An Algorithm for Charge-Integration, Pulse-Shape Discrimination and Estimation of Neutron/Photon Misclassification in Organic Scintillators

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Abstract

Organic scintillators are frequently used for measurements that require sensitivity to both photons and fast neutrons because of their pulse shape discrimination capabilities. In these measurement scenarios, particle identification is commonly handled using the charge-integration pulse shape discrimination method. This method works particularly well for high-energy depositions, but is prone to misclassification for relatively low-energy depositions. A novel algorithm has been developed for automatically performing charge-integration pulse shape discrimination in a consistent and repeatable manner. The algorithm is able to estimate the photon and neutron misclassification corresponding to the calculated discrimination parameters, and is capable of doing so using only the information measured by a single organic scintillator. This paper describes the algorithm and assesses its performance by comparing algorithm-estimated misclassification to values computed via a more traditional time-of-flight estimation. A single data set was processed using four different low-energy thresholds: 40, 60, 90, and 120 keVee. Overall, the results compared well between the two methods; in most cases, the algorithm-estimated values fell within the uncertainties of the TOF-estimated values.

22 **Keywords:** *organic scintillators, pulse shape discrimination, neutron and photon misclassification, time*
23 *of flight*

24 **1. Introduction**

25 The accurate detection of neutrons is important in many fields including nuclear safeguards and security,
26 reactor instrumentation, particle physics, material science, dosimetry, and astrophysics [1]. Organic
27 scintillators are a good candidate for neutron measurement systems due to their sensitivity to fast
28 neutrons and their pulse shape discrimination (PSD) properties, which allow for reasonably accurate
29 identification of detected particle type [2-4]. The PSD performance of organic scintillators also makes
30 them especially useful for applications in which simultaneous detection of neutrons and photons is
31 desirable [5, 6].

32 Several PSD methods exist, but the charge-integration method is frequently used due to its simplicity
33 and performance [7-10]. In particular, the charge-integration method allows for highly accurate
34 discrimination between photons and neutrons at high-energy depositions. However, at low-energy
35 depositions (below ~1 MeV neutron energy deposited), discriminating between photons and neutrons
36 becomes increasingly difficult and eventually particle misclassification becomes unavoidable. In certain
37 applications, such as the measurement of special nuclear material (SNM), measured data often include a
38 large number of low-energy depositions. To properly analyze these low-energy depositions, it is
39 important to accurately estimate the extent of particle misclassification.

40 PSD misclassification has been evaluated previously by using information gained from time-of-flight
41 (TOF) measurements [11]. The large difference in the velocity of photons and neutrons allows for a
42 particle to be classified based on the time between its emission and subsequent detection. The TOF
43 classifications can be used as a reference to assess the performance of a PSD method. However, particle

44 TOF can only be obtained through specific experimental setups that are impractical or impossible to
45 utilize in the uncontrolled environments often found in field measurements. As such, it is advantageous
46 to develop methods that are capable of evaluating PSD performance while making use of readily
47 available information.

48 An algorithm was developed that is capable of automatically performing charge-integration pulse shape
49 discrimination (CIPSD) in a methodical and consistent manner. This algorithm is also capable of
50 estimating the fraction of misclassified photons and neutrons while using only the information measured
51 by a single scintillator cell. The algorithm has been wrapped into a fully functional MATLAB graphical
52 user interface (GUI) called “Auto Slice PSD”, and has been successfully used in several studies [12-14].
53 The GUI is capable of loading and processing measured data sets of various formats. The data can be
54 visualized in various ways before and after data processing and the user has the option to save an image
55 at any point. After processing, relevant information on particle discrimination and misclassification is
56 provided to the user with the option to save a detailed report.

57 This paper will give a detailed description of the algorithm utilized in Auto Slice PSD and will assess its
58 ability to estimate photon and neutron misclassification in the absence of TOF information. The
59 discussion will begin with an overview of the CIPSD method. This overview will be followed by an in-
60 depth description of the four main components of the algorithm. The acquisition and processing of the
61 TOF-tagged data set used for assessing the performance of the algorithm will be subsequently discussed.
62 Finally, Auto-Slice-PSD-estimated photon and neutron misclassification values will be presented for
63 comparison to TOF-estimated values. This comparison will be made in light of the known statistical and
64 systematic uncertainties associated with the TOF methodology, and conclusions will be drawn on the
65 relative accuracy of the Auto Slice PSD algorithm.

66 **2. Charge-Integration Pulse-Shape-Discrimination**

67 The algorithm utilized in Auto Slice PSD is based on the CIPSD principle. In CIPSD, particles are
68 identified based on the fraction of pulse that falls within the “tail” region of the pulse. This fraction is
69 dictated by the amount of phosphorescent and delayed fluorescent light produced, which is dependent on
70 the density of triplet states induced along the charged-particle interaction path [1]. Heavier charged
71 particles will produce a higher density of triplet states because they exhibit a higher rate of energy loss,
72 dE/dx [1]. For equivalent energy depositions, recoil protons resulting from neutron interactions will
73 induce a larger tail (slow) component than recoil electrons resulting from photon interactions [1]. In
74 CIPSD, a pulse is integrated over two regions to determine the fraction of the pulse that occurs in the tail.
75 The first region includes the entire pulse and, for fast organic scintillators, typically ranges from several
76 nanoseconds prior to the peak of the pulse to several hundred nanoseconds after the peak of the pulse
77 [15]. The integral of this region is referred to as the “total integral”. The second region includes only the
78 tail portion of the pulse and, for fast organic scintillators, typically begins several nanoseconds after the
79 pulse maximum and extends to the same time as the total integral region [15]. The integral of this region
80 will be referred to as the “tail integral”. The definition of the integration regions is important to the
81 overall performance of the CIPSD method and should be optimized for the detector being used [15].

82 With the computed tail and total integrals, it is possible to generate a scatter plot of pulses on the tail-
83 integral-vs.-total-integral axes. This scatter plot will show two clusters, as seen in Fig. 1. The points in
84 the upper cluster signify pulses with a higher relative fraction of light in the tail region and represent
85 pulses from heavier particles. Conversely, the points in the lower cluster represent pulses with a lower
86 relative fraction of light in the tail region. Throughout this paper, it will be assumed that the upper
87 cluster contains pulses from neutron interactions and the lower cluster contains pulses from photon
88 interactions. A curve (or line) can be created that divides the neutron and photon cluster; this curve will

89 be referred to as a “discrimination curve”. It is possible to discriminate between pulses resulting from
90 different particle interactions by designating pulses that fall above the discrimination curve to be coming
91 from neutron interactions and pulses below the discrimination curve to be coming from photon
92 interactions.

