

## APPENDIX A

### BETA SINGLES MODEL

*Many people have set up computer models of things, and have discovered that they learned more while setting up the model than while actually looking at the output of the eventual program.* –Donald Knuth [3]

The purpose of the beta singles model is to determine the number of  $\beta$  decays from trapped ions of interest, observed in an experimental dataset. For us this analytical task was complicated by the presence of contaminant nuclei among the trapped ions and by the presence of untrapped nuclei that, despite being located away from the trap center, still emitted  $\beta$ 's that were detected with some efficiency. We start with a brief overview of these complications and their causes.

1. We injected some amount of nearest-neighbor isobaric contaminants into the trap along with the species of interest. These contaminants are also  $\beta$  emitters having different lifetimes that are typically  $\sim 10\times$  different from those of the species of interest. This is an unwelcome effect that hopefully will be eliminated in the future.
2. Each ion bunch delivered to the BPT was not captured with perfect efficiency. Ions not captured are instead scattered by unstable interactions with the trap rf and may come to rest just about anywhere in the BPT chamber. Though it may be difficult, one can imagine eliminating this effect by realizing a capture efficiency of  $\approx 100\%$ .
3. The trapped ions in our experiment suffered from a finite “trap lifetime,” meaning they were neutralized through charge-exchange with contaminant molecules in the buffer gas, at rates that were sometimes comparable to the  $\beta$ -decay rates. This effect provides a non-radioactive channel through which trapped ions become untrapped continuously, modifying the apparent half-life of each trapped species in a chemistry-dependent way. The populations of  $\beta$  emitters that become untrapped in this way evolve differently

in time than the emitters lost during capture (the latter changing discontinuously at the moment of injection) and presumably have a different spatial distribution. This also is an unwelcome effect. It was present in our particular installation due to an undiscovered vacuum leak. Ordinarily the trap lifetime is effectively infinite, and we expect this will be achieved again in any future installation.

4. The  $\beta$ -decay recoil-nuclei, which are themselves  $\beta$  emitters, remain in the BPT volume and detectable. The populations of these recoils are also continuous functions of time and are presumably also distributed differently spatially from the other untrapped groups, in addition to now being another nuclear species. This effect seems inevitable, given our basic method and apparatus, so we expect it to be present even in refined future iterations of the experiment.
5. Many of the  $\beta$ -decay recoils are neutron-emitters, and therefore a fraction of the resulting untrapped nuclei will be of the  $\beta n$  resultant species and have a different lifetime. This also seems unavoidable.
6. For trapped ions the  $\beta$  detection efficiency is known, but untrapped atoms have unknown detection efficiencies that, following the points above, almost certainly depend on how they came to be untrapped.

These are the known issues with our measurement. As we build up the model we will treat them all, except (5). We will also address the possibility that some fraction of trapped ions are lost when a new bunch comes in, and the possibility that the populations of untrapped nuclei may also undergo non-radioactive decay. The omission of the  $\beta n$  resultant nuclei is the primary shortcoming of the model presented here, in the author's opinion.

## A.1 Definitions

We consider a  $\beta$ -decay chain of three ion species delivered to the BPT, enumerating them such that Species 1 is the parent of Species 2, which in turn is the parent of Species 3. Species  $i$  has a population  $T_i(t)$  that is trapped at the center of the BPT and a population  $U_i(t)$  that is untrapped, ie. scattered about the BPT such that its  $\beta$ 's are still detectable.

Symbol	Description	Units
$r_1$	Rate of Species 1 ion injection to BPT	ions/sec
$r_2$	Rate of Species 2 ion injection to BPT	ions/sec
$r_3$	Rate of Species 3 ion injection to BPT	ions/sec
$p$	Capture efficiency of all species in BPT	# in $[0,1]$

**Table A.1:** Essential parameters in describing the evolution of trapped and untrapped ion populations during experiment.

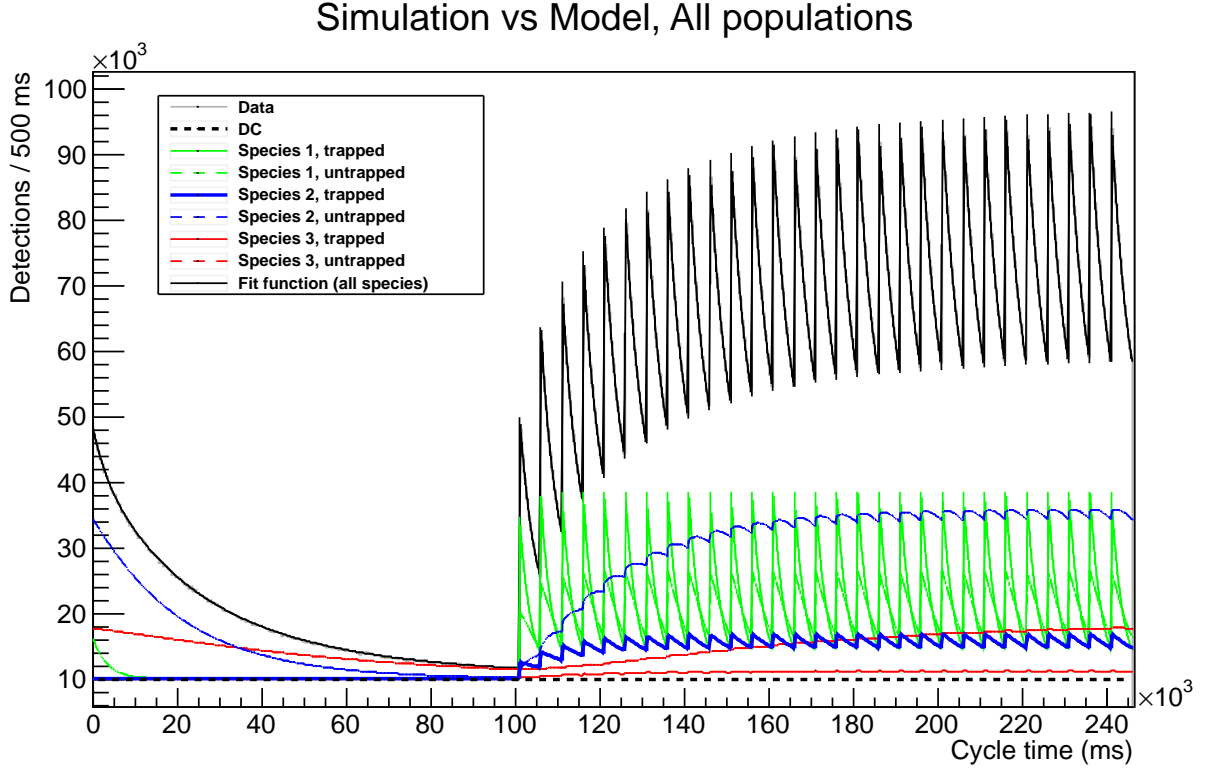
Species 2 denotes the BDN precursor we want to measure, and the other two species are nearest-neighbor contaminants which are not eliminated by the isobar separator. Our goal is learn the number of  $\beta$  decays of trapped Species 2 nuclei, belonging to the  $T_2$  population. A picture of this is given in Figure A.1, which shows the total signal as it relates to the trapped and untrapped components of all three species.

It is worth emphasizing that the dynamical variables of the model are the populations of different types of ions, while the data we must fit are the integrated rates of detected  $\beta$  decays associated with each population. Treating the populations allows us to build the model around the most physically obvious parameters and a set of dynamics that must be present in the experiment. It is easy to derive the  $\beta$  rates once the populations are determined.

The model takes as fixed the time structure of the measurement cycle used for a given dataset. Recalling ?? and using  $t$  to denote the cycle-time variable, we let  $t = 0$  be the time at which all trapped ions are ejected from the BPT. The background interval is then  $t = 0$  to  $t_B$ , and the trapping interval is  $t = t_B$  to  $t_C$ . Ions are injected at intervals of  $t_A$ , so that the times of injection are given by

$$t_n \equiv t_B + (n - 1)t_A, \quad n = 1, 2, \dots, N. \quad (\text{A.1})$$

The model is built around 4 essential parameters described in Table A.1. In an ideal version of the experiment these parameters, together with the known radioactive lifetimes and a set of reasonable assumptions, would be sufficient to describe the evolution of all 6 populations. Other parameters will be introduced as needed. The full list of parameters (including the values used to generate our illustrations) is given in Table A.2.



**Figure A.1:** Illustrative data generated by a Monte Carlo simulation as described in section A.9, modeled after the cycle and decay characteristics of the  $^{137}\text{I}07$  dataset. The data (gray histogram) includes contributions from trapped and untrapped populations of three different nuclear species, and these contributions (colored lines) must be estimated from a model of the overall signal (black line). A constant background rate (DC) is shown by the dashed black line, and the colored lines are drawn using this DC as their 0. The critical output of the model is the area under the solid blue curve, corresponding to the number of  $\beta$  decays by the trapped species of interest in the presence of nearest-neighbor isobaric contaminants as well as untrapped populations of all three species. The parameter values used in this run of the simulation can be found in section A.11. The perfect agreement between the simulation and the model provides strong confirmation that both are implemented correctly.

## A.2 Assumptions

1. There are no trapped ions in the trap during the background measurement:  $T_i(t) = 0$  for  $0 \leq t < t_B$ . This fact is regarded as extremely reliable.
2. The untrapped populations are continuous between BPT cycles:  $U_i(0) = U_i(t_C)$ . This is also considered extremely reliable, so long as the time in which the untrapped ions build up is marginalized.
3. The rates of ion injection do not vary during the course of the trapping period.
4. Injected ions of all three species are captured in the BPT with the same efficiency. This is ensured by the nearly identical masses of the species.
5. Trapped ions of all three species are retained in the BPT, during the capture of an incoming bunch, with the same efficiency  $\rho$ . This seems to be as good as Assumption 4.
6. Every radioactive decay of a trapped or untrapped ion of Species  $i$  produces an untrapped ion of Species  $i + 1$ .

## A.3 Fitting to data

Given the time-dependent trapped and untrapped species populations,  $T_i$  and  $U_i$ , we will need to match these functions to data. The data will be in the form of an histogram with bin width  $\Delta t$ , containing the frequency of some type of event that is linked to the species population (such as  $\beta$  detection) versus “cycle-time,” or the time elapsed since the most recent BPT ejection pulse. The data are summed over a number  $N_C$  of cycles. We did not synchronize our data-taking with cycle-time, so  $N_C$  is neither guaranteed to be an integer nor even guaranteed to be a constant across the summed histogram. As a reminder, this histogram should generally be corrected for deadtime, as the overall trigger rate in the experiment generally varies with respect to cycle-time. This histogram includes detections of  $\beta$ ’s from an unknown combination of all populations. We call the height of each bin  $y(t)$

and denote the rate of detections as  $D(t)$ , so that

$$y(t) = N_C D(t) \Delta t. \quad (\text{A.2})$$

We build the total detection rate  $D$  from the six ion populations and a constant background rate  $D_0$ . The detection rates are just the products of decay rates (population/lifetime) and detection efficiencies  $\varepsilon$ ,

$$D_{Ti} = \varepsilon_T T_i / \tau_i \quad (\text{A.3})$$

$$D_{Ui} = \varepsilon_U U_i / \tau_i. \quad (\text{A.4})$$

This is the aforementioned link between population and event rate, though in principle the relation could have a different form. The lifetimes  $\tau_i$  in these expressions are radioactive only, as only a radioactive decay produces a  $\beta$  detection. Note that we are allowing the detection efficiencies to differ between trapped and untrapped ions, but they do not vary per the nuclear species. So our fitting function is

$$y(t) = N_C \left[ D_0 + \varepsilon_T \sum_{i=1}^3 T_i(t) / \tau_i + \varepsilon_U \sum_{i=1}^3 U_i(t) / \tau_i \right] \Delta t. \quad (\text{A.5})$$

Here we see three new model parameters that were not included in our initial list:  $D_0$ ,  $\varepsilon_T$ , and  $\varepsilon_U$ . There are more secondary parameters to come, and they will cause a lot more trouble than these did.

On that score, we will be subdividing the untrapped populations into components  $V_i$ ,  $W_i$ ,  $Z_i$ ,  $X_i$ , and  $Y_i$ . With those components, the fitting function is

$$\begin{aligned} y(t) = & N_C \left[ D_0 + \varepsilon_T \sum_{i=1}^3 T_i(t) / \tau_i + \varepsilon_U \sum_{i=1}^3 (\varepsilon_V V_i(t) + \varepsilon_W W_i(t) + \varepsilon_Z Z_i(t)) / \tau_i \right. \\ & \left. + \varepsilon_U \sum_{i=2}^3 (\varepsilon_X X_i(t) + \varepsilon_Y Y_i(t)) / \tau_i \right] \Delta t. \end{aligned} \quad (\text{A.6})$$

Each component gets its own (species-independent) detection efficiency. The overall untrapped efficiency  $\varepsilon_U$  is kept as a computational convenience for setting all untrapped com-

ponents equal. It is intended that  $\varepsilon = 1$  be used whenever the component efficiencies are set to different values, but in any case the working model uses the product  $\varepsilon_U \varepsilon_V$  for the  $V_i$  efficiencies, and so on.

## A.4 Dynamics

All of the dynamics that we consider will come from the first-order linear equation,

$$\frac{df}{dt} + \frac{f(t)}{\tau} = g(t). \quad (\text{A.7})$$

This equation is well known and can be solved, for any integrable function  $g$ , using an integrating factor. (See, for example, page 442 of [1]). With an initial value  $f(t_0)$ , we have

$$f(t) = f(t_0)e^{-(t-t_0)/\tau} + e^{-t/\tau} \int_{t_0}^t g(s)e^{s/\tau} ds. \quad (\text{A.8})$$

The variety we will encounter in our solutions is due only to the variety we will see in the source term  $g$ .

We will continually make use of the linearity of Equation A.7, so that when the source is the sum of multiple components  $g = g_1 + g_2$  we can decompose a solution into components  $f = f_1 + f_2$  such that each component is also a solution:

$$\begin{cases} f_1(t) &= f_1(t_0)e^{-(t-t_0)/\tau} + e^{-t/\tau} \int_{t_0}^t g_1(s)e^{s/\tau} ds \\ f_2(t) &= f_2(t_0)e^{-(t-t_0)/\tau} + e^{-t/\tau} \int_{t_0}^t g_2(s)e^{s/\tau} ds. \end{cases} \quad (\text{A.9})$$

One important application of this will be to decompose the untrapped populations into a “trapping component”  $f_A$  and a “background component”  $f_B$ , such that

$$f(t) = \begin{cases} f_B(t), & 0 \leq t \leq t_B \\ f_B(t) + f_A(t), & t_B < t \leq t_C \end{cases}. \quad (\text{A.10})$$

This will be helpful because the untrapped populations have source terms  $g_A$  that are present only on the trapping interval. The trapping component  $f_A$  comprises the contributions of “injection” terms  $g_A/\tau_g$  that are present only on the trapping interval, and the background component  $f_B$  comprises the contribution of source terms  $g_B/\tau_g$  present throughout the cycle. We may therefore write

$$\begin{cases} \frac{df_A}{dt} + \frac{f_A}{\tau_f} = \frac{g_A}{\tau} & \text{if } t_B < t \leq t_C \\ \frac{df_B}{dt} + \frac{f_B}{\tau_f} = \frac{g_B}{\tau} & \text{always.} \end{cases} \quad (\text{A.11})$$

For notational simplicity, although we will be using this decomposition continually, we will avoid using the  $A$  and  $B$  subscripts in the work ahead. When we come to analyzing the trapping components of various untrapped populations, we will instead use the lower case, eg. the trapping component of the  $V_2$  population will be  $v_2(t)$ .

