions will shift the guiding center?
Line 654-655: Thus, the radial ion current is expected to be significantly higher than the radial electron current, $->$ Please clarify "Thus" i.e. how this statement is connected to the ones preceding it.

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Figure 13 caption: Absolute radial particle current towards the beam tube in longitudinal direction. $->$ This is awkward wording. Do you mean "current towards the beam tube as a function of longitudinal position along the beam tube"? Please rephrase.
Line 662: is in the same order of magnitude than the current of the electrons $->$ is of the same order of magnitude as that for the electrons is this the intended meaning?
Line 664: This means that there must be a non-negligible amount of charge transfer reactions, or that enough T + 2 is created close to the beam tube walls. $->$ Why? Please clarify in the text.
Line 666-667: Thus, it must be assumed in first order that both effects play a role. $->$ I assume that by both effects you mean charge transfer reactions and production close to the tube wall. This looks like repetition unless there is some additional insight to be gained from the shape comparison. Please clarify.

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Line 699: electron spectrum in the source $->$ electron spectrum in the KATRIN source
Line 671: time spent in the simulation domain $->$ What is meant by this statement. Please clarify.
Line 672: The spectrum was therefore derived independent of the position in the source and can $->$ I think that you mean "Position dependence of the spectrum was not included and therefore the spectrum can"
Line 676-677: Please give the energy range used for the normalization.
Line 679: The general shape of these regions is similar to our simulation. $->$ I don't agree with this statement – in the thermal region there is a displacement in energy as well as a different shape which is masked by being plotted on a logarithmic scale. Please comment.
Line 682: differences of the spectrum $->$ differences in the spectrum
Line 685: show, that $->$ show that
Line 685: please expand the text to indicate where this conclusion comes from
Line 687: Thus, different a different plasma description is necessary, which must also include high energy electrons. $->$ Thus, a different a different plasma description is necessary, which must also include high energy electrons. Also please state why it must also include high energy electrons

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Line 688-689: which is not existent in our simulation − > which does not appear in our simulation
Line 692: delete sentence "We assume therefore that it originated from statistical uncertainty."
Line 692-694: To test whether statistical fluctuations could produce such a peak, we performed our simulations with different random number seeds. No peak was found. replace this text if you agree.
Line 695-696: The maximum of the thermal region of Nastoyashchii et al. is not at the expected maximum of the Maxwell-Boltzmann distribution. − > please overlay the expected distribution on Figure 14 and reference how it is determined.

Page 33

Line 703-704: Vice versa, the simulation can now be used to probe favorable source conditions. − > This simulation can also be used to probe favorable source parameters.
Line 707-708: But when decreasing the density down to 10% of the original value, the shape of the spectrum changes such that there is no discernible thermal region anymore.. − > This is awkward English, please rephrase.
Line 714-715: could now show, that − > show that
Line 718: the simulated current towards − > the calculated current towards or just the current since the whole paper is about simulated currents
Line 721: in contrast to the simulations of Nastoyashchii et al. − > Please add text supporting this statement or if it was not part of the Nastoyashchii simulation rephrase accordingly

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Figure 16: − > pleased make the figure axis descriptions match the caption e.g. Density − > Ion Density
Line 730: until they are destroyed − > particles can also leave the source? Also please indicate the ways by which particles can be destroyed.

Page 36

Line 734: showed a trisection: a beta-region, − > show three regions: a beta-decay region
Line 736: We determined the density of electrons and ions depending on the position in the source. − > this repeats the sentence immediately preceding it. Please delete.

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Line 741: Now the electron spectrum can be determined depending on the position $->$ Notably, the electron spectrum can be determined depending on the position

Line 744-745: Additionally, investigations of the influence of the interactions and their cross section can be performed now. $->$ Investigations of the influence of the interactions and their cross section can also be performed.

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