93

94 **Fig. 1. Typical tail-integral-vs.-total-integral scatter plot resulting from the CIPSD method applied to Cf-252 data. Inset**
95 **emphasizes cluster overlap at the low-energy-deposition region. Pulses were collected with an EJ-309 organic-liquid scintillator and**
96 **processed using a 30-keVee measurement-threshold. Data are available out to approximately 9 V·ns in total integral and 1.8 V·ns**
97 **in tail integral but are not shown due to the relative sparsity at these higher energy depositions. It should be noted that the data set**
98 **shown here differs from the data set that will be described in section 4.**

99 Ideally, the neutron and photon clusters would be fully separated and allow for straightforward
100 discrimination. However, at low total-integral values, which correspond to small energy deposition
101 (below ~1 MeV neutron energy deposited), the clusters begin to overlap. This overlap is emphasized in
102 the inset of Fig. 1. Cluster overlap is undesirable because it results in misclassification when using a
103 discrimination curve for particle identification. The degree to which the clusters overlap can be reduced

104 and practically completely removed by increasing the measurement threshold. However, increasing the
105 measurement threshold will always result in a loss of low-energy information. While using a
106 discrimination curve with cluster overlap will always result in some amount of misclassification, it is
107 reasonable to assume that in some applications there is an acceptable level of misclassification that can
108 be tolerated in order to retain the low-energy information. The algorithm described in this paper is
109 intended for use in such applications. The algorithm attempts to minimize the number of misclassified
110 particles, subject to a set of user-defined parameters, and estimates the particle misclassification
111 resulting from the calculated discrimination curve. This estimation is performed using only the
112 information measured by a single organic scintillator.

113 **3. Auto Slice PSD Algorithm**

114 Auto Slice PSD determines a discrimination curve by using a multi-step process that includes slicing the
115 data into smaller subsets, fitting the distribution of tail-to-total-integral ratios in each slice, and using the
116 fits to find the optimal discrimination points that minimize misclassification in each slice. Once
117 identified, these points can be used to fit a discrimination curve through the data set. Additionally, by
118 analyzing the slice-by-slice fits it is possible to estimate the fraction of neutrons and photons
119 misclassified by the discrimination curve.

120 **3.1. Slicing the Data**

121 The first step in determining a discrimination curve is to divide the full data set into smaller subsets by
122 using linear slices. By slicing the data, it is possible for the discrimination points to be chosen such that
123 they optimally separate a local region; this optimization process will be discussed in section 3.3. A
124 histogram of the ratio of tail-to-total integrals for the pulses contained in a slice can be accurately fit as a
125 sum of two Gaussians, where one Gaussian models the neutron cluster and another models the photon

126 cluster. The peaks are Gaussian in nature as a result of the stochastic processes inherent to converting an
127 energy deposition to an output signal in a detector and photomultiplier tube. It should be noted that
128 although a similar histogram can be computed for the full data set, it generally cannot be modeled as a
129 sum of two Gaussians due to the shift in the means of the clusters as a function of total integral.

130 The slices used by this algorithm are linear and are defined by a slope and width, which are selected by
131 the user and provided as inputs. Auto Slice PSD numbers slices in ascending order beginning with the
132 slice that contains the pulses with the lowest total-integral. When comparing two or more slices in terms
133 of location, slices with a larger slice number will be considered “to the right of” or “above” slices of a
134 lower slice number.

135 The slope should be chosen such that the slices are as perpendicular to the data clusters as possible. This
136 will help to preserve the Gaussian nature of each cluster when the slice is projected onto the ratio-
137 histogram axes. As the photon and neutron clusters are neither parallel nor perfectly linear, it is not
138 possible to be fully perpendicular to all regions of both clusters simultaneously. However, if the slice
139 angle is reasonably close to the true perpendicular angle and the slice is sufficiently narrow, the
140 Gaussian nature of the clusters will be maintained.

141 The width of the slices is defined as the distance between where the slice edges intercept the total-
142 integral axis. Ideally, the width of the slices should be as narrow as possible to allow for a large number
143 of points through which to fit the discrimination curve. However, in practice the width of the slices
144 should be balanced such that the slices are wide enough to contain enough pulses for the ratio histogram
145 to be accurately fit, while still being narrow enough to avoid a significant shift in cluster mean.

146 Although the slope and width of the slices are currently provided as user inputs, there is a plan for future
147 software versions to automatically compute the optimal slice parameters.

Figure 2 (a) shows the same data set seen in Fig. 1 overlaid with slices having a width of 0.1 V·ns and a slope of -6. The slope is approximately perpendicular to the clusters and was calculated by taking the value half way between the mean slopes for the aggregate neutron and photon clusters. The aspect ratio was changed from Fig. 1 to prevent the illusion of the slices appearing too steep. Figure 2 (b) shows the tail-to-total integral ratio histogram for the fifth slice in Fig. 2 (a), which has been highlighted. Tail-to-total integral ratios can fall between 0 and 1 in theory; however the pulses evaluated in this study do not typically fall within the upper third of this range. As such the ratio histograms presented in this paper will be displayed over a constrained range for clarity.

157

Fig. 2. Tail-integral-vs.-total-integral scatter plot from Fig. 1 overlaid with slices having a width of 0.1 V·ns and a slope of -6 (a). Tail-to-total integral ratio histogram for the fifth (highlighted) slice in of the tail-integral-vs.-total-integral scatter plot (b). Error bars are excluded from the ratio histogram because they would be smaller than the data point. (Color image available online).

3.2. Fitting the Slices

161

162 Once the data have been subdivided into slices, an integral ratio histogram is computed for each slice, as
163 shown in Fig. 2 (b). In general, these histograms will appear as two peaks, with the lower ratio peak
164 representing the photon data and the higher ratio peak representing the neutron data. As such, the full
165 histogram can be well modeled as a sum of two Gaussians. This is accomplished using a built-in curve-
166 fitting routine in MATLAB [16], which utilizes a nonlinear optimization method to find the six
167 parameters required to define two Gaussian curves: the amplitudes (a_1 and a_2), the means (b_1 and b_2),
168 and c_1 and c_2 , which are related to the widths. To assist with finding the most accurate solution, the
169 routine can be supplied upper and/or lower bounds as well as initial guesses for each of the six
170 parameters. For clarity, the parameters associated with the fit of the photon cluster will be denoted as a_γ ,
171 b_γ , and c_γ while the parameters associated with the fit of the neutron cluster will be denoted as a_n , b_n , and
172 c_n . If it is important to specify the slice number, s , of a parameter, the slice number will be denoted as a
173 parenthetical superscript (e.g. $a_n^{(s)}$).

174 This fitting routine works very well for slice histograms with two easily distinguishable peaks. This is
175 true even when no information is provided about the expected parameter values (although the fit is
176 found more quickly if some initial information is provided). However, when using sufficiently low
177 energy thresholds the photon and neutron clusters begin to overlap in the low-energy-deposition region.
178 Predictably, as this overlap occurs, the two peaks in the ratio histograms begin to move closer together
179 (through descending slices) and eventually appear as a single peak. If it is assumed that the slices with
180 overlapping data clusters do in fact contain pulses from both neutron and photon interactions, then it is
181 still reasonable to fit the ratio histogram as a sum of two Gaussians. However, it is difficult for the
182 MATLAB fitting routine to fit histograms of this nature unless it is provided with estimates of the
183 expected amplitudes, means, and widths of the two Gaussians. It is possible to estimate this required

184 information reasonably well by using parameters from the previously fit slice as well as information
185 gained from analyzing the data set as a whole.