Several forms of Equation A.7 will need needed below. First is a source that is a  $\delta$  function, which models the ion injection:

$$\frac{df}{dt} + \frac{f(t)}{\tau} = A\delta(t - t_1). \quad (\text{A.12})$$

The solution is

$$f(t) = \begin{cases} f(t_0)e^{-(t-t_0)/\tau}, & t < t_1 \\ f(t_0)e^{-(t-t_0)/\tau} + Ae^{-(t-t_1)/\tau}, & t \geq t_1 \end{cases}. \quad (\text{A.13})$$

Next consider a population  $g$  being fed continuously by the decays of another population  $h$  at a rate  $1/\tau_{hg}$ , so that

$$\frac{dg}{dt} + \frac{g(t)}{\tau_g} = \frac{h(t)}{\tau_{hg}}. \quad (\text{A.14})$$

We will want the solution in the case

$$h(t) = h(t_0)e^{-(t-t_0)/\tau_h}, \quad (\text{A.15})$$

Using the symbol

$$\Gamma_B^A \equiv \frac{1}{\tau_A} - \frac{1}{\tau_B} = \frac{\tau_B - \tau_A}{\tau_A \tau_B} \quad (\text{A.16})$$



the solution for  $g$  is

$$g(t) = g(t_0)e^{-(t-t_0)/\tau_g} + h(t_0) \cdot \frac{e^{-(t-t_0)/\tau_g} - e^{-(t-t_0)/\tau_h}}{\tau_{hg}\Gamma_h^g}. \quad (\text{A.17})$$

Next we will want the population  $f$  that is fed by  $g$ , with

$$\frac{df}{dt} + \frac{f(t)}{\tau_f} = \frac{g(t)}{\tau_{gf}}. \quad (\text{A.18})$$

The general solution to this is

$$\begin{aligned} f(t) = & f(t_0)e^{-(t-t_0)/\tau_f} + g(t_0) \cdot \frac{e^{-(t-t_0)/\tau_f} - e^{-(t-t_0)/\tau_g}}{\tau_{gf}\Gamma_g^f} \\ & + \frac{h(t_0)}{\tau_{hg}\Gamma_h^g} \cdot \left[ \frac{e^{-(t-t_0)/\tau_f} - e^{-(t-t_0)/\tau_g}}{\tau_{gf}\Gamma_g^f} - \frac{e^{-(t-t_0)/\tau_f} - e^{-(t-t_0)/\tau_h}}{\tau_{gf}\Gamma_h^f} \right]. \end{aligned} \quad (\text{A.19})$$

We now have seen all the solutions that will be needed in the following sections. It is time to start finding the populations.

## A.5 Trapped Populations

The trapped populations have source terms for the ion injections into the trap. Ions are injected in bunches at intervals of  $t_A$  during the trapping period, starting at  $t = t_B$ . Species  $i$  is injected into the BPT chamber at a time-averaged rate  $r_i$  and trapped at the BPT center with trapping efficiency  $p$ , so that each bunch contains a number  $pr_i t_A$  of Species  $i$  nuclei. Each injection takes  $20 \mu\text{s}$ , and with intervals of  $t_A \geq 100 \text{ ms}$  the injection is aptly modeled as a  $\delta$  function in the source term.

For a given experimental case the cycle times  $t_A$ ,  $t_B$ , and  $t_C$  are fixed, and the ion injection takes place at times  $t_n$  given by Equation A.1. The dynamical equation for  $T_i$  can be written as

$$\dot{T}_i + T_i/\tau_{Ti} = A_{Ti} \sum_{k=1}^N \delta(t - t_k), \quad (\text{A.20})$$

with  $A_{Ti} \equiv pr_i t_A$  and  $N$  the number of injections in each cycle. Here is the modified lifetime  $\tau_{Ti}$  that combines all radioactive and non-radioactive channels. We apply Equation A.13

with  $t_0 = 0$  and  $f(t_0) = 0$ , so that  $T_i(t) = 0$  on the background interval. Each such solution is the contribution of a single ion bunch, and the solution to Equation A.20 is a sum of these contributions from  $t_1$  to  $t$ . Denoting the tooth number at time  $t$  as  $n$ , we have

$$\begin{aligned} T_i(t) &= A_{Ti} \sum_{k=1}^n \exp\left(-\frac{t-t_k}{\tau_{Ti}}\right) \\ &= A_{Ti} \cdot \frac{1 - \exp(-nt_A/\tau_{Ti})}{1 - \exp(-t_A/\tau_{Ti})} \cdot \exp\left(-\frac{t-t_n}{\tau_{Ti}}\right), \end{aligned} \quad (\text{A.21})$$

where we have done a little juggling in the exponent and used the identity

$$\sum_{k=1}^n a^{n-k} = \sum_{k=0}^{n-1} a^k = \frac{1 - a^n}{1 - a}. \quad (\text{A.22})$$

There are several notational conventions at work here that we will use throughout the remaining analysis. The first is Equation A.1, in which we have chosen to index the injections as  $n = 1, 2, \dots, N$ . We often call the injections “teeth” due to their sawtooth shape in a graph. The tooth number  $n$  may be treated as an index or as the time-dependent variable

$$n(t) \equiv \text{ceiling}\left(\frac{t-t_B}{t_A}\right) \quad (\text{A.23})$$

interchangeably. The latter form is necessary for computing the species populations as functions of time. The number of injections in a cycle is then

$$N \equiv n(t_C) = \text{ceiling}\left(\frac{t_C - t_B}{t_A}\right). \quad (\text{A.24})$$

There are various ways to produce the step function  $n(t)$ , and the choice of the ceiling function here is not arbitrary. The floor function was initially chosen as its behavior at  $t = t_n$  was considered more pleasing, but it produces different values for  $N = n(t_C)$  depending on whether  $(t_C - t_B)/t_A$  is already an integer. As we will see below, this quantity is used to enforce the cyclic boundary condition, so its value at  $t = t_C$  matters to the untrapped populations.

Computationally, the discontinuities at should be treated with some care. The data

should be binned such that the injection times  $t_n$  are bin edges, so that the adjacent bins capture the whole difference in ion populations upon capture. The bin sizes should also be large enough that the 20- $\mu$ s injection event is negligible. In practice this is no problem as we have found it unnecessary to go smaller than 10 ms in any case, and undesirable as it slows down the fit. If it were necessary, one can imagine correcting the bin containing the injection window for the missing time or using a parameter to model it.

When regressing the model, the objective function (eg.  $\chi^2$ ) should not depend on the values at the discontinuities. This can be avoided by evaluating the fitting function at the bin-centers, as is done by default in ROOT's TMinuit fitter. We have also learned that it is safe to use TMinuit's 'I' option [2], which causes the regression to compare the integral of the fitting function to the areas of the bins. The bottom line is that we are making an arbitrary choice of what the populations are at the exact moments of injection, and we must avoid giving these points any special importance in the computed model.

### A.5.1 Capture retention

We now introduce the “capture retention” parameter  $\rho$ , which is the fraction (0 to 1) of already-trapped ions retained during a capture pulse. A value  $\rho < 1$  will appear in a graph as teeth that become shorter as the number of previous captures increases. The first tooth, arising from injection to an empty trap, never suffers from this loss mechanism. Including  $\rho$  in the model is not a response to any evidence we have seen that compels us to account for it (unlike the  $\tau_{Ti}$ ). Rather we include it to enable us to statistically search for its presence.

With this parameter our injection coefficients will now include a term proportional to the populations themselves:

$$\dot{T}_i + T_i/\tau_{Ti} = (A_{Ti} - (1 - \rho)T_i) \sum_{k=1}^N \delta(t - t_k), \quad (\text{A.25})$$

The populations in the injection terms are to be evaluated in the limit  $t \rightarrow t_k$  from the left, since the capture-retention loss acts only on previously-trapped ions. Thus, again, the first capture of the cycle must be unaffected by this term.

The extension of Equation A.21 to include the capture retention can easily be produced

once it is recognized that  $\rho$  acts just like the per-injection decay factor  $\exp(-t_A/\tau_{Ti})$ . The population just after the  $(n+1)^{\text{th}}$  injection is related to that on the  $n^{\text{th}}$  by

$$T_i(t_{n+1}) = A_{Ti} + \rho e^{-t_A/\tau_{Ti}} T_i(t_n). \quad (\text{A.26})$$

This recursion relation comprises several scalar operations on  $T_i(t_n)$ : first the population is decayed over one tooth; then it is reduced to a fraction  $\rho$ ; and then the next injection  $A_{Ti}$  is added. The first two operations are both multiplication by a constant and therefore just multiply each other. When  $\rho \rightarrow 1$ , Equation A.26 reduces to a statement that is true of our previous solution.

We will use the notations

$$a_{Ti} \equiv \exp(-t_A/\tau_{Ti}) \quad (\text{A.27})$$

and

$$\sigma_{Ti}(n) \equiv \frac{1 - (\rho a_{Ti})^n}{1 - \rho a_{Ti}}, \quad (\text{A.28})$$

and write the complete trapped-ion solutions as

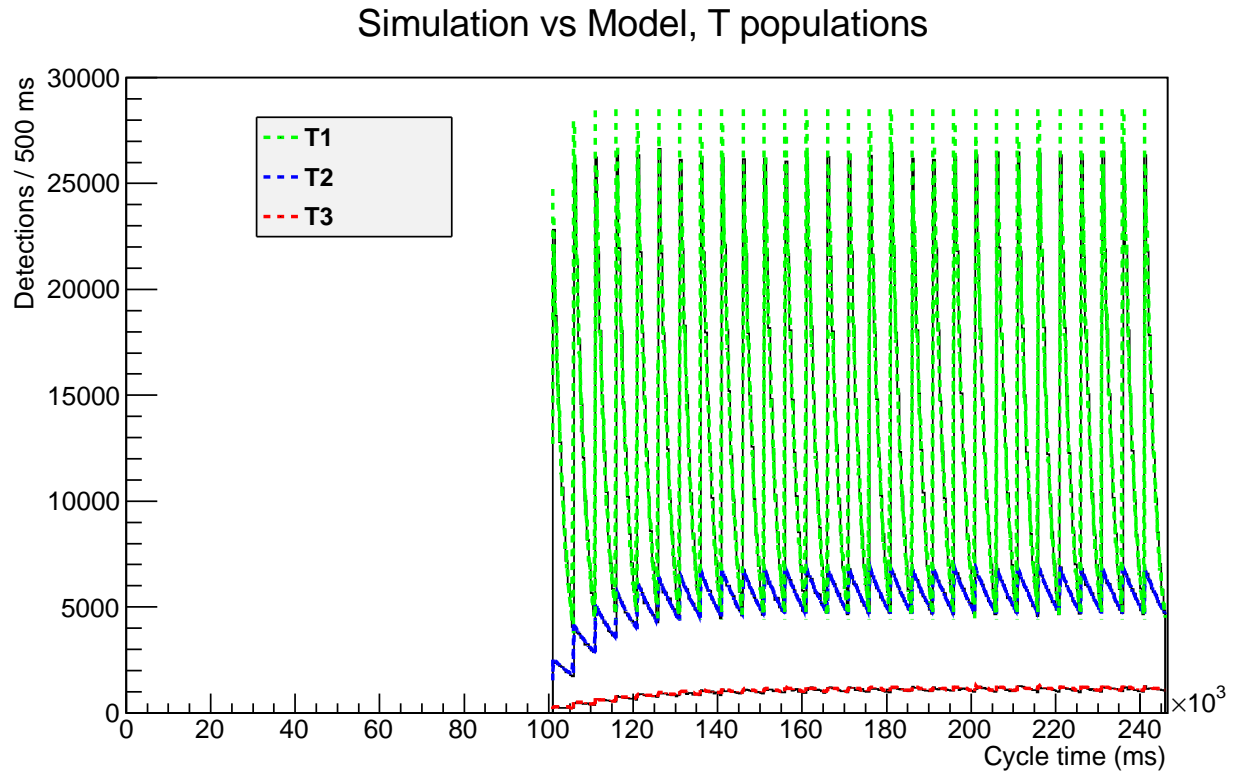
$$T_i(t) = A_{Ti} \sigma_{Ti}(n) \exp\left(-\frac{t - t_n}{\tau_{Ti}}\right). \quad (\text{A.29})$$

Examples of the  $T$  populations are shown in Figure A.2.

## A.6 Untrapped populations

In this section we will give a preliminary treatment of the overall untrapped populations. In later sections we will subdivide these, so the  $U_i$  populations derived here are never used as such in the model. The analysis presented in this section follows the lines of our first approach to building the model and still seems well suited as a means of showing how the full solutions are built. The methods we explain here will be relied upon throughout the analyses that follow.

Following Equation A.11, we decompose the untrapped populations  $U_i$  into background components  $U_i^B$  and trapping components  $U_i^A$ . The expression we find for  $U_i^B$  in subsection A.6.1 will be enough for all subdivided populations. The expressions for  $U_i^A$  in subsec-



**Figure A.2:** Comparison of simulated  $\beta$  detections to those calculated by the model, for  $T_1$ ,  $T_2$  and  $T_3$  populations. The functions are discontinuous due to direct feeding from  $\delta$ -function source terms associated with each capture event. The background component of  $T_i$  is always zero by definition, and this leads to the overall experimental signal not obeying the cyclic boundary condition. The parameter values used in this run of the simulation can be found in section A.11. This example shows the effect of both a modified lifetime and imperfect retention.

tion A.6.2, on the other hand, merely resemble the trapping components used in the model, and they are presented for their expository value. The amplitudes of the  $U_i^B$  will naturally depend on those of the  $U_i^A$ , and we will show how to put these together in ??.

### A.6.1 Background components

The feeding in the background components is represented by the coupled rate equations

$$\dot{U}_1^B + U_1^B/\tau_{U1} = 0 \quad (\text{A.30})$$

$$\dot{U}_2^B + U_2^B/\tau_{U2} = U_1^B/\tau_1 \quad (\text{A.31})$$

$$\dot{U}_3^B + U_3^B/\tau_{U3} = U_2^B/\tau_2. \quad (\text{A.32})$$

Note that the feeding depends only on the radioactive lifetime, since only the radioactive decay converts species. The intrinsic population decay follows the net lifetime  $\tau_{U_i}$ .

We solve Equations A.30–A.32 sequentially, plugging the first solution into the second equation and so on. This procedure follows that of Equations A.17 and A.19, with  $t_0 = 0$ ,  $h = U_1$ ,  $\tau_{hg} = \tau_1$ ,  $g = U_2$ ,  $\tau_{gf} = \tau_2$ ,  $f = U_3$ . The solutions are

$$U_1^B(t) = U_1(0) \exp\left(-\frac{t}{\tau_{U1}}\right) \quad (\text{A.33})$$

$$U_2^B(t) = U_2(0) \exp\left(-\frac{t}{\tau_{U2}}\right) \quad (\text{A.34})$$

$$\begin{aligned} & + U_1(0) \cdot \frac{1}{\tau_1 \Gamma_{U2}^{U1}} \cdot \left[ \exp\left(-\frac{t}{\tau_{U2}}\right) - \exp\left(-\frac{t}{\tau_{U1}}\right) \right] \\ U_3^B(t) & = U_3(0) \exp\left(-\frac{t}{\tau_{U3}}\right) \quad (\text{A.35}) \\ & + U_2(0) \cdot \frac{1}{\tau_2 \Gamma_{U3}^{U2}} \cdot \left[ \exp\left(-\frac{t}{\tau_{U3}}\right) - \exp\left(-\frac{t}{\tau_{U2}}\right) \right] \\ & + U_1(0) \cdot \frac{1}{\tau_1 \Gamma_{U2}^{U1}} \cdot \frac{1}{\tau_2 \Gamma_{U3}^{U2}} \cdot \left[ \exp\left(-\frac{t}{\tau_{U3}}\right) - \exp\left(-\frac{t}{\tau_{U2}}\right) \right] \\ & - U_1(0) \cdot \frac{1}{\tau_1 \Gamma_{U2}^{U1}} \cdot \frac{1}{\tau_2 \Gamma_{U3}^{U1}} \cdot \left[ \exp\left(-\frac{t}{\tau_{U3}}\right) - \exp\left(-\frac{t}{\tau_{U1}}\right) \right]. \end{aligned}$$

The pattern of how feeding works is evident here, and this is an opportune point for the reader to ensure he or she understands them. The initial values  $U_i(0)$  are determined in ??.

### A.6.2 Trapping components

The trapping components  $U_i^A$  are fed directly by the  $\propto (1 - p)$  ions that are not captured during injection, and by the radioactive decays of both the trapped parent populations  $T_{i-1}$  and the trapping components of the untrapped parent populations  $U_{i-1}^A$ . For now we neglect feeding by the non-radioactive decay, or continuous losses, of the trapped populations or by imperfect trap retention  $\rho$ . So the rate equations are

$$\dot{U}_1^A + U_1^A/\tau_{U1} = A_{U1} \sum_{k=1}^N \delta(t - t_k) \quad (\text{A.36})$$

$$\dot{U}_2^A + U_2^A/\tau_{U2} = A_{U2} \sum_{k=1}^N \delta(t - t_k) + T_1(t)/\tau_1 + U_1^A(t)/\tau_1 \quad (\text{A.37})$$

$$\dot{U}_3^A + U_3^A/\tau_{U3} = A_{U3} \sum_{k=1}^N \delta(t - t_k) + T_2(t)/\tau_2 + U_2^A(t)/\tau_2 \quad (\text{A.38})$$

with the amplitudes

$$A_{Ui} \equiv (1 - p)r_i t_A. \quad (\text{A.39})$$

The  $\delta$ -function terms produce solutions that are exactly analogous to the trapped populations with  $\rho = 1$  (Equation A.21), and since  $U_1^A$  only includes this term, we can immediately write down the solution

$$U_1^A(t) = A_{U1} \cdot \sigma_{U1}(n) \cdot \exp\left(-\frac{t - t_n}{\tau_{U1}}\right), \quad (\text{A.40})$$

where now the population decay term is

$$a_{Ui} \equiv \exp(-t_A/\tau_{Ui}) \quad (\text{A.41})$$

and

$$\sigma_{Ui}(n) \equiv \frac{1 - a_{Ui}^n}{1 - a_{Ui}}. \quad (\text{A.42})$$

To handle the  $T_i$  and  $U_i^A$  terms we express the solution on an arbitrary tooth, where  $\sigma_{Ti}$  and  $\sigma_{Ui}$  are constant so that again we can apply Equations A.17 and A.19. The resulting expressions will be sums of many terms all following those patterns, and they will be valid

on every tooth given the right value of  $n$  from Equation A.23. They are

$$\begin{aligned}
U_2^A(t) &= A_{U2} \cdot \sigma_{U2}(n) \cdot \exp\left(-\frac{t-t_n}{\tau_{U2}}\right) \\
&+ A_{T1} \cdot \sigma_{T1}(n) \cdot \frac{1}{\tau_1 \Gamma_{U2}^{T1}} \cdot \left[ \exp\left(-\frac{t-t_n}{\tau_{U2}}\right) - \exp\left(-\frac{t-t_n}{\tau_{T1}}\right) \right] \\
&+ A_{U1} \cdot \sigma_{U1}(n) \cdot \frac{1}{\tau_1 \Gamma_{U2}^{U1}} \cdot \left[ \exp\left(-\frac{t-t_n}{\tau_{U2}}\right) - \exp\left(-\frac{t-t_n}{\tau_{U1}}\right) \right]
\end{aligned} \tag{A.43}$$

and

$$\begin{aligned}
U_3^A(t) &= A_{U3} \cdot \sigma_{U3}(n) \cdot \exp\left(-\frac{t-t_n}{\tau_{U3}}\right) \\
&+ A_{T2} \cdot \sigma_{T2}(n) \cdot \frac{1}{\tau_2 \Gamma_{U3}^{T2}} \cdot \left[ \exp\left(-\frac{t-t_n}{\tau_{U3}}\right) - \exp\left(-\frac{t-t_n}{\tau_{T2}}\right) \right] \\
&+ A_{U2} \cdot \sigma_{U2}(n) \cdot \frac{1}{\tau_2 \Gamma_{U3}^{U2}} \cdot \left[ \exp\left(-\frac{t-t_n}{\tau_{U3}}\right) - \exp\left(-\frac{t-t_n}{\tau_{U2}}\right) \right] \\
&+ A_{T1} \cdot \sigma_{T1}(n) \cdot \frac{1}{\tau_1 \Gamma_{U2}^{T1}} \cdot \frac{1}{\tau_2 \Gamma_{U3}^{U2}} \cdot \left[ \exp\left(-\frac{t-t_n}{\tau_{U3}}\right) - \exp\left(-\frac{t-t_n}{\tau_{U2}}\right) \right] \\
&- A_{T1} \cdot \sigma_{T1}(n) \cdot \frac{1}{\tau_1 \Gamma_{U2}^{T1}} \cdot \frac{1}{\tau_2 \Gamma_{U3}^{T1}} \cdot \left[ \exp\left(-\frac{t-t_n}{\tau_{U3}}\right) - \exp\left(-\frac{t-t_n}{\tau_{T1}}\right) \right] \\
&+ A_{U1} \cdot \sigma_{U1}(n) \cdot \frac{1}{\tau_1 \Gamma_{U2}^{U1}} \cdot \frac{1}{\tau_2 \Gamma_{U3}^{U2}} \cdot \left[ \exp\left(-\frac{t-t_n}{\tau_{U3}}\right) - \exp\left(-\frac{t-t_n}{\tau_{U2}}\right) \right] \\
&- A_{U1} \cdot \sigma_{U1}(n) \cdot \frac{1}{\tau_1 \Gamma_{U2}^{U1}} \cdot \frac{1}{\tau_2 \Gamma_{U3}^{U1}} \cdot \left[ \exp\left(-\frac{t-t_n}{\tau_{U3}}\right) - \exp\left(-\frac{t-t_n}{\tau_{U1}}\right) \right]
\end{aligned} \tag{A.44}$$

### A.6.3 Full solution

To build the complete solution for the untrapped populations, we compose the full function as

$$U_i(t) = \begin{cases} U_i^B(t), & 0 \leq t \leq t_B \\ U_i^B(t) + U_i^A(t), & t_B < t \leq t_C. \end{cases} \tag{A.45}$$

The initial values  $U_i(0)$  are found sequentially. The cyclic boundary condition of Assumption 2 allows us to substitute  $t = 0$  on the LHS, and  $t = t_C$  on the RHS, of Equation A.33. Solving for  $U_i(0)$  yields

$$U_1(0) = A_{U1} \cdot \sigma_{U1}(N) \cdot \frac{\exp[-(t_C - t_N)/\tau_{U1}]}{1 - \exp(-t_C/\tau_{U1})}, \tag{A.46}$$



which is fully determined by known constants and model parameters. With  $U_1(0)$  in hand we can then follow the same procedure with Equation A.34 to find  $U_2(0)$ , and so on for  $U_3(0)$ . Generally we can write

$$U_i(0) = \frac{U_i(t_C) - U_i(0) \exp(-t_C/\tau_{Ui})}{1 - \exp(-t_C/\tau_{Ui})}, \quad (\text{A.47})$$

understanding that the RHS can be evaluated without having to know  $U_i(0)$ . These initial values are recalculated whenever the parameters are changed during the model regression.

The cyclic boundary condition assumes that an effectively infinite number of cycles is observed, relative to the longest population lifetime. Consider that a long-lived untrapped population, viewed versus real time, builds up from cycle to cycle just as the trapped populations build up from tooth to tooth: starting from 0 in the first cycle and reaching steady state after many cycles. The decay factor of the untrapped population over one cycle is  $\exp(-t_C/\tau_{Ui})$ , which is typically non-negligible for Species 3 since the cycle time is tuned to the shorter lifetime of Species 2. The sum of an infinite number of these decay factors is  $1/(1 - \exp(-t_C/\tau_{Ui}))$ , which of course is exactly what the cyclic boundary condition requires. This impact of Assumption 2 should be kept in mind, because an effectively infinite number of observed cycles is not guaranteed.

## A.7 Components of untrapped populations

Until now we have treated the untrapped populations as monolithic, even though  $U_2$  and especially  $U_3$  can be made from two very different sources: inefficient capture and feeding. By lumping all these into a single population we have been resigned to giving all these ions the same detection efficiency. But that treatment is not necessarily justified. A recoiling ion can be lost from the chamber entirely if it emerges along the BPT axis and drifts down the beamline, or otherwise come to rest where it has no line of sight to a  $\beta$  detector. For these ions the  $\beta$  detection efficiency is nearly 0. On the other hand, one can imagine the recoil ion coming to rest on the foil in front of the  $\beta$  detector, resulting in a multifold enhancement in detection efficiency relative to a trapped ion. Or the ion could come to rest on the tip of one of the trap electrodes, resulting in an intermediary efficiency, closer to that of the

trapped ions. By subdividing the untrapped populations based on the various dynamics that may lead to their being untrapped, we can easily assign different efficiencies to each subpopulation. It also has the secondary benefit of allowing us to validate each untrapped component individually using a Monte Carlo simulation of the populations. The untrapped components are broken down as

$$U_1 = V_1 + W_1 + Z_1 \quad (\text{A.48})$$

$$U_2 = V_2 + W_2 + Z_2 + X_2 + Y_2 \quad (\text{A.49})$$

$$U_3 = V_3 + W_3 + Z_3 + X_3 + Y_3 \quad (\text{A.50})$$

where

$V_i \equiv$  Ions immediately lost from each injected bunch due to imperfect capture (fed by  $T_i$ )

$W_i \equiv$  Previously-trapped ions that become untrapped during a capture pulse (fed by  $T_i$ )

$Z_i \equiv$  Ions that become untrapped due to shortened trap lifetime (fed by  $T_i$ )

$X_i \equiv$   $\beta$ -decay children of trapped parent isotopes (fed by  $T_{i-1}$ )

$Y_i \equiv$   $\beta$ -decay children of untrapped parents (fed by  $U_{i-1}$ ).

All of these populations are assumed to have the same net lifetime  $\tau_{U_i}$ , depending only on their species and their being untrapped.

The linearity property Equation A.9 means that each of these components can be regarded as a separate population obeying Equation A.7 and having its own trapping and background component. With the exception of the  $Y_i$  populations, the background component of each of these populations has the simple form of Equation A.33. Therefore in the analysis that follows we will discuss only the trapping components until we get to the  $Y_i$  populations, so we may drop the superscript  $A$  if it feels cumbersome.

### A.7.1 The $V_1, V_2, V_3$ populations

The  $V_i$  populations are fed only by any imperfect capture efficiency, and they obey

$$\dot{V}_i + V_i/\tau_{Ui} = A_{Vi} \sum_{k=1}^N \delta(t - t_k) \quad (\text{A.51})$$

with

$$A_{Vi} = (1 - p)r_i t_A. \quad (\text{A.52})$$

This of course is just the trapped-population equation with  $\tau_{Ti} \rightarrow \tau_{Ui}$ ,  $p \rightarrow (1 - p)$ , and  $\rho \rightarrow 1$ . The trapping component is therefore

$$V_i^A(t) = A_{Vi} \sigma_{Vi}(n) \exp\left(-\frac{t - t_n}{\tau_{Ui}}\right) \quad (\text{A.53})$$

using

$$\sigma_{Vi}(n) \equiv \frac{1 - a_{Ui}^n}{1 - a_{Ui}}. \quad (\text{A.54})$$

Examples of the  $V$  populations are shown in Figure A.3.