186 Although there is only a small fraction of slices contained in the overlapping region, it is important to
187 accurately fit the histograms for these slices because a small shift in the discrimination point can result
188 in a significant change in particle misclassification. This is contrary to slices in region of high cluster
189 separation in which a small shift in the discrimination point may not change the number of misclassified
190 particles at all. Additionally, because the slices in the overlapping region contain a comparatively large
191 number of pulses, proper fitting is required to get an accurate estimate of misclassification for the full
192 data set. Due to the importance of fitting the slices in the overlapping region, several steps are taken
193 within the processing algorithm to provide the MATLAB fitting routine with as much information as
194 possible on the expected parameter values. This is done by executing a pre-fitting algorithm on the full
195 data set that results in an estimate of the mean value for both clusters in each slice. The slice-fitting
196 algorithm is then executed beginning with a slice that shows reasonable separation and moving down
197 through the overlapping region before fitting the remainder of the well-separated slices. By starting with
198 a slice that can be reliably fit with minimal input (and using the resulting fit information to work
199 backwards) it is possible to provide enough information to the MATLAB fitting routine to accurately fit
200 slices with strongly overlapping peaks.

201 **3.2.1. Pre-fitting Algorithm**

202 Prior to fitting the individual slices, a pre-fitting algorithm is used to estimate the mean values of the
203 photon and neutron clusters as a function of total integral. This is done by choosing a linear
204 discriminator based on the ratio histogram for the full data set and temporarily classifying pulses above
205 the curve as neutrons and pulses below the curve as photons. The temporary neutron and photon clusters

206 can then be fit with separate second order polynomials that reasonably estimate where the Gaussian
 207 means will be located in a slice's ratio histogram. An example of these fits can be seen in Fig. 3. It is
 208 important to note that the estimates of the Gaussian means derived from the quadratic fits will only be
 209 used as input parameters to bound the search region and accelerate the fitting routine. These estimated
 210 means are not the same as means used for defining the Gaussians, b_γ and b_n , which are determined by the
 211 fitting routine.

212
 213 **Fig. 3. Temporary classification of particles into neutrons and photons based on the linear discriminator chosen by the pre-fitting**
 214 **algorithm. The curves show the second-order polynomials that have been fit to each cluster in an attempt to estimate the means of**
 215 **the Gaussian fits during the slice-fitting algorithm. (Color image available online).**

216 The linear discriminator is found by computing an integral-ratio histogram for the full data set and using
 217 a peak finding routine to find the valley minimum located between the neutron and photon peaks. If the
 218 peak finding routine does not identify two well-defined peaks, the pulses from lowest slice number are
 219 removed and the ratio histogram is recomputed. This process is repeated until either two peaks are
 220 identified or all slices have been removed. In the latter case, the fitting process ends and an error is

221 generated stating that two data clusters could not be found. A flowchart detailing the operation of the
222 pre-fitting algorithm is shown in Fig. 4. In this flowchart, s represents the current slice number and S
223 represents the total number of slices.

Fig. 4. Flowchart describing the pre-fitting algorithm, which is used to find reasonable estimates for the means of the Gaussian fits that will be computed during the slice-fitting algorithm.

227 3.2.2. Slice-fitting Algorithm

228 The slice-fitting algorithm functions very similarly on each slice. The first step is to compute the
229 estimated Gaussian means for the slice by finding where the previously computed photon and neutron
230 cluster fits intercept the centerline of the slice and calculating the corresponding ratios. These values will
231 be referred to as $\tilde{b}_\gamma$ and $\tilde{b}_n$, respectively. The MATLAB fitting routine is then invoked using upper
232 bounds, lower bounds, and start points for the Gaussian means based on the expected means. The quality
233 of the fit is assessed using the coefficient of determination, R^2 , which is defined as the ratio of the sum
234 of squares of the fit about the mean and the sum of squares of the data about the mean. The R^2 of the fit
235 is checked against a threshold value of 0.95, below which the fit is not reliable for use in determining the
236 optimal discrimination point. If the fit is deemed to be inaccurate, the slice histogram is refit using
237 parameter constraints and start points based on the parameters of the nearest slice that has been
238 previously fit. If the quality of the fit is still poor, the slice histogram is fit a third time using only a non-
239 negativity constraint on the six parameters. If the starting slice must be refit, only the second refitting
240 step is used because no other slice information is available. If either refitting step is utilized, the fit with
241 the highest R^2 value is kept, regardless of whether it falls above or below the threshold.¹

242 The parameters being fed to the fitting routine for the initial fit in each slice vary slightly depending on
243 where along the clusters the slice is located. The four location categories that a slice can fall into are the
244 starting slice, the slice immediately above the starting slice, slices where the clusters have completely

¹ Fits with an R^2 value below the threshold typically occur at relatively high total-integral values where the low number of counts makes it difficult to achieve a statistically sound fit. The fits for these slices are kept because the separation of the clusters allows for fits that provide acceptable representations of both the neutron and photon peaks in spite of the associated R^2 values. While any slice's contribution to the discrimination curve can be removed by the user, the fits of every slice will be used when computing misclassification.

245 overlapped and could be misconstrued as a single peak, and all other slices. The third region will be
246 referred to as the “single-mean region” and may or may not exist, depending on the data set.

247 The starting slice is chosen to be the slice closest to 10% of the total number of slices. This percentage
248 value was selected because it is typically high enough to be in the range of reasonably well-separated
249 clusters while still being low enough to contain enough counts for reliable fitting. While this value is
250 currently hard coded at 10%, it is worth noting that future revisions of the code could automatically find
251 a suitable starting slice.

252 Existence of a single-mean region is triggered if a slice is found in which the falling edge of the photon
253 fit crosses the half maximum of the neutron fit at a ratio larger than mean of the neutron fit. All slices
254 below an existing trigger slice will be considered to be in the single-mean region. An example of a slice
255 that would trigger the single-mean region can be seen in Fig. 5. In this slice, the photon fit evaluates to
256 283, which is the half-maximum of the neutron fit, at a ratio of approximately 0.287. This ratio is greater
257 than the ratio of the neutron mean, which occurs at 0.169.

Fig. 5. Example of a slice in the single-mean region. In this slice, it is clear that the photon fit does not fall below the half-maximum of the neutron fit until well after the mean of the neutron fit. Error bars on the individual data points are not shown because they would be smaller than the data points themselves. (Color image available online).