We will continue to use  $\sigma(n)$ 's to represent the piecewise-constant parts of the populations. These will be increasingly complex sums that depend on the decay factors  $a_{Ti}$  and  $a_{Ui}$ . Note that both  $\sigma_{Ti}$  and  $\sigma_{Vi}$  are manifestations of the same form which we will call

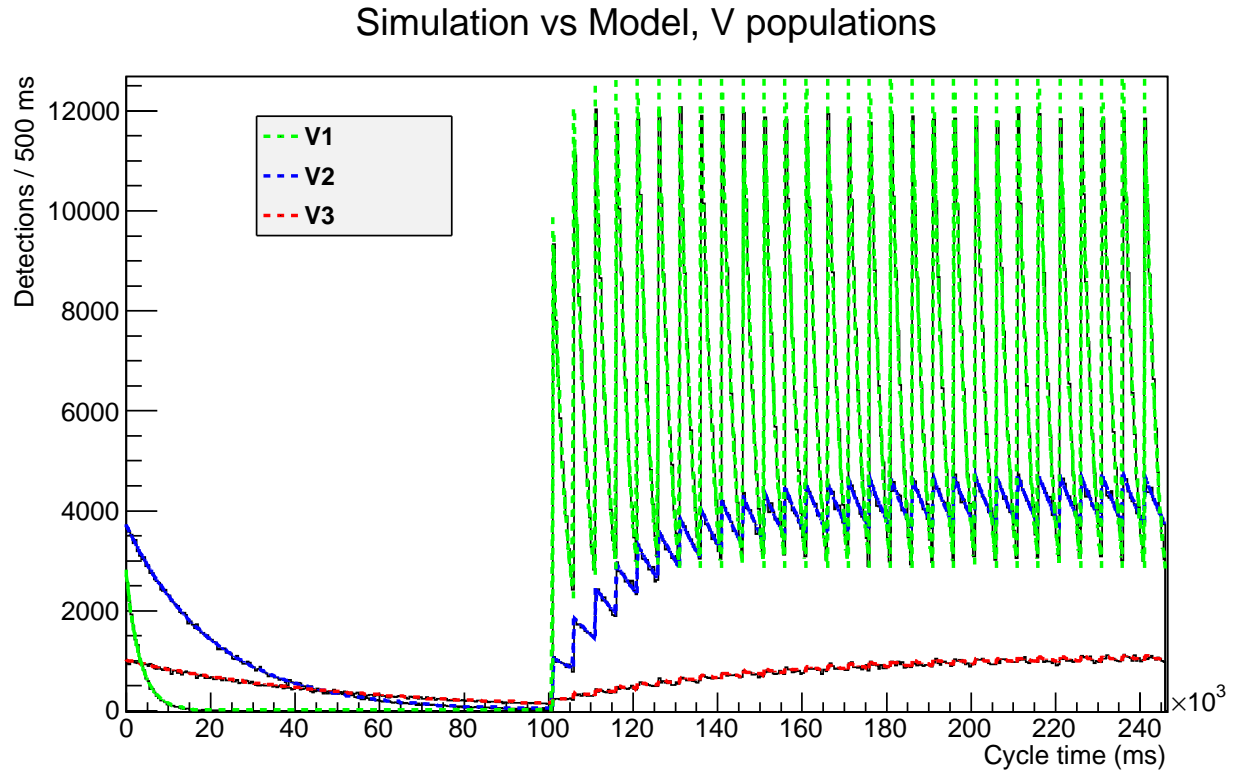
$$\sigma_I(\rho, a, n) \equiv \frac{1 - (\rho a)^n}{1 - \rho a}. \quad (\text{A.55})$$

This notation will be useful as we build up the more complex sums that appear in other populations.

### A.7.2 The $W_1, W_2, W_3$ populations

The  $W_i$  populations are fed by imperfect trapped-ion-retention during capture, so their source terms are complementary to those of Equation A.25,

$$\dot{W}_i + W_i/\tau_{Ui} = (1 - \rho)T_i \sum_{k=1}^N \delta(t - t_k), \quad (\text{A.56})$$



**Figure A.3:** Comparison of simulated  $\beta$  detections to those calculated by the model, for  $V_1$ ,  $V_2$  and  $V_3$  populations. The functions are discontinuous due to direct feeding from  $\delta$ -function source terms associated with each capture event. The trapping component of  $V_i$  has the same form as  $T_i$ , but of course  $V_i$  also has a non-zero background component. The parameter values used in this run of the simulation can be found in section A.11.

where again the population  $T_i$  is evaluated at the from-the-left limit at each discontinuity.

It is tempting to reason that the trapping component  $W_i^A$  is equal to the difference between “ $T_i$  with  $\rho = 1$ ” and “ $T_i$  with  $\rho = \rho$ ,” but this is incorrect because the population lifetime changes ( $\tau_{Ti} \rightarrow \tau_{Ui}$ ) when the ions become untrapped. To find the solution we use Equation A.13 to see that our solution must have the form  $W_i^A(t_n) \exp(-(t - t_n)/\tau_{Ui})$  and that we need only to find the initial values  $W_i^A(t_n)$ .

Since no previously-trapped ions can be lost in the first injection, the first tooth in  $W_i^A$  will always be zero:

$$W_i^A(t_1) = W_i^A(t_B) = 0, \quad (\text{A.57})$$

recalling the definition of  $t_n$  in Equation A.1. The first contribution to  $W_i^A$  will be the ions from  $T_i$  during the second injection, so that the initial value of the second tooth is

$$\begin{aligned} W_i^A(t_2) &= (1 - \rho)T_i(t_1)e^{-t_A/\tau_{Ti}} \\ &= (1 - \rho)A_{Ti}\sigma_{Ti}(1)a_{Ti}. \end{aligned} \quad (\text{A.58})$$

Here we are cheating slightly in our notation. Strictly speaking,  $T_i(t_1) = 0$  with the definition of  $n(t)$  as given in Equation A.23. But immediately after this point  $T_i(t_1 + \epsilon)$  assumes values described accurately by Equation A.57, and that is the region of interest. The same is true of the initial values  $W_i^A(t_n)$  and those of other population we will analyze in the following sections. As we said earlier, we apply the model in such a way that the exact behavior at the discontinuities doesn't matter.

The next initial value is

$$\begin{aligned} W_i^A(t_3) &= a_{Ui}W_i^A(t_2) + a_{Ti}(1 - \rho)T_i(t_2) \\ &= (1 - \rho)A_{Ti}a_{Ti}[\sigma_{Ti}(1)a_{Ui} + \sigma_{Ti}(2)], \end{aligned} \quad (\text{A.59})$$

which can be understood operationally as taking  $W_i^A(t_2)$ , decaying it by  $a_{Ui}$ , and then adding the unretained part of  $T_i$  during the 3rd capture which is the fraction  $(1 - \rho)$  of  $T_i(t_2)$  decayed by  $a_{Ti}$ , or  $a_{Ti}(1 - \rho)T_i(t_2) = a_{Ti}(1 - \rho)A_{Ti}\sigma_{Ti}(2)$ . The presence of  $a_{Ti}$  and  $a_{Ui}$  multiplying each other is a sign that we're on the right track.

For good measure we write out one more term,

$$\begin{aligned} W_i^A(t_4) &= a_{Ui}W_i^A(t_3) + (1 - \rho)a_{Ti}T_i(t_3) \\ &= A_{Wi}a_{Ti} [\sigma_{Ti}(1)a_{Ui}^2 + \sigma_{Ti}(2)a_{Ui} + \sigma_{Ti}(3)], \end{aligned} \quad (\text{A.60})$$

with the  $W_i^A$  amplitude defined as

$$A_{Wi} \equiv (1 - \rho)A_{Ti} \equiv (1 - \rho)pr_i t_A. \quad (\text{A.61})$$

Now we can see clearly the pattern that the initial conditions obey. We have a sum of contributions to the  $n^{\text{th}}$  tooth in  $W_i^A$ . The latest contribution was lost on the  $n^{\text{th}}$  capture and carries a factor of  $\sigma_{Ti}(n - 1)a_{Ui}^0$ . The previous contribution was lost on the  $(n - 1)^{\text{th}}$  capture and carries a factor of  $\sigma_{Ti}(n - 2)a_{Ui}^1$ . And this pattern continues over the  $n - 1$  captures that have lost ions until the first contribution carrying the factor  $\sigma_{Ti}(1)a_{Ui}^{n-2}$ . All the contributions are decayed by the  $a_{Ti}$  of the first tooth spent in the trap.

So the initial values can be expressed as

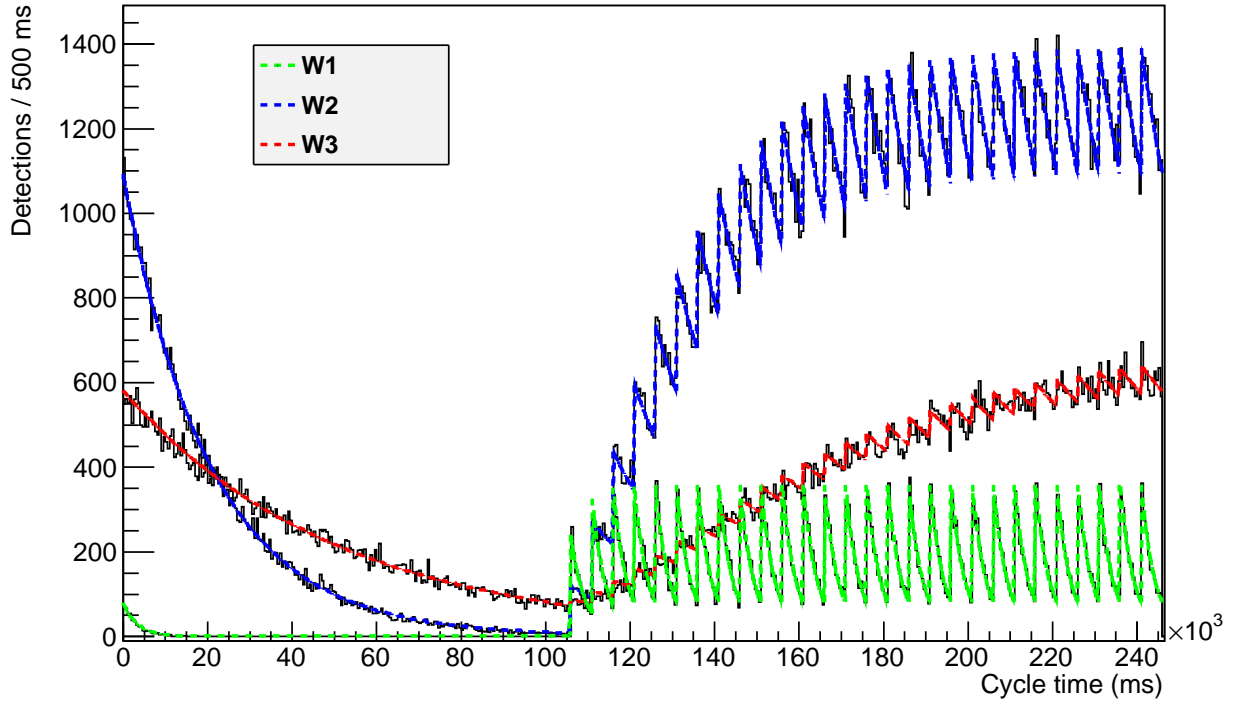
$$\begin{aligned} W_i^A(t_n) &= A_{Wi}a_{Ti} \sum_{k=1}^{n-1} \sigma_{Ti}(k)a_{Ui}^{n-1-k} \\ &= A_{Wi}a_{Ti} \sum_{k=1}^{n-1} \sigma_I(\rho, a_{Ti}, k)a_{Ui}^{n-1-k} \\ &\equiv A_{Wi}a_{Ti}\sigma_{II}(\rho, a_{Ti}, a_{Ui}, n) \\ &\equiv A_{Wi}\sigma_{Wi}(n) \end{aligned} \quad (\text{A.62})$$

where evaluating the sum involves some algebra that is summarized in section A.10. With this the trapping component is

$$W_i^A(t) = A_{Wi}\sigma_{Wi}(n) \exp\left(-\frac{t - t_n}{\tau_{Ui}}\right). \quad (\text{A.63})$$

Examples of the  $W$  populations are shown in Figure A.4.

### Simulation vs Model, W populations



**Figure A.4:** Comparison of simulated  $\beta$  detections to those calculated by the model, for  $W_1$ ,  $W_2$  and  $W_3$  populations. The functions are discontinuous due to direct feeding from  $\delta$ -function source terms. The  $W$  populations get their first contribution in the 2nd tooth of the cycle as they wait for the first ion bunch to be captured and then possibly leaked during the following capture. The parameter values used in this run of the simulation can be found in section A.11.

### A.7.3 The $Z_1, Z_2, Z_3$ populations

The radioactive and non-radioactive decay channels of  $T_i$  feed the  $X_{i+1}$  and  $Z_i$  populations, respectively. (The radioactive decay causes the ion to change species.) The non-radioactive decay is assumed to be exponential, and the dynamics of the  $X_{i+1}$  and  $Z_i$  populations will therefore be the same. In this section we will find  $Z_i(t)$ , and in the next we will transform this into  $X_i(t)$ .

We will denote the net lifetime of any non-radioactive channels as  $\theta_{Ti}$  and write

$$\frac{1}{\tau_{Ti}} \equiv \frac{1}{\tau_i} + \frac{1}{\theta_{Ti}}. \quad (\text{A.64})$$

In the computed model we instead use the loss-rate parameters

$$\gamma_{Ti} = 1/\theta_{Ti} \quad (\text{A.65})$$

since these will be 0, rather than  $\infty$ , when there is no effect. In this appendix we use  $\gamma_{Ti}$  and  $1/\theta_{Ti}$  interchangeably.

Using this notation we can write the rate equations,

$$\dot{Z}_1 + Z_1/\tau_{U1} = T_1/\theta_{T1} \quad (\text{A.66})$$

$$\dot{Z}_2 + Z_2/\tau_{U2} = T_2/\theta_{T2} \quad (\text{A.67})$$

$$\dot{Z}_3 + Z_3/\tau_{U3} = T_3/\theta_{T3} \quad (\text{A.68})$$

where the source terms together account for feeding from all continuous decays of the trapped populations.

As with the  $W_i$  populations our approach will be to find the initial values of each tooth. But here our source terms are not  $\delta$  functions but are the discontinuous functions  $T_i$ . Our solutions will be continuous with discontinuous first derivatives, as shown ???. This shape is given by Equation A.17 with  $g(t_0) = Z_i^A(t_n)$ ,  $h(t_0) = T_i(t_n)$ ,  $\tau_g = \tau_{Ui}$ ,  $\tau_h = \tau_{Ti}$ , and  $\tau_{hg} = \theta_{Ti}$ , so that the solution on one tooth is

$$Z_i^A(t) = Z_i^A(t_n) \exp\left(-\frac{t-t_n}{\tau_{Ui}}\right) + A_{Zi}\sigma_{Ti}(n) \left[ \exp\left(-\frac{t-t_n}{\tau_{Ui}}\right) - \exp\left(-\frac{t-t_n}{\tau_{Ti}}\right) \right], \quad (\text{A.69})$$



where we have defined the  $Z_i$  amplitude

$$A_{Zi} \equiv \frac{A_{Ti}}{\theta_{Ti}} \frac{\tau_{Ti}\tau_{Ui}}{\tau_{Ui} - \tau_{Ti}} = pr_i t_A \frac{\gamma_{Ti}}{\gamma_{Ti} - \gamma_{Ui}}. \quad (\text{A.70})$$

As with  $W_i^A$ , the initial values for  $Z_i^A$  obey a recursion relation

$$\begin{cases} Z_i^A(t_1) &= Z_i^A(t_B) = 0 \\ Z_i^A(t_{n+1}) &= Z_i^A(t_n)a_{Ui} + A_{Zi}\sigma_{Ti}(n)(a_{Ui} - a_{Ti}). \end{cases} \quad (\text{A.71})$$

This can be discerned directly from Equation A.69, since substituting  $t = t_{n+1}$  on the LHS just turns the exp's on the RHS into corresponding decay factors. (No such shortcut for  $W_i^A$  is obvious to this author, since in that case the effect of the  $\delta$  functions is put in by hand.) This recursion relation corresponds to the closed form

$$\begin{aligned} Z_i^A(t_n) &= A_{Zi}(a_{Ui} - a_{Ti}) \sum_{k=1}^{n-1} \sigma_{Ti}(k) a_{Ui}^{n-1-k} \\ &= A_{Zi}(a_{Ui} - a_{Ti}) \sum_{k=1}^{n-1} \sigma_I(\rho, a_{Ti}, k) a_{Ui}^{n-1-k} \\ &\equiv A_{Zi}(a_{Ui} - a_{Ti}) \sigma_{II}(\rho, a_{Ti}, a_{Ui}, n) \\ &\equiv A_{Zi} \sigma_{Zi}(n). \end{aligned} \quad (\text{A.72})$$

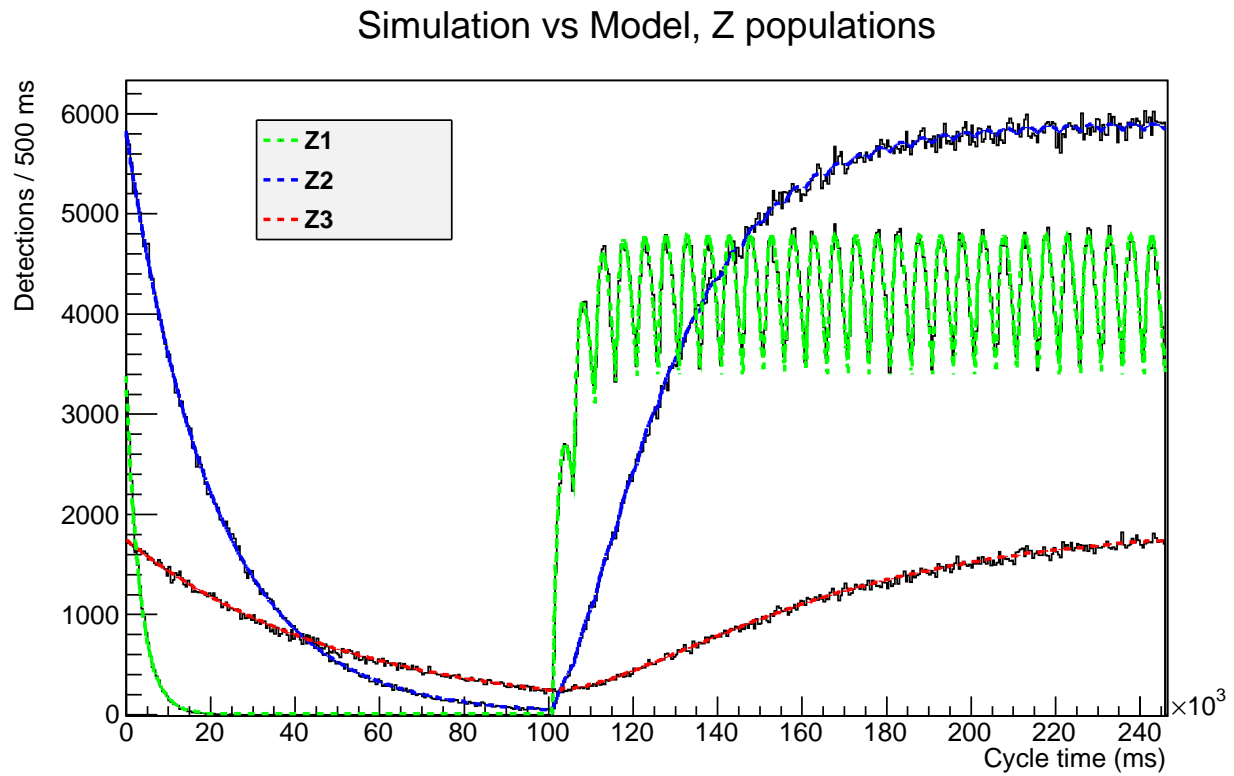
So the trapping component is

$$\begin{aligned} Z_i^A(t) &= A_{Zi} \sigma_{Zi}(n) \exp\left(-\frac{t - t_n}{\tau_{Ui}}\right) \\ &+ A_{Zi} \sigma_{Ti}(n) \left[ \exp\left(-\frac{t - t_n}{\tau_{Ui}}\right) - \exp\left(-\frac{t - t_n}{\tau_{Ti}}\right) \right]. \end{aligned} \quad (\text{A.73})$$

Examples of the  $Z$  populations are shown in Figure A.5.

A reader comparing Equation A.73 to our code should note that `sigmaZi[n]` in our code is what we will call

$$\sigma'_{Zi}(n) \equiv (a_{Ui} - a_{Ti}) \sigma_{II}(\rho, a_{Ti}, a_{Ui}, n) + \sigma_{Ti}(\rho, a_{Ti}, n) \quad (\text{A.74})$$



**Figure A.5:** Comparison of simulated  $\beta$  detections to those calculated by the model, for  $Z_1$ ,  $Z_2$  and  $Z_3$  populations. The functions are continuous with discontinuities in the 1st derivative due to the feeding from a the discontinuous  $T$  populations. The parameter values used in this run of the simulation can be found in section A.11.

in this appendix. This saves on the number of calls to the `TMath::Exp()` function. And later in this appendix it will save integrations and space on the page. We do the same thing with  $\sigma'_{Xi}(n) = \text{sigmaXi}[n]$ . These alternate definitions are also listed in section A.10.

As always trapping component applies only on the trapping interval and is zero elsewhere. Following subsection A.6.3, the cyclic boundary condition is

$$Z_i(0) = Z_i^A(t_C)/(1 - \exp(t_C/\tau_{Ui})), \quad (\text{A.75})$$

and the full solution is

$$Z_i(t) = Z_i(0) \exp\left(-\frac{t - t_n}{\tau_{Ui}}\right) + Z_i^A(t). \quad (\text{A.76})$$

The  $Z_i$  population contains a removable 0/0 discontinuity in the parameter space where  $\gamma_{Ti} = \gamma_{Ui}$ . This causes the program, wrongly but without complaining, to find  $Z_i = 0$  and propagate this into  $Y_{i+1}$ . Although this condition is extremely unlikely to appear during a regression, the user may want to fix  $\gamma_{Ti} = \gamma_{Ui}$ . This problem showed up during testing for  $\gamma_{Ti} = \gamma_{Ui} \neq 0$ , which is a condition we do not expect to be needed since  $\gamma_{Ti}$  and  $\gamma_{Ui}$  presumably model very different mechanisms with different rates. For our tests the  $\gamma_{Ti} = \gamma_{Ui} = 0$  condition gave the correct result of  $A_{Zi} = 0$ , but it's possible this correct behavior was compiler-dependent and therefore not to be relied upon. The latter case is important, as it is expected to be true in future experiments.

While this discontinuity could be handled using L'Hospital's rule to rewrite the offending factor

$$\lim_{\gamma_{Ui} \rightarrow \gamma_{Ti}} \frac{a_{Ui} - a_{Ti}}{\gamma_{Ti} - \gamma_{Ui}} = a_{Ti} t_A, \quad (\text{A.77})$$

we found it sufficient simply to hard-code a tiny offset into each  $\gamma_{Ui}$ . Similar offsets are used in certain ratios appearing in the  $\sigma$ 's, as noted in section A.10. There are many other instances in which the modified lifetimes may produce 0/0-type removable discontinuities, but the author believes that none of them have any special importance and that they will effectively never occur during a fit.

Before moving on we note that the connection between Equation A.69 and Equation A.72 is particularly important. We will be using the same procedure repeatedly in deriving  $Y_2^A$

and  $Y_3^A$ .

#### A.7.4 The $X_2$ , $X_3$ populations

The rate equations for the  $X$  populations are

$$\dot{X}_2 + X_2/\tau_{U_2} = T_1/\tau_1 \quad (\text{A.78})$$

$$\dot{X}_3 + X_3/\tau_{U_3} = T_2/\tau_2. \quad (\text{A.79})$$

The source terms here are the same as in Equation A.66 and Equation A.67, up to constants. Therefore the  $X_2$  will be the same as  $Z_1$ , and  $X_3$  the same as  $Z_2$ , up to a the following set of substitutions:

$$\begin{aligned} Z_i &\rightarrow X_{i+1} \\ A_{Ti} &\rightarrow A_{Ti} \quad (\text{same source species}) \\ \theta_{Ti} &\rightarrow \tau_i \quad (\text{different decay channel}) \\ \tau_{Ui} &\rightarrow \tau_{U(i+1)} \quad (\text{different resulting species}). \end{aligned}$$

Notably the  $A_{Ti}$  and  $\tau_{Ti}$  factors are preserved, since the same species  $T_i$  is feeding  $Z_i$  and  $Z_{i+1}$ .

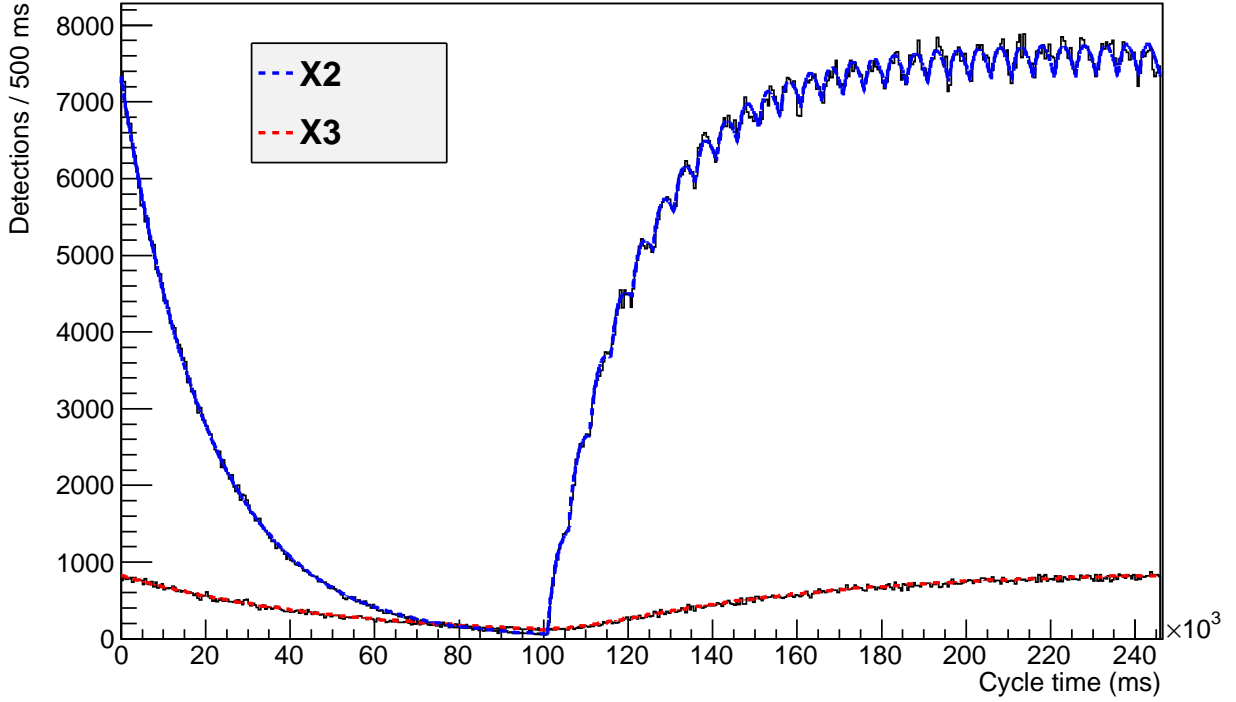
The  $X_i$  amplitude, found by applying these substitutions to Equation A.70 is

$$A_{Xi} \equiv \frac{A_{T(i-1)}}{\tau_{(i-1)}} \frac{\tau_{T(i-1)}\tau_{Ui}}{\tau_{Ui} - \tau_{T(i-1)}}. \quad (\text{A.80})$$

Because the species changes in this feeding channel, both the simplification into  $\gamma$ 's and the likelihood of a 0/0 discontinuity are removed from  $A_{Xi}$ . With the partial sum defined by

$$\sigma_{Xi}(n) \equiv (a_{Ui} - a_{T(i-1)})\sigma_{II}(\rho, a_{T(i-1)}, a_{Ui}, n), \quad (\text{A.81})$$

### Simulation vs Model, X populations



**Figure A.6:** Comparison of simulated  $\beta$  detections to those calculated by the model, for  $X_2$  and  $X_3$  populations. The functions are continuous with discontinuities in the 1st derivative at the capture events. The parameter values used in this run of the simulation can be found in section A.11.

the trapping component is

$$\begin{aligned}
 X_i^A(t) = & A_{X_i} \sigma_{X_i}(n) \exp\left(-\frac{t-t_n}{\tau_{U_i}}\right) \\
 & + A_{X_i} \sigma_{T(i-1)}(n) \left[ \exp\left(-\frac{t-t_n}{\tau_{U_i}}\right) - \exp\left(-\frac{t-t_n}{\tau_{T(i-1)}}\right) \right]. \quad (\text{A.82})
 \end{aligned}$$

Examples of the  $X$  populations are shown in Figure A.6.