All slices bound the fit amplitudes, a_γ and a_n , by 0 and the total number of pulses in the slice. Additionally, all slices bound the widths, c_γ and c_n , by 0 and 0.5, which prevents unrealistically wide fits. For slices outside of the single-mean region, the fit means, b_γ and b_n , are restricted to fall between $\pm 25\%$ of $\tilde{b}_\gamma$ and $\tilde{b}_n$ respectively. If the slice is within the single-mean region, b_γ is allowed to range between 0 and 125% of $\tilde{b}_\gamma$, which allows for the photon fit to capture the low ratio pulses found in the early slices. Alternatively, b_n in the single-mean region must fall between 50% and 110% of b_n from the above slice. The estimated mean, $\tilde{b}_n$ is not used in the single-mean region because the quadratic fit used is not able to capture the rapid decrease in ratio of the neutron cluster. The asymmetric window around b_n is used to encourage the mean to move towards lower ratio values. Neither of the aforementioned refitting steps is used in the single-mean region due to the unique fitting parameters required for these slices.

273 The fit routine is generally provided an initial guess for each of the six parameters to encourage accurate
274 and efficient fitting. The initial guesses for the peak amplitudes are equal to the amplitudes of the
275 previously fit slice scaled by the ratio of the number of pulses contained in each slice. The initial guesses
276 for the means are $\tilde{b}_\gamma$ and $\tilde{b}_n$ unless the slice is in the single-mean region where the initial guess for both
277 means is $\tilde{b}_\gamma$. The initial guesses for the width parameters are the widths from the previously fit slice. The
278 slice immediately above the starting slice differs from most slices in that it uses information from the
279 starting slice rather than the most recently fit slice (which would be slice 1). Initial guesses are not fed to
280 the starting slice or to any slice that follows a slice with an $R^2 < 0.95$.

281 Figure 6 shows the flowchart for the fitting algorithm. In this flowchart, s is a vector containing the slice
282 processing order, S is the total number of slices, and i is a counter that can hold integer values between 1
283 and S . This notation varies slightly from the rest of the paper in that $s[i]$ (rather than s) denotes the
284 number of the slice currently being processed. Additionally, s_0 is the starting slice, $N^{(s[i])}$ is the number of
285 pulses in slice $s[i]$, and $w^{(s[i])}$ and $d^{(s[i])}$ are related to the weighting of the slice and are defined in Section
286 3.4.

Fig. 6. Flowchart describing the operation of the slice-fitting algorithm.

The fitting algorithm described leads to reliable fits throughout all regions of the data, even in the presence of overlap. Fig. 7 shows a progression of slice fits through the overlapping region of the sample data set shown in Figs. 1-3. The histograms being fit come from slices that have a slope of -6 and a width of 0.025 V·ns, which is narrower than the width of the slices shown in Fig. 2. The ‘X’ shown in each histogram marks the optimal discrimination point, which will be described further in section 3.3.

Each of the six fits shown have an $R^2 > 0.999$ for the full histogram. It is important to note that while all of the slices shown have between approximately 75,000 and 150,000 counts, fits with an $R^2 > 0.990$ can be consistently obtained for slices with more than approximately 500 counts, and usable fits can be obtained for slices with approximately 100 counts. The ability to accurately fit slices with a low number of counts is a result of the previously known fit data being passed forward to each new slice. Therefore, the slice widths should be adjusted such that the starting slice contains on the order of one thousand counts, which will allow the fitting algorithm to begin with a reliably fit slice.

301

Fig. 7. Six slice histograms from the low-energy-deposition region of a tail-integral-vs.-total-integral scatter plot. Fits are shown for the full histogram (sum of two Gaussians) as well as for individual photon and neutron clusters (individual Gaussians). The 'X' marks the optimal discrimination point derived from analyzing the fits. All six full-histogram fits have an $R^2 > 0.999$. Error bars on the individual data points are not shown because they would be smaller than the data points themselves. (Color image available online).

309

310 **3.3. Choosing the Discrimination Points**

311 The Auto Slice PSD algorithm uses the fit data to determine the optimal discrimination point within
 312 each slice, which is defined as the ratio that minimizes particle misclassification while accounting for
 313 any bias or normalization desired by the user. This ratio, x_{opt} , is found by solving

$$314 \quad x_{opt} = \arg \min_{x \in [0,1]} \left(\frac{k_\gamma}{M_\gamma} \int_x^1 a_\gamma e^{-\left(\frac{x'-b_\gamma}{c_\gamma}\right)^2} dx' + \frac{k_n}{M_n} \int_0^x a_n e^{-\left(\frac{x'-b_n}{c_n}\right)^2} dx' \right), \quad (1)$$

315 where M_γ and M_n are normalization factors, k_γ and k_n are bias parameters, and the remaining parameters
 316 are given by the fitting routine. The normalization factors and bias parameters will be described in the
 317 following paragraphs. The first integral in Eq. (1) computes the portion of the photon fit that will be
 318 misclassified when setting x as the discrimination point and the second integral computes the portion of
 319 the neutron fit that will be misclassified.

320 The normalization factors can be set either to unity (for the unnormalized case) or to

$$321 \quad M_j = \int_0^1 a_j e^{-\left(\frac{x-b_j}{c_j}\right)^2} dx, \quad j = \gamma, n. \quad (2)$$

322 The unnormalized case will compute the optimal discrimination point by finding the ratio that
 323 misclassifies the smallest number of particles in the slice. However, if the data set contains an
 324 overwhelming number of pulses from one type of particle, the unnormalized minimization could result
 325 in a discrimination point that misclassifies a large percentage of the less prevalent particle. In the
 326 extreme case, where the fit of the less prevalent particle is strictly less than the fit of the more prevalent
 327 particle for all ratios, the discrimination point would misclassify all of the less prevalent particles. In
 328 some scenarios it may be desirable to account for the imbalance in particle types, which is accomplished

329 by utilizing the normalization factors from Eq. (2). These normalization factors are the integral of each
330 fit over the total range of possible tail-to-total-integral ratios, [0,1]. Using these factors allows for the
331 minimization step in Eq. (1) to equally penalize the misclassification of each particle type.

332 In some applications, it may also be advantageous to tune the weighting of each particle type to
333 accomplish a specific goal. Particle weighting can be accomplished by using the bias parameters, k_γ and
334 k_n , to adjust the penalization ratio during the minimization step. For example, if it is important to
335 accurately detect neutrons, k_n could be increased such that it is more penalizing to misclassify neutrons
336 than photons. Of course, increasing k_n would result in an increase of misclassified photons because
337 optimal discrimination point would be pushed towards 0. The bias parameters can be used to find the
338 appropriate balance between neutron and photon misclassification for a given application.