#### A.7.5 The $Y_2$ population

The  $Y$  populations are fed only by the radioactive decays of untrapped parent ions. The  $Y_2$  function will be continuous with discontinuous first (due to  $V_1$  and  $W_1$ ) and second (due to  $Z_1$ ) derivatives. They can be analyzed following the example of subsection A.7.3. The  $Y_2$

rate equation is

$$\dot{Y}_2 + Y_2/\tau_{U2} = (V_1 + W_1 + Z_1)/\tau_1. \quad (\text{A.83})$$

The  $Y$  populations are the only populations that are fed by untrapped populations and therefore have a background components of the more complex forms we found in subsection A.6.1. Using Equation A.34 we can immediately find the  $Y_2$  background component

$$\begin{aligned} Y_2^B(t) &= Y_2(0) \cdot \exp\left(-\frac{t}{\tau_{U2}}\right) \\ &+ U_1(0) \cdot \frac{1}{\tau_1 \Gamma_{U2}^{U1}} \cdot \left[ \exp\left(-\frac{t}{\tau_{U2}}\right) - \exp\left(-\frac{t}{\tau_{U1}}\right) \right]. \end{aligned} \quad (\text{A.84})$$

For the trapping component we use Equation A.43 repeatedly to write

$$\begin{aligned} Y_2^A(t) &= Y_2^A(t_n) \cdot \exp\left(-\frac{t-t_n}{\tau_{U2}}\right) \\ &+ \frac{A_{V1}\sigma_{V1}(n) + A_{W1}\sigma_{W1}(n) + A_{Z1}\sigma'_{Z1}(n)}{\tau_1 \Gamma_{U2}^{U1}} \cdot \left[ \exp\left(-\frac{t-t_n}{\tau_{U2}}\right) - \exp\left(-\frac{t-t_n}{\tau_{U1}}\right) \right] \\ &- \frac{A_{Z1}\sigma_{T1}}{\tau_1 \Gamma_{U2}^{T1}} \cdot \left[ \exp\left(-\frac{t-t_n}{\tau_{U2}}\right) - \exp\left(-\frac{t-t_n}{\tau_{T1}}\right) \right] \end{aligned} \quad (\text{A.85})$$

where our job again is to find the initial values  $Y_2^A(t_n)$ . To do this we follow the example of the  $Z_i^A$  analysis, writing the recursion relation

$$\left\{ \begin{aligned} Y_2^A(t_1) &= Y_2^A(t_B) = 0 \\ Y_2^A(t_{n+1}) &= Y_2^A(t_n) \cdot a_{U2} \\ &+ \frac{1}{\tau_1 \Gamma_{U2}^{U1}} \cdot [A_{V1} \cdot \sigma_{V1}(n) + A_{W1} \cdot \sigma_{W1}(n) + A_{Z1} \cdot \sigma'_{Z1}(n)] \cdot (a_{U2} - a_{U1}) \\ &- \frac{1}{\tau_1 \Gamma_{U2}^{T1}} \cdot A_{Z1} \cdot \sigma_{T1}(n) \cdot (a_{U2} - a_{T1}). \end{aligned} \right.$$

Each appearance of a  $\sigma$  here will lead to a sum of the form

$$\sum_{k=1}^{n-1} \sigma(k) a_{U2}^{n-1-k}, \quad (\text{A.86})$$

which we evaluate using the algebra of section A.10. We will call the resulting sums  $\sigma_{Y2V1}$ ,

$\sigma_{Y_2W_1}$ , and  $\sigma_{Y_2Z_1}$ , according to the source terms giving rise to them. These sums will constitute an overall  $\sigma_{Y_2}$  which we define as

$$\begin{aligned}\sigma_{Y_2}(n) &\equiv A_{V_1} \cdot \sigma_{Y_2V_1}(n) + A_{W_1} \cdot \sigma_{Y_2W_1}(n) + A_{Z_1} \cdot \sigma_{Y_2Z_1}(n) \\ &= Y_2^A(t_n),\end{aligned}\tag{A.87}$$

and which, as noted, is the needed initial value. Note that  $\sigma_{Y_2}$  includes amplitudes, whereas the  $\sigma$ 's seen previously were dimensionless.

The component sums are

$$\begin{aligned}\sigma_{Y_2V_1}(n) &\equiv \frac{a_{U_2} - a_{U_1}}{\tau_1 \Gamma_{U_2}^{U_1}} \cdot \sum_{k=1}^{n-1} \sigma_{V_1}(k) a_{U_2}^{n-1-k} \\ &= \frac{a_{U_2} - a_{U_1}}{\tau_1 \Gamma_{U_2}^{U_1}} \cdot \sum_{k=1}^{n-1} \sigma_I(1, a_{U_1}, k) a_{U_2}^{n-1-k} \\ &= \frac{a_{U_2} - a_{U_1}}{\tau_1 \Gamma_{U_2}^{U_1}} \cdot \sigma_{II}(1, a_{U_1}, a_{U_2}, n)\end{aligned}\tag{A.88}$$

$$\begin{aligned}\sigma_{Y_2W_1}(n) &\equiv \frac{a_{U_2} - a_{U_1}}{\tau_1 \Gamma_{U_2}^{U_1}} \cdot \sum_{k=1}^{n-1} \sigma_{W_1}(k) a_{U_2}^{n-1-k} \\ &= \frac{a_{U_2} - a_{U_1}}{\tau_1 \Gamma_{U_2}^{U_1}} \cdot a_{T_1} \cdot \sum_{k=1}^{n-1} \sigma_{II}(\rho, a_{T_1}, a_{U_1}, k) a_{U_2}^{n-1-k} \\ &= \frac{a_{U_2} - a_{U_1}}{\tau_1 \Gamma_{U_2}^{U_1}} \cdot a_{T_1} \cdot \sigma_{III}(\rho, a_{T_1}, a_{U_1}, a_{U_2}, n)\end{aligned}\tag{A.89}$$

$$\begin{aligned}
\sigma_{Y_2 Z_1}(n) &\equiv \frac{a_{U_2} - a_{U_1}}{\tau_1 \Gamma_{U_2}^{U_1}} \cdot \sum_{k=1}^{n-1} \sigma'_{Z_1}(k) a_{U_2}^{n-1-k} - \frac{a_{U_2} - a_{T_1}}{\tau_1 \Gamma_{U_2}^{T_1}} \cdot \sum_{k=1}^{n-1} \sigma_{T_1}(k) a_{U_2}^{n-1-k} \\
&= \frac{(a_{U_2} - a_{U_1})(a_{U_1} - a_{T_1})}{\tau_1 \Gamma_{U_2}^{U_1}} \cdot \sum_{k=1}^{n-1} \sigma_{II}(\rho, a_{T_1}, a_{U_1}, k) a_{U_2}^{n-1-k} \\
&\quad + \left( \frac{a_{U_2} - a_{U_1}}{\tau_1 \Gamma_{U_2}^{U_1}} - \frac{a_{U_2} - a_{T_1}}{\tau_1 \Gamma_{U_2}^{T_1}} \right) \cdot \sum_{k=1}^{n-1} \sigma_I(\rho, a_{T_1}, k) a_{U_2}^{n-1-k} \\
&= \frac{(a_{U_2} - a_{U_1})(a_{U_1} - a_{T_1})}{\tau_1 \Gamma_{U_2}^{U_1}} \cdot \sigma_{III}(\rho, a_{T_1}, a_{U_1}, a_{U_2}, n) \\
&\quad + \left( \frac{a_{U_2} - a_{U_1}}{\tau_1 \Gamma_{U_2}^{U_1}} - \frac{a_{U_2} - a_{T_1}}{\tau_1 \Gamma_{U_2}^{T_1}} \right) \cdot \sigma_{II}(\rho, a_{T_1}, a_{U_2}, n). \tag{A.90}
\end{aligned}$$

With the above definitions, the trapping component of  $Y_2$  is

$$\begin{aligned}
Y_2^A(t) &= \sigma_{Y_2}(n) \exp\left(-\frac{t - t_n}{\tau_{U_2}}\right) \\
&\quad + \frac{1}{\tau_1 \Gamma_{U_2}^{U_1}} \cdot \left[ A_{V_1} \sigma_{V_1}(n) + A_{W_1} \sigma_{W_1}(n) + A_{Z_1} \sigma'_{Z_1}(n) \right] \cdot \left[ e^{-\frac{t-t_n}{\tau_{U_2}}} - e^{-\frac{t-t_n}{\tau_{U_1}}} \right] \\
&\quad - \frac{1}{\tau_1 \Gamma_{U_2}^{T_1}} \cdot A_{Z_1} \sigma_{T_1}(n) \cdot \left[ e^{-\frac{t-t_n}{\tau_{U_2}}} - e^{-\frac{t-t_n}{\tau_{T_1}}} \right]. \tag{A.91}
\end{aligned}$$

### A.7.6 The $Y_3$ population

The  $Y_3$  rate equation is

$$\dot{Y}_3 + Y_3/\tau_{U_3} = (V_2 + W_2 + Z_2 + X_2 + Y_2)/\tau_2. \tag{A.92}$$

Following Equation A.35, the background component of  $Y_3$  is

$$\begin{aligned}
Y_3^B(t) &= Y_3(0) \cdot \exp\left(-\frac{t}{\tau_{U_3}}\right) \\
&\quad + U_2(0) \cdot \frac{1}{\tau_2 \Gamma_{U_3}^{U_2}} \cdot \left[ \exp\left(-\frac{t}{\tau_{U_3}}\right) - \exp\left(-\frac{t}{\tau_{U_2}}\right) \right] \\
&\quad + U_1(0) \cdot \frac{1}{\tau_1 \Gamma_{U_2}^{U_1}} \cdot \frac{1}{\tau_2 \Gamma_{U_3}^{U_2}} \cdot \left[ \exp\left(-\frac{t}{\tau_{U_3}}\right) - \exp\left(-\frac{t}{\tau_{U_2}}\right) \right] \\
&\quad - U_1(0) \cdot \frac{1}{\tau_1 \Gamma_{U_2}^{U_1}} \cdot \frac{1}{\tau_2 \Gamma_{U_3}^{U_1}} \cdot \left[ \exp\left(-\frac{t}{\tau_{U_3}}\right) - \exp\left(-\frac{t}{\tau_{U_1}}\right) \right], \tag{A.93}
\end{aligned}$$



with

$$U_1(0) = V_1(0) + W_1(0) + Z_1(0) \quad (\text{A.94})$$

$$U_2(0) = V_2(0) + W_2(0) + Z_2(0) + X_2(0) + Y_2(0). \quad (\text{A.95})$$

As a reminder, the  $Y_3^B$  component incorporates the feeding from  $V_2^B$ ,  $W_2^B$ ,  $Z_2^B$ ,  $X_2^B$ , and  $Y_2^B$ , but all the boundary values depend also on the trapping components evaluated at  $t = t_C$ .

The  $Y_3$  trapping component is found by integrating Equation A.91, making repeated use of Equation A.19. This yields the initial value solution

$$\begin{aligned} Y_3^A(t) &= Y_3^A(t_n) \cdot e^{-\frac{t-t_n}{\tau_{U3}}} \\ &+ A_{V2} \cdot \frac{\sigma_{V2}(n)}{\tau_2 \Gamma_{U3}^{U2}} \cdot \left( e^{-\frac{t-t_n}{\tau_{U3}}} - e^{-\frac{t-t_n}{\tau_{U2}}} \right) \\ &+ A_{W2} \cdot \frac{\sigma_{W2}(n)}{\tau_2 \Gamma_{U3}^{U2}} \cdot \left( e^{-\frac{t-t_n}{\tau_{U3}}} - e^{-\frac{t-t_n}{\tau_{U2}}} \right) \\ &+ A_{Z2} \cdot \left[ \frac{\sigma'_{Z2}(n)}{\tau_2 \Gamma_{U3}^{U2}} \cdot \left( e^{-\frac{t-t_n}{\tau_{U3}}} - e^{-\frac{t-t_n}{\tau_{U2}}} \right) - \frac{\sigma_{T2}(n)}{\tau_2 \Gamma_{U3}^{T2}} \cdot \left( e^{-\frac{t-t_n}{\tau_{U3}}} - e^{-\frac{t-t_n}{\tau_{T2}}} \right) \right] \\ &+ A_{X2} \cdot \left[ \frac{\sigma'_{X2}(n)}{\tau_2 \Gamma_{U3}^{U2}} \cdot \left( e^{-\frac{t-t_n}{\tau_{U3}}} - e^{-\frac{t-t_n}{\tau_{U2}}} \right) - \frac{\sigma_{T1}(n)}{\tau_2 \Gamma_{U3}^{T1}} \cdot \left( e^{-\frac{t-t_n}{\tau_{U3}}} - e^{-\frac{t-t_n}{\tau_{T1}}} \right) \right] \\ &+ A_{V1} \cdot \frac{\sigma_{Y2V1}(n)}{\tau_2 \Gamma_{U3}^{U2}} \cdot \left( e^{-\frac{t-t_n}{\tau_{U3}}} - e^{-\frac{t-t_n}{\tau_{U2}}} \right) \\ &+ A_{V1} \cdot \frac{\sigma_{V1}(n)}{\tau_1 \Gamma_{U2}^{U1}} \cdot \left[ \frac{1}{\tau_2 \Gamma_{U3}^{U2}} \cdot \left( e^{-\frac{t-t_n}{\tau_{U3}}} - e^{-\frac{t-t_n}{\tau_{U2}}} \right) - \frac{1}{\tau_2 \Gamma_{U3}^{U1}} \cdot \left( e^{-\frac{t-t_n}{\tau_{U3}}} - e^{-\frac{t-t_n}{\tau_{U1}}} \right) \right] \\ &+ A_{W1} \cdot \frac{\sigma_{Y2W1}(n)}{\tau_2 \Gamma_{U3}^{U2}} \cdot \left( e^{-\frac{t-t_n}{\tau_{U3}}} - e^{-\frac{t-t_n}{\tau_{U2}}} \right) \\ &+ A_{W1} \cdot \frac{\sigma_{W1}(n)}{\tau_1 \Gamma_{U2}^{U1}} \cdot \left[ \frac{1}{\tau_2 \Gamma_{U3}^{U2}} \cdot \left( e^{-\frac{t-t_n}{\tau_{U3}}} - e^{-\frac{t-t_n}{\tau_{U2}}} \right) - \frac{1}{\tau_2 \Gamma_{U3}^{U1}} \cdot \left( e^{-\frac{t-t_n}{\tau_{U3}}} - e^{-\frac{t-t_n}{\tau_{U1}}} \right) \right] \\ &+ A_{Z1} \cdot \frac{\sigma_{Y2Z1}(n)}{\tau_2 \Gamma_{U3}^{U2}} \cdot \left( e^{-\frac{t-t_n}{\tau_{U3}}} - e^{-\frac{t-t_n}{\tau_{U2}}} \right) \\ &+ A_{Z1} \cdot \frac{\sigma'_{Z1}(n)}{\tau_1 \Gamma_{U2}^{U1}} \cdot \left[ \frac{1}{\tau_2 \Gamma_{U3}^{U2}} \cdot \left( e^{-\frac{t-t_n}{\tau_{U3}}} - e^{-\frac{t-t_n}{\tau_{U2}}} \right) - \frac{1}{\tau_2 \Gamma_{U3}^{U1}} \cdot \left( e^{-\frac{t-t_n}{\tau_{U3}}} - e^{-\frac{t-t_n}{\tau_{U1}}} \right) \right] \\ &- A_{Z1} \cdot \frac{\sigma_{T1}(n)}{\tau_1 \Gamma_{U2}^{T1}} \cdot \left[ \frac{1}{\tau_2 \Gamma_{U3}^{U2}} \cdot \left( e^{-\frac{t-t_n}{\tau_{U3}}} - e^{-\frac{t-t_n}{\tau_{U2}}} \right) - \frac{1}{\tau_2 \Gamma_{U3}^{T1}} \cdot \left( e^{-\frac{t-t_n}{\tau_{U3}}} - e^{-\frac{t-t_n}{\tau_{T1}}} \right) \right], \end{aligned} \quad (\text{A.96})$$

with the Species 1 source terms are coming through  $Y_2^A$ . We will skip the writing of the

recursion relation for  $Y_3^A(t_n)$  and go straight to the  $\sigma$ 's for  $Y_3^A$ . As with  $Z_i^A$ ,  $X_i^A$ , and  $Y_2^A$ ,  $Y_3^A$  is continuous with  $Y_3^A(t_B) = 0$ . The feeding from  $V_2^A$ ,  $W_2^A$ , and  $Z_2^A$  into  $Y_3^A$  is exactly analogous to the feeding of  $Y_2^A$  from  $V_1^A$ ,  $W_1^A$ , and  $Z_1^A$ . The feeding of  $Y_3^A$  by  $X_2^A$  is the same as the feeding of  $Y_2^A$  by  $Z_1^A$  under the substitution rules given in subsection A.7.4. So we can describe these first four sources using the following sums, which are formally the same as the ones we calculated for  $Y_2^A$ :

$$\sigma_{Y_3V_2}(n) \equiv \frac{a_{U3} - a_{U2}}{\tau_2 \Gamma_{U3}^{U2}} \cdot \sigma_{\text{II}}(1, a_{U2}, a_{U3}, n) \quad (\text{A.97})$$

$$\sigma_{Y_3W_2}(n) \equiv \frac{a_{U3} - a_{U2}}{\tau_2 \Gamma_{U3}^{U2}} \cdot a_{T2} \cdot \sigma_{\text{III}}(\rho, a_{T2}, a_{U2}, a_{U3}, n) \quad (\text{A.98})$$

$$\begin{aligned} \sigma_{Y_3Z_2}(n) \equiv & \frac{(a_{U3} - a_{U2})(a_{U2} - a_{T2})}{\tau_2 \Gamma_{U3}^{U2}} \cdot \sigma_{\text{III}}(\rho, a_{T2}, a_{U2}, a_{U3}, n) \\ & + \left( \frac{a_{U3} - a_{U2}}{\tau_2 \Gamma_{U3}^{U2}} - \frac{a_{U3} - a_{T2}}{\tau_2 \Gamma_{U3}^{T2}} \right) \cdot \sigma_{\text{II}}(\rho, a_{T2}, a_{U3}, n) \end{aligned} \quad (\text{A.99})$$

$$\begin{aligned} \sigma_{Y_3X_2}(n) \equiv & \frac{(a_{U3} - a_{U2})(a_{U2} - a_{T1})}{\tau_2 \Gamma_{U3}^{U2}} \cdot \sigma_{\text{III}}(\rho, a_{T1}, a_{U2}, a_{U3}, n) \\ & + \left( \frac{a_{U3} - a_{U2}}{\tau_2 \Gamma_{U3}^{U2}} - \frac{a_{U3} - a_{T1}}{\tau_2 \Gamma_{U3}^{T1}} \right) \cdot \sigma_{\text{II}}(\rho, a_{T1}, a_{U3}, n) \end{aligned} \quad (\text{A.100})$$

The remaining sums come through the feeding from  $Y_2^A$ . To find them we continue to use the procedure from the  $Z_i$  populations. That is, we take each term in Equation A.96 and turn each  $\exp(-(t - t_n)/\tau_X)$  into the decay factor  $a_X = \exp(-t_A/\tau_X)$  to represent the time evolution from one injection to the next. We then sum the  $n$ -dependent part, the  $\sigma$ , over previous injections multiplied by the number of  $a_{U3}$  decay factors that are picked up with  $Y_3^A(t_n)$  by the recursion over previous teeth. We first write down these terms and then use the algebra from section A.10 to evaluate them. This procedure yields

$$\begin{aligned}
\sigma_{Y3V1}(n) &\equiv \frac{a_{U3} - a_{U2}}{\tau_2 \Gamma_{U3}^{U2}} \cdot \sum_{k=1}^{n-1} \sigma_{Y2V1}(k) a_{U3}^{n-1-k} \\
&\quad + \frac{1}{\tau_1 \Gamma_{U2}^{U1}} \cdot \left( \frac{a_{U3} - a_{U2}}{\tau_2 \Gamma_{U3}^{U2}} - \frac{a_{U3} - a_{U1}}{\tau_2 \Gamma_{U3}^{U1}} \right) \cdot \sum_{k=1}^{n-1} \sigma_{V1}(k) a_{U3}^{n-1-k} \\
&= \frac{a_{U3} - a_{U2}}{\tau_2 \Gamma_{U3}^{U2}} \cdot \sum_{k=1}^{n-1} \frac{a_{U2} - a_{U1}}{\tau_1 \Gamma_{U2}^{U1}} \sigma_{II}(1, a_{U1}, a_{U2}, k) a_{U3}^{n-1-k} \\
&\quad + \frac{1}{\tau_1 \Gamma_{U2}^{U1}} \cdot \left( \frac{a_{U3} - a_{U2}}{\tau_2 \Gamma_{U3}^{U2}} - \frac{a_{U3} - a_{U1}}{\tau_2 \Gamma_{U3}^{U1}} \right) \cdot \sum_{k=1}^{n-1} \sigma_I(1, a_{U1}, k) a_{U3}^{n-1-k} \\
&= \frac{1}{\tau_1 \Gamma_{U2}^{U1}} \cdot \left[ \frac{(a_{U3} - a_{U2})(a_{U2} - a_{U1})}{\tau_2 \Gamma_{U3}^{U2}} \cdot \sigma_{III}(1, a_{U1}, a_{U2}, a_{U3}, n) \right. \\
&\quad \left. + \left( \frac{a_{U3} - a_{U2}}{\tau_2 \Gamma_{U3}^{U2}} - \frac{a_{U3} - a_{U1}}{\tau_2 \Gamma_{U3}^{U1}} \right) \cdot \sigma_{II}(1, a_{U1}, a_{U3}, n) \right], \tag{A.101}
\end{aligned}$$

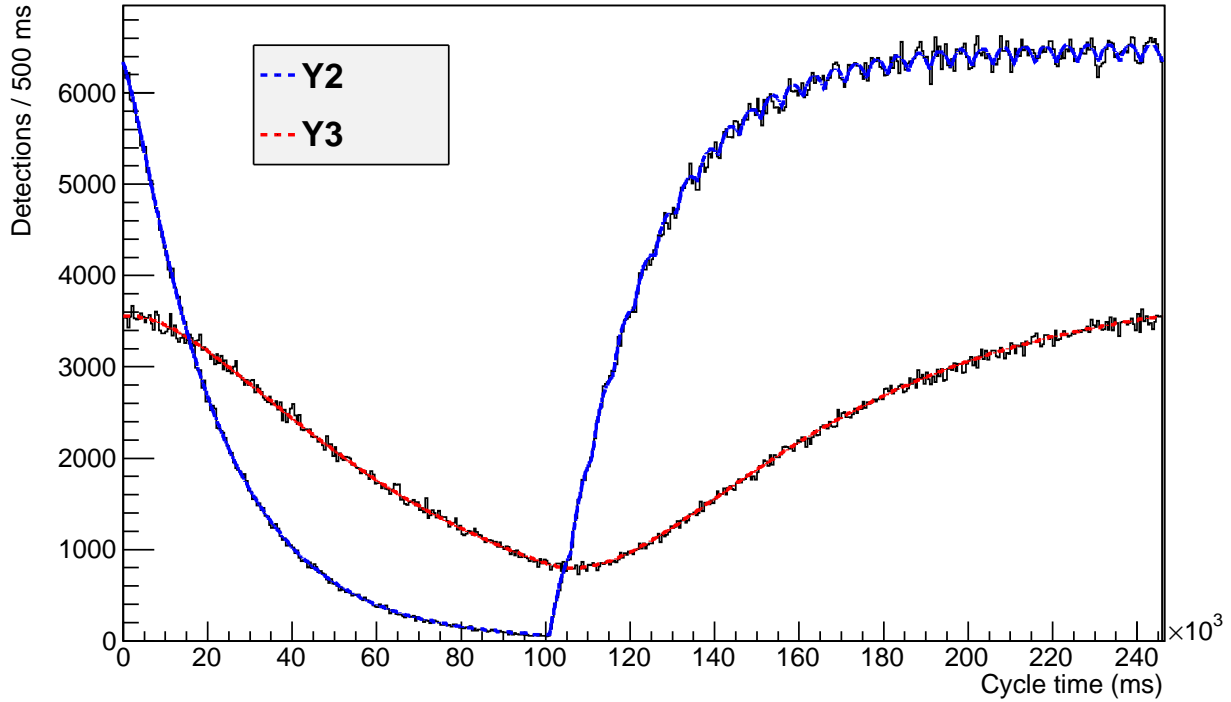
$$\begin{aligned}
\sigma_{Y3W1}(n) &\equiv \frac{a_{U3} - a_{U2}}{\tau_2 \Gamma_{U3}^{U2}} \cdot \sum_{k=1}^{n-1} \sigma_{Y2W1}(k) a_{U3}^{n-1-k} \\
&\quad + \frac{1}{\tau_1 \Gamma_{U2}^{U1}} \cdot \left( \frac{a_{U3} - a_{U2}}{\tau_2 \Gamma_{U3}^{U2}} - \frac{a_{U3} - a_{U1}}{\tau_2 \Gamma_{U3}^{U1}} \right) \cdot \sum_{k=1}^{n-1} \sigma_{W1}(k) a_{U3}^{n-1-k} \\
&= \frac{a_{U3} - a_{U2}}{\tau_2 \Gamma_{U3}^{U2}} \cdot \sum_{k=1}^{n-1} \frac{a_{U2} - a_{U1}}{\tau_1 \Gamma_{U2}^{U1}} a_{T1} \sigma_{III}(\rho, a_{T1}, a_{U1}, a_{U2}, k) a_{U3}^{n-1-k} \\
&\quad + \frac{1}{\tau_1 \Gamma_{U2}^{U1}} \cdot \left( \frac{a_{U3} - a_{U2}}{\tau_2 \Gamma_{U3}^{U2}} - \frac{a_{U3} - a_{U1}}{\tau_2 \Gamma_{U3}^{U1}} \right) \cdot \sum_{k=1}^{n-1} a_{T1} \sigma_{II}(\rho, a_{T1}, a_{U1}, k) a_{U3}^{n-1-k} \\
&= \frac{a_{T1}}{\tau_1 \Gamma_{U2}^{U1}} \cdot \left[ \frac{(a_{U3} - a_{U2})(a_{U2} - a_{U1})}{\tau_2 \Gamma_{U3}^{U2}} \cdot \sigma_{IV}(\rho, a_{T1}, a_{U1}, a_{U2}, a_{U3}, n) \right. \\
&\quad \left. + \left( \frac{a_{U3} - a_{U2}}{\tau_2 \Gamma_{U3}^{U2}} - \frac{a_{U3} - a_{U1}}{\tau_2 \Gamma_{U3}^{U1}} \right) \cdot \sigma_{III}(\rho, a_{T1}, a_{U1}, a_{U3}, n) \right], \tag{A.102}
\end{aligned}$$

$$\begin{aligned}
\sigma_{Y3Z1}(n) &\equiv \frac{a_{U3} - a_{U2}}{\tau_2 \Gamma_{U3}^{U2}} \cdot \sum_{k=1}^{n-1} \sigma_{Y2Z1}(k) a_{U3}^{n-1-k} \\
&+ \frac{1}{\tau_1 \Gamma_{U2}^{U1}} \cdot \left( \frac{a_{U3} - a_{U2}}{\tau_2 \Gamma_{U3}^{U2}} - \frac{a_{U3} - a_{U1}}{\tau_2 \Gamma_{U3}^{U1}} \right) \cdot \sum_{k=1}^{n-1} \sigma'_{Z1}(k) a_{U3}^{n-1-k} \\
&- \frac{1}{\tau_1 \Gamma_{U2}^{T1}} \cdot \left( \frac{a_{U3} - a_{U2}}{\tau_2 \Gamma_{U3}^{U2}} - \frac{a_{U3} - a_{T1}}{\tau_2 \Gamma_{U3}^{T1}} \right) \cdot \sum_{k=1}^{n-1} \sigma_{T1}(k) a_{U3}^{n-1-k} \\
&= \frac{a_{U3} - a_{U2}}{\tau_2 \Gamma_{U3}^{U2}} \cdot \sum_{k=1}^{n-1} \left[ \frac{(a_{U2} - a_{U1})(a_{U1} - a_{T1})}{\tau_1 \Gamma_{U2}^{U1}} \cdot \sigma_{\text{III}}(\rho, a_{T1}, a_{U1}, a_{U2}, k) \right. \\
&\quad \left. + \left( \frac{a_{U2} - a_{U1}}{\tau_1 \Gamma_{U2}^{U1}} - \frac{a_{U2} - a_{T1}}{\tau_1 \Gamma_{U2}^{T1}} \right) \cdot \sigma_{\text{II}}(\rho, a_{T1}, a_{U2}, k) \right] a_{U3}^{n-1-k} \\
&+ \frac{1}{\tau_1 \Gamma_{U2}^{U1}} \cdot \left( \frac{a_{U3} - a_{U2}}{\tau_2 \Gamma_{U3}^{U2}} - \frac{a_{U3} - a_{U1}}{\tau_2 \Gamma_{U3}^{U1}} \right) \cdot \sum_{k=1}^{n-1} (a_{U1} - a_{T1}) \sigma_{\text{II}}(\rho, a_{T1}, a_{U1}, k) a_{U3}^{n-1-k} \\
&+ \frac{1}{\tau_1 \Gamma_{U2}^{U1}} \cdot \left( \frac{a_{U3} - a_{U2}}{\tau_2 \Gamma_{U3}^{U2}} - \frac{a_{U3} - a_{U1}}{\tau_2 \Gamma_{U3}^{U1}} \right) \cdot \sum_{k=1}^{n-1} \sigma_{\text{I}}(\rho, a_{T1}, k) a_{U3}^{n-1-k} \\
&- \frac{1}{\tau_1 \Gamma_{U2}^{T1}} \cdot \left( \frac{a_{U3} - a_{U2}}{\tau_2 \Gamma_{U3}^{U2}} - \frac{a_{U3} - a_{T1}}{\tau_2 \Gamma_{U3}^{T1}} \right) \cdot \sum_{k=1}^{n-1} \sigma_{\text{I}}(\rho, a_{T1}, k) a_{U3}^{n-1-k} \\
&= \frac{a_{U3} - a_{U2}}{\tau_2 \Gamma_{U3}^{U2}} \cdot \frac{a_{U2} - a_{U1}}{\tau_1 \Gamma_{U2}^{U1}} \cdot (a_{U1} - a_{T1}) \cdot \sigma_{\text{IV}}(\rho, a_{T1}, a_{U1}, a_{U2}, a_{U3}, n) \\
&+ \frac{a_{U3} - a_{U2}}{\tau_2 \Gamma_{U3}^{U2}} \cdot \left( \frac{a_{U2} - a_{U1}}{\tau_1 \Gamma_{U2}^{U1}} - \frac{a_{U2} - a_{T1}}{\tau_1 \Gamma_{U2}^{T1}} \right) \cdot \sigma_{\text{III}}(\rho, a_{T1}, a_{U2}, a_{U3}, n) \\
&+ \frac{1}{\tau_1 \Gamma_{U2}^{U1}} \cdot \left( \frac{a_{U3} - a_{U2}}{\tau_2 \Gamma_{U3}^{U2}} - \frac{a_{U3} - a_{U1}}{\tau_2 \Gamma_{U3}^{U1}} \right) \cdot (a_{U1} - a_{T1}) \cdot \sigma_{\text{III}}(\rho, a_{T1}, a_{U1}, a_{U3}, n) \\
&+ \frac{1}{\tau_1 \Gamma_{U2}^{U1}} \cdot \left( \frac{a_{U3} - a_{U2}}{\tau_2 \Gamma_{U3}^{U2}} - \frac{a_{U3} - a_{U1}}{\tau_2 \Gamma_{U3}^{U1}} \right) \cdot \sigma_{\text{II}}(\rho, a_{T1}, a_{U3}, n) \\
&- \frac{1}{\tau_1 \Gamma_{U2}^{T1}} \cdot \left( \frac{a_{U3} - a_{U2}}{\tau_2 \Gamma_{U3}^{U2}} - \frac{a_{U3} - a_{T1}}{\tau_2 \Gamma_{U3}^{T1}} \right) \cdot \sigma_{\text{II}}(\rho, a_{T1}, a_{U3}, n). \tag{A.103}
\end{aligned}$$

The initial value is then

$$\begin{aligned}
Y_3^A(t_n) &= \sigma_{Y3}(n) \\
&\equiv A_{V2} \sigma_{Y3V2}(n) + A_{W2} \sigma_{Y3W2}(n) + A_{Z2} \sigma_{Y3Z2}(n) + A_{X2} \sigma_{Y3X2}(n) \\
&+ A_{V1} \sigma_{Y3V1}(n) + A_{W1} \sigma_{Y3W1}(n) + A_{Z1} \sigma_{Y3Z1}(n), \tag{A.104}
\end{aligned}$$

## Simulation vs Model, Y populations



**Figure A.7:** Comparison of simulated  $\beta$  detections to those calculated by the model, for  $Y_2$  and  $Y_3$  populations. Slight discontinuities in the 1st and 2nd derivatives are present in the trapping components of both functions. The presence of feeding from background components, visible in the curvature of the background decay, is unique to the  $Y$  populations. The parameter values used in this run of the simulation can be found in section A.11.

and with this we have the complete solution for  $Y_3$ . The  $Y$  populations from our simulated example are shown in Figure A.7. Examples of the  $Y$  populations are shown in Figure A.7.