339 **3.4. Fitting a Discrimination Curve and Estimating Particle Misclassification**

340 Once a discrimination point has been chosen for each slice, the corresponding tail and total integral
341 values are found by mapping the ratios to the midlines of the slice. A discrimination curve can be fit
342 through the points on the tail-integral-vs.-total-integral scatter plot. This discriminator can take on a
343 variety of forms including linear, quadratic, and two-function; a two-function discriminator is a
344 combination of a quadratic curve in the low-energy-deposition region and a linear discriminator in the
345 high-energy deposition region. During the fitting of the discrimination curve, each slice is assigned a
346 weighting parameter,

$$347 \quad w^{(s)} = \left| (d^{(s)})^{-3} \right|, \quad (3)$$

348 where $d^{(s)}$ is the Euclidean distance between the cluster means on the tail-integral-vs.-total-integral
349 scatter plot. The exponent in Eq. (3) was chosen to be negative to give higher importance to slices in

350 which the data clusters are relatively close or overlapping. The magnitude of the exponent was chosen
 351 heuristically by assessing the tightness of the fit in the low-energy-deposition region over several data
 352 sets. This weighting parameter encourages a tighter fit in the overlapping region at the expense of
 353 allowing more freedom in regions of good separation. This tradeoff is acceptable because an inaccurate
 354 fit in the overlapping region can significantly impact misclassification, while an inaccurate fit in regions
 355 of good separation will have a negligible impact.

356 After the discrimination curve has been determined, it is possible to estimate the aggregate detection and
 357 misclassification ratios. Because the discrimination curve has been fit through the discrimination points,
 358 the true discrimination ratio may not be equivalent to the optimal discrimination ratio found during the
 359 minimization procedure. The true discrimination ratios can be determined by finding where the fit
 360 crosses the midline of each slice. The integral ratio associated with each of these intersection points will
 361 be denoted as $x^{\dagger(s)}$. Then, for a particular slice s , the following values can be computed:

$$362 \quad \hat{p}_t^{(s)} = \int_0^1 a_\gamma^{(s)} e^{-\left(\frac{x-b_\gamma^{(s)}}{c_\gamma^{(s)}}\right)^2} dx \quad (4)$$

$$363 \quad \hat{p}_d^{(s)} = \int_0^{x^{\dagger(s)}} a_\gamma^{(s)} e^{-\left(\frac{x-b_\gamma^{(s)}}{c_\gamma^{(s)}}\right)^2} dx \quad (5)$$

$$364 \quad \hat{p}_m^{(s)} = \int_{x^{\dagger(s)}}^1 a_\gamma^{(s)} e^{-\left(\frac{x-b_\gamma^{(s)}}{c_\gamma^{(s)}}\right)^2} dx = \hat{p}_t^{(s)} - \hat{p}_d^{(s)} \quad (6)$$

$$365 \quad \hat{n}_t^{(s)} = \int_0^1 a_n^{(s)} e^{-\left(\frac{x-b_n^{(s)}}{c_n^{(s)}}\right)^2} dx \quad (7)$$

$$366 \quad \hat{n}_d^{(s)} = \int_{x^{\dagger(s)}}^1 a_n^{(s)} e^{-\left(\frac{x-b_n^{(s)}}{c_n^{(s)}}\right)^2} dx \quad (8)$$

367

$$\hat{n}_m^{(s)} = \int_0^{x^{\dagger(s)}} a_n^{(s)} e^{-\left(\frac{x-b_n^{(s)}}{c_n^{(s)}}\right)^2} dx = \hat{n}_t^{(s)} - \hat{n}_d^{(s)}, \quad (9)$$

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371

where Eq. (4) estimates the total number of photons in slice s , Eq. (5) estimates the number of detected photons in slice s , Eq. (6) estimates the number of misclassified photons in slice s , and Eqs. (7)-(9) compute the same values for neutrons. Using these values, the aggregate software-estimated detection and misclassification ratios are defined as:

372

$$\hat{p}_d = \frac{\sum_s \hat{p}_d^{(s)}}{\sum_s \hat{p}_t^{(s)}} \quad (10)$$

373

$$\hat{p}_m = \frac{\sum_s \hat{p}_m^{(s)}}{\sum_s \hat{p}_t^{(s)}} \quad (11)$$

374

$$\hat{n}_d = \frac{\sum_s \hat{n}_d^{(s)}}{\sum_s \hat{n}_t^{(s)}} \quad (12)$$

375

$$\hat{n}_m = \frac{\sum_s \hat{n}_m^{(s)}}{\sum_s \hat{n}_t^{(s)}}. \quad (13)$$

376

4. Acquisition of Test Data

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A TOF-tagged-data set was used to assess the performance of the Auto Slice PSD software with regards to estimation of particle detection and misclassification. A discrimination curve generated by Auto Slice PSD was used to classify particles in the TOF-tagged-data set as either photons or neutrons. The TOF distributions for the discriminated photons and neutrons were then compared to the total TOF distribution. By analyzing reasonable photon and neutron TOF regions within these distributions, it was possible to compute TOF-based detection and misclassification ratios for comparison against the software generated ratios.

384 **4.1. Time-of-Flight Measurement**

385 A TOF measurement of a ^{252}Cf source was performed at Ohio University's Edwards Accelerator
386 Laboratory. The strength of the ^{252}Cf was approximately 18 μCi . The emitted radiation was detected
387 using a 3"-diameter-by-3"-thick cylindrical EJ-309 organic-liquid scintillator. A standoff distance of
388 216.5 cm was used between the source and the front face of the detector. The detector was used as a
389 trigger and particle TOF was calculated relative to the signal from an ion chamber, which contained the
390 ^{252}Cf source. Waveforms were recorded using a 250 MHz CAEN V1720 digitizer with 12-bit dynamic
391 range. 404 samples, which is equivalent to 1612 ns, were collected for each waveform.

392 The TOF experiment was performed twice, once with a shadow bar present in front of the detector and
393 once without the shadow bar present. These experiments will be referred to the "shadow-bar" and "bare"
394 experiments respectively. The shadow bar was constructed of brass and was used to eliminate the
395 majority of uncollided neutrons interacting in the detector in an attempt to measure the contribution of
396 scattered neutrons to the bare experiment. Both experiments had total run times of 82.5 hours.
397 Schematics of the measurement setup can be seen in Fig. 8.

Fig. 8. Schematics of the measurement setup. The shadow bar is designated with a dashed line because it is not present in the bare experiment.

Prior to analysis, both data sets were cleaned of saturated and double pulses. Additionally, low-energy thresholds of 40, 60, 90, and 120 keVee were applied during post-processing to assess the software's performance for various levels of cluster overlap. The number of counts available after cleaning and applying low-energy thresholds is shown in Table 1 for each data set. The TOF for a pair of events was computed by taking the difference between the trigger times for each pulse, which were set to be at 20% of the pulse maximum. A linear interpolator was used to increase the accuracy of the trigger times. However, there is still some digitization error present, which causes the TOF peaks to appear jagged in 4-ns intervals.

410

411 **Table 1. Number of pulses available for analysis in each of the eight data sets after post-processing. Raw data was post-processed**
412 **by cleaning out saturated and double pulses and by applying four different low-energy thresholds.**

Threshold (keVee)	Bare (pulses)	Shadow Bar (pulses)
40	1.88×10^6	6.98×10^5
60	1.61×10^6	5.60×10^5
90	1.33×10^6	4.29×10^5
120	1.14×10^6	3.53×10^5

413

414 **4.2. Misclassification Assessment in Time-of-Flight Data**

415 The bare and shadow-bar TOF distributions were used to compute detection and misclassification ratios
416 for a PSD curve generated by Auto Slice PSD. The general method for computing these values is
417 outlined below and described in more detail in the following paragraphs.

- 418 1. Subtract the shadow-bar distribution from the bare distribution.
- 419 2. Compute the mean baseline value for positive and negative TOF regions.
- 420 3. Sum the number of counts in a predefined photon region of interest (ROI) and subtract
421 the expected number of counts due to the negative TOF baseline.
- 422 4. Sum the number of counts in a predefined neutron ROI and subtract the expected
423 number of counts due to the positive TOF baseline.
- 424 5. Use a discrimination curve to subdivide the data sets into PSD-tagged neutrons and
425 photons. Do this separately for both the bare and shadow-bar data sets.
- 426 6. Repeat steps 1-4 for both the PSD-tagged neutron and PSD-tagged photon data
427 subdivisions.
- 428 7. Compute the detection and misclassification ratios for photons and neutrons by
429 comparing the ROIs computed using the data subdivisions to the ROIs computed prior
430 to PSD.

431

432 Figure 9 shows the TOF-distributions for the bare and shadow-bar data sets when processed using a 40-
433 keVee threshold. In these distributions, the photon peak is centered at the expected value of 7.2 ns. In
434 the bare TOF distribution, the neutron peak can be seen between approximately 40 and 250 ns. A small
435 peak can also be seen in both data sets around 15 ns. This peak is likely a photon peak due to scatter off

the laboratory floor. A similar, but less obvious, effect is present in the neutron peak and takes the form of a low amplitude plateau that can be seen in the shadow-bar distribution. The result is a delayed return to the baseline, which makes it difficult to accurately compute the average contribution from accidentals. It should be noted that data are available for TOF values between approximately -150 and 1500 ns and that all available data were used during analysis of the distributions. However, the TOF range in Figs. 9 and 10 is constricted to emphasize the photon and neutron regions and the impact of neutron scatter on the return of a distribution to its baseline. It can be assumed that a distribution continues along its depicted trend outside the visualized range.

444

445 **Fig. 9. TOF distributions (using 1 ns bins) for the bare and shadow-bar data sets. Data were processed using a 40-keVee threshold.**
 446 (Color image available online).

447 To minimize the impact of scattered particles, the shadow-bar TOF distribution was subtracted from the
 448 bare distribution prior to computing the baselines and summing the ROIs. The shadow-bar-subtracted
 449 data set can not have a discrimination curve applied directly to it because individual pulse information
 450 can not be retained during the subtraction and it is therefore not possible to create a tail-integral-vs.-

451 total-integral scatter plot of the shadow-bar-subtracted TOF distribution. To obtain discriminated,
 452 shadow-bar-subtracted TOF distributions, the same discrimination curve was applied separately to both
 453 the bare and shadow-bar data sets and the resulting subdivided distributions were appropriately
 454 subtracted. Although the two data sets come from separate measurements, it is reasonable to use the
 455 same discrimination curve because the measurement setup was identical aside from the presence of the
 456 shadow bar. Fig. 10 shows how shadow-bar subtraction impacts the TOF distributions, before and after
 457 pulse shape discrimination, for the same data shown in Fig. 9. It is clear that the shadow-bar subtraction
 458 procedure significantly reduced the impact of scattered particles and accidental coincidences.

459

Fig. 10. TOF distributions (using 1 ns bins) for the bare, shadow-bar, and shadow-bar-subtracted data sets. Distributions are shown for the full, pre-discrimination, data set (a) as well as for the PSD-tagged neutron data set (b) and the PSD-tagged photon data set (c). Data were processed using a 40-keVee threshold. (Color image available online).

The total number of TOF tagged photons and neutrons in each distribution were computed by summing the number of counts, less the mean baseline contribution, in the photon and neutron ROIs of the

shadow-bar-subtracted distributions. The photon baseline was computed by taking the mean of the TOF distribution between -120 ns and the beginning of the photon ROI, while the neutron baseline was computed by taking the mean of the TOF distribution between the end of the neutron ROI and 1450 ns. The photon ROI was set to be between 0 and 14 ns, which was chosen by finding when the leading edge of the photon peak begins to rise from the baseline and assuming symmetry around the 7 ns peak. The lower bound of the neutron ROI was found to be approximately 39 ns by determining where the leading edge of the neutron peak begins to rise in the shadow bar subtracted data sets. In contrast to the photon ROI, which was constant for all thresholds, the upper bound of the neutron ROI was set to be the theoretical TOF limit for the threshold being evaluated. To find this value, the threshold was converted to energy deposition by numerically inverting the light-output response-function described in [17],

$$L = 0.81723E - 2.6290(1 - e^{-0.29686E}), \quad (14)$$

where L corresponds to the amount of light created in MeVee from a neutron energy deposition of E MeV on a proton. This energy value corresponds to the slowest possible neutron that could deposit its full energy during a single scatter on a proton and produce a pulse above the processing threshold (in the absence of detector resolution). As such, the time required for a neutron of this energy to travel 216.5 cm should be a reasonable value for the right bound of the neutron ROI. The minimum detectable energies and corresponding TOF values are summarized in Table 2 for the four thresholds investigated.

Table 2. Minimum detectable neutron energy and corresponding TOF for various measurement thresholds and a 216.5 cm flight path.

Threshold (keVee)	Energy (keV)	TOF _{max} (ns)
40	457	231
60	591	203
90	760	179
120	904	164

487 By assessing the photon and neutron ROIs in the full and discriminated TOF distributions, it was
 488 possible to estimate the fraction of detected and misclassified particles as follows:

$$489 \quad \tilde{p}_d = \frac{\sum_{TOF=0}^{14} \mathcal{P}}{\sum_{TOF=0}^{14} \mathcal{T}} \quad (15)$$

$$490 \quad \tilde{p}_m = \frac{\sum_{TOF=0}^{14} \mathcal{N}}{\sum_{TOF=0}^{14} \mathcal{T}} \quad (16)$$

$$491 \quad \tilde{n}_d = \frac{\sum_{TOF=39}^{TOF_{max}} \mathcal{N}}{\sum_{TOF=39}^{TOF_{max}} \mathcal{T}} \quad (17)$$

$$492 \quad \tilde{n}_m = \frac{\sum_{TOF=39}^{TOF_{max}} \mathcal{P}}{\sum_{TOF=39}^{TOF_{max}} \mathcal{T}}, \quad (18)$$

493 In Eqs. (15)-(18) $\mathcal{T}$, $\mathcal{P}$, and $\mathcal{N}$ signify the shadow-bar and baseline-subtracted TOF distributions for the
 494 total, the PSD-classified photon, and the PSD-classified neutron data subsets respectively. TOF_{max} varies
 495 with threshold, as shown in Table 2.