## A.8 Program

The model as described in this appendix was implemented in a C++ program called `BFit2`, that uses ROOT libraries to handle the histograms, functions, fitting, and plotting. The program takes two arguments from the command line. The first argument is the name of a `BDNCase` object which contains the radioactive lifetimes of the measured species measured and information about the measurement cycle. The second argument is the name of a `BFitCase` which contains initial parameter values and a toggle to fix or vary each parameter,

as well as a number of other options to control the program including the options string given to ROOT's fitting algorithm.

The full populations correspond to functions  $T_{tot}(i, a, t)$ ,  $U_{tot}(i, a, t)$ ,  $V_{tot}(i, a, t)$ , ...,  $Y_{tot}(i, a, t)$ , that take the species number  $i$ , a pointer  $a$  to the array of parameter values, and the cycle time  $t$ . For an untrapped population this function calculates the background and trapping components separately. The trapping component is calculated in a separate function, eg.  $Y_{cap}(i, a, t)$ . For the  $Y$  populations the background components are calculated in  $Y_{bkgd}(i, a, t)$ .

The program uses these populations for fitting, event counting, and plotting. The event counting is done by taking the integral of the time-dependent  $\beta$ -detection rate of that population. This rate is returned by a function named with a leading  $r$ , eg. the function  $rT2(t, a)$  returns the detection rate of events attributed to the  $T_{tot}(2, a, t)$  population, which is

$$rT2(t, a) = (\# \text{ of cycles}) * (T \text{ efficiency}) * T_{tot}(2, a, t) / (\text{rad. tau}^2). \quad (\text{A.105})$$

These rate functions correspond to the  $D(t)$  functions in section A.3, up to the factor of  $N_C = n_{Cyc}$  needed to account for summing over many cycles in the data.

To produce something that can be plotted against a histogram we multiply this rate by the histogram's bin width to produce the counting functions

$$yT2(t, a) = rT2(t, a) * (\text{bin width}). \quad (\text{A.106})$$

An offset function  $oT2(t, a) = yT2(t, a) + yDC(t, a)$ , where  $yDC(t, a) = rDC * (\text{bin width})$  is the counting function of the DC event rate  $rDC$ , is used to produce a nicer visualization as in Figure A.1, where the per-population event rates are shown as if the DC rate were 0 for easier comparison to the sum.

The function that is regressed on the data is called  $yA11(t, a)$  and calculated as

$$yA11(t, a) = yDC(t, a) + yT1(t, a) + yT2(t, a) + yT3(t, a) \quad (A.107)$$

$$+ (U \text{ efficiency}) * (yU1(t, a) + yU2(t, a) + yU3(t, a)),$$

$$yU1(t, a) = yV1(t, a) + yW1(t, a) + yZ1(t, a) \quad (A.108)$$

$$yU2(t, a) = yV2(t, a) + yW2(t, a) + yZ2(t, a) + yX2(t, a) + yY2(t, a) \quad (A.109)$$

$$yU3(t, a) = yV3(t, a) + yW3(t, a) + yZ3(t, a) + yX3(t, a) + yY3(t, a). \quad (A.110)$$

Note that, as indicated in section A.3, we have an extra efficiency factor for all untrapped populations, in addition to the efficiencies in each untrapped counting function. This is included as a convenience and should be used with care.

The populations contain many complex quantities that depend only on the parameters. In first building the model, these quantities were included as needed in every population. Although this was a sensible approach, the end result was very inefficient computationally. To evaluate each population once, with fixed parameters, on an array of  $\sim 10000$  time-points required at least one recalculation of each parameter-dependent quantity at each point. To amend this, the  $yA11$  function tests the parameters in  $a$  against a global last-known set of values. When any parameter is changed,  $yA11$  calls the function `ComputeParameterDependentVals(a)`, and the modified lifetimes, decay factors,  $\sigma$ 's, and boundary values (eg.  $Y_3(0)$ ) are recalculated before the populations are evaluated over all  $t$  values. This requires some careful handling of the global parameter array in the program. This reorganization to avoid redundancy is the essential difference between `BFit` and `BFit2`.

## A.9 Validation

Given the degree of mathematical and computational complexity in the model, we created a Monte Carlo simulation that used all the model dynamics to randomly generate and decay each population in a long series of small time steps. For each model population, both the number of members and the number of radioactive decays per time-step are stored in histograms over both real time (many trap cycles) and cycle time (summed over all cycles). The decays-versus-cycle-time histograms had the same form as the data from our

experiment and were used to test the model. The first test was to see that giving the same model parameters to both the simulation and the model produced histograms and functions that overlapped. Because of dissimilarity of the analytical approach of the model from the numerical approach of the simulation, the agreement of the two is a strong confirmation that the dynamics proffered here as representing the real evolution of populations in the experiment are at least correctly implemented in both the simulation and the model. These comparisons have been shown throughout this appendix.

The second test is a statistical one. Does the regression, operating on the sum of many exponential functions having different and perhaps varying lifetimes, produce accurate inferences about known data? By using the simulated data we knew the true number of decay events attributable to every ion population, and we found that the regression was able to find the correct values within the errors derived from the fit covariance matrix.

The model's success under these tests gave us confidence in using it in the applications presented in this thesis.



## A.10 Algebra

$$a_X \equiv \exp(-t_A/\tau_X) \quad (\text{A.111})$$

$$\sigma_{Ti}(n) \equiv \sigma_I(\rho, a_{Ti}, n) \quad (\text{A.112})$$

$$\sigma_{Vi}(n) \equiv \sigma_I(1, a_{Ui}, n) \quad (\text{A.113})$$

$$\sigma_{Wi}(n) \equiv a_{Ti}\sigma_{II}(\rho, a_{Ti}, a_{Ui}, n) \quad (\text{A.114})$$

$$\sigma_{Zi}(n) \equiv (a_{Ui} - a_{Ti})\sigma_{II}(\rho, a_{Ti}, a_{Ui}, n) \quad (\text{A.115})$$

$$\sigma'_{Zi}(n) \equiv (a_{Ui} - a_{Ti})\sigma_{II}(\rho, a_{Ti}, a_{Ui}, n) + \sigma_{Ti}(n) \quad (\text{A.116})$$

$$\sigma_{Xi}(n) \equiv (a_{Ui} - a_{T(i-1)})\sigma_{II}(\rho, a_{T(i-1)}, a_{Ui}, n) \quad (\text{A.117})$$

$$\sigma'_{Xi}(n) \equiv (a_{Ui} - a_{T(i-1)})\sigma_{II}(\rho, a_{T(i-1)}, a_{Ui}, n) + \sigma_{T(i-1)}(n) \quad (\text{A.118})$$

$$\sigma_I(\rho, a, n) \equiv \frac{1 - (\rho a)^n}{1 - \rho a} \quad (\text{A.119})$$

$$\sigma_{II}(\rho, a_T, a_U, n) \equiv \sum_{k=1}^{n-1} \sigma_I(\rho, a_T, k) a_U^{n-1-k} \quad (\text{A.120})$$

$$= \frac{1}{1 - \rho a_T} \left( \frac{1 - a_U^{n-1}}{1 - a_U} - \rho a_T \frac{a_U^{n-1} - (\rho a_T)^{n-1} + \varepsilon}{a_U - \rho a_T + \varepsilon} \right)$$

$$\sigma_{III}(\rho, \tau_{T1}, \tau_{U1}, \tau_{U2}, n) \equiv \sum_{k=1}^{n-1} \sigma_{II}(\rho, a_{T1}, a_{U1}, k) a_{U2}^{n-1-k} \quad (\text{A.121})$$

$$= \frac{1}{1 - \rho a_{T1}} \left[ \frac{1}{1 - a_{U1}} \left( \frac{1 - a_{U2}^{n-1}}{1 - a_{U2}} - \frac{a_{U2}^{n-1} - a_{U1}^{n-1}}{a_{U2} - a_{U1}} \right) \right. \\ \left. - \frac{\rho a_{T1} + \varepsilon}{a_{U1} - \rho a_{T1} + \varepsilon} \left( \frac{a_{U2}^{n-1} - a_{U1}^{n-1}}{a_{U2} - a_{U1}} - \frac{a_{U2}^{n-1} - (\rho a_{T1})^{n-1}}{a_{U2} - \rho a_{T1}} \right) \right]$$

$$\begin{aligned}
\sigma_{\text{IV}}(\rho, a_{T1}, a_{U1}, a_{U2}, a_{U3}, n) &\equiv \sum_{k=1}^{n-1} \sigma_{\text{III}}(\rho, a_{T1}, a_{U1}, a_{U2}, k) a_{U3}^{n-1-k} \quad (\text{A.122}) \\
&= \frac{1}{1 - \rho a_{T1}} \left\{ \frac{1}{1 - a_{U1}} \left[ \frac{1}{1 - a_{U2}} \left( \frac{1 - a_{U3}^{n-1}}{1 - a_{U3}} - \frac{a_{U3}^{n-1} - a_{U2}^{n-1}}{a_{U3} - a_{U2}} \right) \right. \right. \\
&\quad \left. \left. - \frac{1}{a_{U2} - a_{U1}} \left( \frac{a_{U3}^{n-1} - a_{U2}^{n-1}}{a_{U3} - a_{U2}} - \frac{a_{U3}^{n-1} - a_{U1}^{n-1}}{a_{U3} - a_{U1}} \right) \right] \right. \\
&\quad \left. - \frac{\rho a_{T1} + \varepsilon}{a_{U1} - \rho a_{T1} + \varepsilon} \left[ \frac{1}{a_{U2} - a_{U1}} \left( \frac{a_{U3}^{n-1} - a_{U2}^{n-1}}{a_{U3} - a_{U2}} - \frac{a_{U3}^{n-1} - a_{U1}^{n-1}}{a_{U3} - a_{U1}} \right) \right. \right. \\
&\quad \left. \left. - \left( \frac{a_{U3}^{n-1} - a_{U2}^{n-1}}{a_{U3} - a_{U2}} - \frac{a_{U3}^{n-1} - (\rho a_{T1})^{n-1}}{a_{U3} - \rho a_{T1}} \right) \right] \right\}
\end{aligned}$$

## A.11 Parameter summary

Hi.

Symbol	Description	Units	Value
Data parameters (from <code>BDNCases.csv</code> ):			
$t_A$	Time between captures	sec	5
$t_B$	Duration of background interval	sec	101
$t_C$	Duration of cycle	sec	246
$\tau_1$	Radioactive lifetime ( $1/e$ ) of Species 1	sec	3.592
$\tau_2$	Radioactive lifetime ( $1/e$ ) of Species 2	sec	35.346
$\tau_3$	Radioactive lifetime ( $1/e$ ) of Species 3	sec	330.493
$n_C$	Number of cycles covered	#	500
Model parameters (from <code>BFitCases.csv</code> ):			
$R_{DC}$	Rate of room background events on $\beta$ detector	events/sec	0.04
$r_1$	Rate of Species 1 ion injection to BPT	ions/sec	0.1
$r_2$	Rate of Species 2 ion injection to BPT	ions/sec	0.1
$r_3$	Rate of Species 3 ion injection to BPT	ions/sec	0.1
$p$	Capture efficiency of all species in BPT	#	0.71349
$\rho$	Retention efficiency of trapped ions during capture	#	0.93553
$\varepsilon_T$	Detection efficiency of $T$ populations	#	1
$\varepsilon_V$	Detection efficiency of $V$ populations	#	1
$\varepsilon_W$	Detection efficiency of $W$ populations	#	1
$\varepsilon_X$	Detection efficiency of $X$ populations	#	1
$\varepsilon_Y$	Detection efficiency of $Y$ populations	#	1
$\varepsilon_Z$	Detection efficiency of $Z$ populations	#	1
$\varepsilon_U$	Auxiliary efficiency of all untrapped populations	#	1
$\gamma_{T1}$	Non-radioactive decay rate ( $1/e$ ) of trapped Species 1	$\text{sec}^{-1}$	1/10
$\gamma_{T2}$	Non-radioactive decay rate ( $1/e$ ) of trapped Species 2	$\text{sec}^{-1}$	1/20
$\gamma_{T3}$	Non-radioactive decay rate ( $1/e$ ) of trapped Species 3	$\text{sec}^{-1}$	1/30
$\gamma_{U1}$	Non-radioactive decay rate ( $1/e$ ) of untrapped Species 1	$\text{sec}^{-1}$	1/40
$\gamma_{U2}$	Non-radioactive decay rate ( $1/e$ ) of untrapped Species 2	$\text{sec}^{-1}$	1/50
$\gamma_{U3}$	Non-radioactive decay rate ( $1/e$ ) of untrapped Species 3	$\text{sec}^{-1}$	1/60

**Table A.2:** Summary of parameters needed to determine the rates of  $\beta$  detection from all populations in the model. The values given in the table are those used to generate the simulated data that appears in the figures in this appendix.

## REFERENCES

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