496 **4.3. Uncertainty in Time-of-Flight-Based Misclassification Estimation**

497 There are several sources of uncertainty that should be considered when estimating misclassification
 498 using the TOF method. The first uncertainty is the Poisson statistical uncertainty associated with the
 499 measured data. The impact the statistical uncertainty has on the estimation of particle misclassification
 500 can be calculated by propagating the Poisson uncertainty of the bare and shadow-bar TOF distributions
 501 through the computations outlined in section 4.2. There is also uncertainty related to the combined effect
 502 of performing the shadow-bar subtraction and the baseline correction. Each point in the post-shadow-
 503 bar-subtraction baseline has a large relative uncertainty as a result of subtracting two Poisson random
 504 variables with similar means. Therefore the mean of a baseline region, which is subtracted from the each
 505 point in the ROI during the baseline correction, also has a large relative uncertainty. The extent to which

506 this uncertainty impacts the summation of the ROI is dependent on the size of the ROI and the relative
507 magnitudes of the ROI and the baseline. The impact of this uncertainty on the estimation of particle
508 misclassification can be determined by varying the mean baseline values using their standard deviation
509 and recomputing the misclassification ratios. This procedure will produce upper and lower bounds on
510 the misclassification ratios that will be tight when the impact of the baseline uncertainty is small and
511 loose when the impact of the baseline uncertainty is large. The final uncertainty that should be
512 considered is the uncertainty related to the ROI boundaries. The impact this uncertainty has on the
513 estimation of particle misclassification can be determined by recomputing the misclassification ratios
514 over a series of systematic shifts on the ROI boundaries. Knowing the impact of each of these
515 uncertainties is an important part in identifying the presence of any systematic uncertainties associated
516 with the Auto Slice PSD algorithm.

517 **5. Results**

518 Auto Slice PSD was used to generate a two-function discrimination curve for the bare data set at each of
519 the four processing thresholds. In all four cases the slice width was set to be 0.025 V·ns and the slope
520 was set to -6; this slope falls in the range of being reasonably perpendicular to both clusters, as discussed
521 in section 3.1. The misclassification points were computed using the fit normalization parameters
522 described in Eq. (2). The discrimination curves were then used to compute the TOF misclassification
523 ratios as described in section 4.2.

524 Figures 11-14 show the tail-integral-vs.-total-integral plot for each threshold along with the computed
525 discrimination curve. The tail-integral-vs.-total-integral plots are shown for both the bare data sets and
526 the shadow-bar data sets. It is important to remember that the same discrimination curve, which was
527 computed using the bare data set, is used for both data sets at a given threshold. Also shown are the pre-

528 and post-discrimination, shadow-bar-subtracted TOF distributions for each of the four thresholds.
529 Similarly to Figs. 9 and 10, Figs. 11-14 show the TOF distributions over a restricted range to emphasize
530 the photon and neutron regions.

531

Fig. 11. PSD discriminated tail-integral-vs.-total-integral plot for the bare data set (a) and the shadow-bar data set (b). Shadow-bar-subtracted TOF distributions (using 1 ns bins) for the pre- and post-discrimination data sets (c). Data were processed with a 40-keVee threshold. (Color image available online).

Fig. 12. PSD discriminated tail-integral-vs.-total-integral plot for the bare data set (a) and the shadow-bar data set (b). Shadow-bar-subtracted TOF distributions (using 1 ns bins) for the pre- and post-discrimination data sets (c). Data were processed with a 60-keVee threshold. (Color image available online).

Fig. 13. PSD discriminated tail-integral-vs.-total-integral plot for the bare data set (a) and the shadow-bar data set (b). Shadow-bar-subtracted TOF distributions (using 1 ns bins) for the pre- and post-discrimination data sets (c). Data were processed with a 90-keVee threshold. (Color image available online).

Fig. 14. PSD discriminated tail-integral-vs.-total-integral plot for the bare data set (a) and the shadow-bar data set (b). Shadow-bar-subtracted TOF distributions (using 1 ns bins) for the pre- and post-discrimination data sets (c). Data were processed with a 120-keVee threshold. (Color image available online).

Table 3 summarizes the comparison between Auto-Slice-PSD-estimated and TOF-estimated photon misclassification ratios while Table 4 summarizes the same comparison for neutrons. Auto-Slice-PSD-estimated misclassification ratios are reported to two significant figures. TOF-estimated misclassification ratios and systematic uncertainties are reported to the number of significant figures required for the associated statistical uncertainty to be reported to two significant figures.

The TOF-estimated misclassification ratios reported in Tables 3 and 4 are calculated using the mean baseline values. The systematic uncertainties report the difference between TOF-estimated misclassification ratios calculated when using the mean baseline values and those calculated when using a two-standard-deviation uncertainty about the mean baseline values. These systematic uncertainties are expected to be asymmetric about the mean value and are therefore reported separately as upper and lower values. This asymmetry is seen in Table 4 (neutrons) but is outside the precision reported in Table 3 (photons). Adding the upper systemic uncertainty to the TOF-estimated misclassification ratio will give the upper bound referred to in section 4.3, while subtracting the lower systematic uncertainty from the TOF-estimated misclassification ratio will give the lower bound. Uncertainties due to the choice of ROI boundaries are not reported because it was determined that the boundaries would need to be shifted unreasonably in either direction for the related uncertainties to approach the magnitude of the reported statistical uncertainties. Detection ratios are not included in Tables 3 and 4 because they are complements of the corresponding misclassification ratios. It should be noted that the misclassification ratios were not optimized for any particular application. As such, their magnitudes are important only to the extent to which they compare between the software and TOF estimation.

At each threshold, the statistical uncertainty was computed separately for each of the three baseline values used. However, these values were found to be equal to within the reported precision regardless of the baseline value. As such, the statistical uncertainty is reported only once for each threshold. Because

the statistical uncertainty was computed directly for the upper and lower bounds, it is not necessary to combine the systematic and statistical uncertainties in quadrature. The software-estimated misclassification ratios are considered to compare well to the TOF-estimated misclassification ratios if they fall within the range defined by the reported misclassification ratio minus the lower systematic uncertainty minus the statistical uncertainty (on the lower end) and the reported misclassification ratio plus the upper systematic uncertainty plus the statistical uncertainty (on the upper end).

Table 3. Comparison between photon misclassification ratios estimated by Auto Slice PSD and those estimated from the TOF data sets. TOF-based misclassification ratios are calculated using the mean baseline values. Systematic uncertainties report the difference between TOF-estimated misclassification ratios calculated when using the mean baseline values and those calculated when using a two-standard-deviation uncertainty about the mean baseline values. Statistical uncertainties are reported at two sigma.

Threshold (keVee)	Misclass. Ratio (Auto Slice PSD)	Misclass. Ratio (TOF)	+ Upper Systematic Uncertainty (TOF)	- Lower Systematic Uncertainty (TOF)	+/- Statistical Uncertainty (TOF)
40	4.5×10^{-2}	3.482×10^{-2}	1.9×10^{-4}	1.9×10^{-4}	5.1×10^{-4}
60	2.7×10^{-2}	2.296×10^{-2}	1.4×10^{-4}	1.4×10^{-4}	4.3×10^{-4}
90	1.3×10^{-2}	1.261×10^{-2}	1.4×10^{-4}	1.4×10^{-4}	3.3×10^{-4}
120	7.6×10^{-3}	8.00×10^{-3}	1.1×10^{-4}	1.1×10^{-4}	2.8×10^{-4}

Table 4. Comparison between neutron misclassification ratios estimated by Auto Slice PSD and those estimated from the TOF data sets. TOF-based misclassification ratios are calculated using the mean baseline values. Systematic uncertainties report the difference between TOF-estimated misclassification ratios calculated when using the mean baseline values and those calculated when using a two-standard-deviation uncertainty about the mean baseline values. Statistical uncertainties are reported at two sigma.

Threshold (keVee)	Misclass. Ratio (Auto Slice PSD)	Misclass. Ratio (TOF)	+ Upper Systematic Uncertainty (TOF)	- Lower Systematic Uncertainty (TOF)	+/- Statistical Uncertainty (TOF)
40	4.0×10^{-2}	4.39×10^{-2}	2.11×10^{-2}	2.22×10^{-2}	2.0×10^{-3}
60	4.0×10^{-2}	3.08×10^{-2}	1.95×10^{-2}	2.04×10^{-2}	1.9×10^{-3}
90	7.5×10^{-3}	2.38×10^{-2}	1.82×10^{-2}	1.90×10^{-2}	1.9×10^{-3}
120	2.8×10^{-3}	2.03×10^{-2}	1.76×10^{-2}	1.84×10^{-2}	1.9×10^{-3}

6. Discussion

The discrimination curves shown in Figs 11-14 behave as expected. The linear segment effectively discriminates the high-energy deposition regions while the quadratic segment attempts to “follow” the bend of the neutron cluster. At 90 and 120 keVee thresholds, the curve appears to cut too far into the photon cluster. This is a result of the slice fit normalization giving too much importance to the neutron fit in a region where the neutron population is low relative to the gamma population. In practice, this discrimination curve could be adjusted by using unnormalized slice fits and/or adding additional bias. However, for the purpose of this paper, the input settings for Auto Slice PSD were left the same for all four thresholds.

The TOF distributions shown in Figs. 11-14 show the expected trends. The full distributions match the PSD-tagged photon distributions well in the photon ROIs and match the PSD-tagged neutron

606 distributions well in the neutron ROIs. Additionally, it is clear from these distributions that the neutron
607 ROI shrinks in width as the threshold is increased.

608 In general, the misclassification ratios generated by Auto Slice PSD compare well to the
609 misclassification ratios based on the TOF information. For photons, reported systematic uncertainty is
610 on the same order of magnitude as the statistical uncertainty. Additionally, both uncertainties are on a
611 lower order of magnitude than the TOF-estimated photon misclassification ratios. The low relative
612 uncertainty suggests that the TOF method is a reasonably accurate way of estimating photon
613 misclassification. At a threshold of 90 keVee the photon misclassification ratios agree to within the
614 reported uncertainties, and at a 120-keVee threshold the photon misclassification ratio estimated by
615 Auto Slice PSD falls just outside the reported uncertainties. However, at thresholds of 40 and 60 keVee,
616 the agreement between photon misclassification ratios is worse and the difference between the values
617 falls well outside the uncertainties on the TOF-based misclassification ratios. This suggests that there
618 may be some systematic uncertainty associated with the Auto Slice PSD algorithm. While the exact
619 source of this uncertainty is under further investigation, it is likely that the uncertainty is related to the
620 difficulty of fitting slices with a great deal of overlap.

621 For neutrons, the misclassification ratios estimated by Auto Slice PSD do not agree well with the TOF-
622 based misclassification ratios calculated using the mean baseline value. However, the reported
623 systematic uncertainty is an order of magnitude higher than the statistical uncertainty and is on the same
624 order of magnitude as the TOF-estimated neutron misclassification ratios computed using the mean
625 baseline value. The systematic uncertainty due to baseline correction is high because the neutron ROI in
626 the PSD-classified-photon data set is close in magnitude to the baseline. The width of the neutron ROI
627 also contributes to the baseline-correction uncertainty. While not reported in Table 4, the systematic
628 uncertainty associated with neutron detection ratios showed a similar trend.

629 The loose misclassification-ratio bounds suggest that the misclassification ratios computed using the
630 mean baseline value might not be a reliable way to assess the performance of Auto Slice PSD for
631 neutron misclassification. However, it is important to note that the Auto Slice PSD estimated neutron
632 misclassification ratios do fall within the TOF-estimated misclassification-ratio bounds for all four
633 thresholds investigated. As such, it can be concluded that the Auto Slice PSD method is comparable to
634 the TOF-based method for the estimation of neutron misclassification. The high level of uncertainty
635 associated with the TOF-estimated neutron misclassification ratios makes it difficult to determine the
636 presence of systemic uncertainty in the Auto Slice PSD estimation of neutron misclassification.
637 However, due to the methods Auto Slice PSD uses to calculate misclassification, it can be safely
638 assumed that any systematic uncertainties impacting the estimation of photon misclassification would
639 also impact the estimation of neutron misclassification.

640 **7. Summary and Conclusions**

641 An algorithm has been developed that is capable of automatically and consistently determining a
642 discrimination curve for use with the CIPSD method for PSD-capable organic scintillation detectors.
643 The algorithm works by slicing the data into smaller subsets and fitting the ratio histogram in each slice
644 to a sum of two Gaussians. The Gaussian fits are analyzed to determine the optimal points, based on the
645 user's input parameters, through which to cut each slice. The points are then fit with a discrimination
646 curve, which is used, along with the Gaussian slice fits, to estimate the neutron and photon detection and
647 misclassification ratios.

648 The algorithm was tested on a TOF-tagged, measured data set, which allowed for Auto-Slice-PSD-
649 estimated misclassification ratios to be compared to TOF-estimated misclassification ratios. In general,
650 the misclassification ratios compared well between methods for both photons and neutrons.

651 Discrepancies between photon misclassification ratios at 40 and 60 keVee thresholds were larger than
652 the uncertainties associated with the TOF-based estimation. These discrepancies suggest that there may
653 be some systematic uncertainty related to the ability of the Auto Slice PSD algorithm to fit slices with a
654 great deal of cluster overlap. While these discrepancies were outside the reported bounds of uncertainty,
655 the estimated misclassification ratios were still reasonably close in magnitude.

656 As a result, Auto Slice PSD is considered a viable method for determining a discrimination curve for use
657 with CIPSD and estimating the detection and misclassification ratios of neutrons and photons measured
658 with PSD-capable organic scintillators. These estimations can be performed using only the data
659 collected from a single detector, which is a significant advantage over using a more traditional TOF
660 approach. As such, the Auto Slice PSD software streamlines the process of tuning misclassification and
661 detection ratios to a desired application.

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