CalcuYield: A Novel Android-Based Software for Radioactivity Yield Calculations

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Abstract. Calculations for predicting the radioactivity yields of radionuclides resulting from an accelerator-based nuclear reaction are necessary for the purpose of evaluation and optimization of irradiation parameters. Moreover, computerized calculations are also needed for time efficiency and avoiding the occurrence of human errors. In this work, for the first time, we have built and developed an Android-based-software (called CalcuYield) to calculate the End of Bombardment (EOB)-yields applicable for cyclotron-based radionuclide production. The calculations benefited from the yield equation by employing the cross-section values of the TALYS-2017 nuclear data library and the stopping power values derived from the SRIM 2013 software. Some experimental data were used to compare and verify the calculated results. It was found that the CalcuYield calculated results agreed with the experimental data with an average error of less than 10%. The CalcuYield is, therefore, well applicable for the EOB yield prediction in cyclotron-based radionuclide production. The CalcuYield was also found to be able to run in android-based devices.

Keywords: CalcuYield, cyclotron, EOB yield, radionuclide production, SRIM, TALYS

1. Introduction

Use of nuclear science and technology by employing accelerators is increasingly being used today. Accelerators are used to accelerate subatomic particles such as neutrons, protons, deuterons, ³He, ⁴He and other heavy particles at sufficient energy levels to be bombarded into the target materials to create nuclear reactions. The purpose of such nuclear reactions is to produce radionuclides which can then be used for various applications including for research, medical and industrial purposes.

One of the important output parameters of a nuclear reaction is the radioactivity or yield of the resulting radionuclides. In theory, the radionuclide activity generated from a nuclear reaction can be calculated. Earlier research has theoretically calculated the radioactivity yield of ⁶⁴Cu and ⁹⁹mTc radionuclides [1,2], though they performed the calculations traditionally using Excel, Visual Basic or Matlab codes. Theoretical calculations are required for the purpose of evaluating the results prior to actual irradiation. With reference to predictive data, the cyclotron researchers and operators can have more precise early information related to the irradiation results to be performed so that the cyclotron operation can be optimized. Computerized calculations are needed for time efficiency and avoiding human errors which might occur during radionuclide production. In previous research, a software was built to perform the calculation [3], though it was limited to the calculation of one particular reaction mode only and for the maximum bombarding particle energy was 20 MeV.
In this investigation, an Android-based software is built and developed with the addition of calculations for several nuclear reaction modes and the energy range of the bombarding particles is added to 30 MeV. The program is built using Android Studio developer software that uses the Java programming language. There are 3 input parameters used as the object of the calculation for this instance, i.e. bombarding particle current, incoming particle energy and duration of bombardment or irradiation. The algorithm applied in the development of the program is highlighted in this report. The results of the CalcuYield calculations are also compared with some experimental data. This research is expected to produce a software that can help cyclotron researchers and operators to predict, optimize and evaluate cyclotron-based radionuclide production.

2. Materials and Methods

2.1 The Yield Equation

The formula employed in this study was the widely known equation for calculating the End-Of-Bombardment (EOB) yield discussed previously elsewhere [1-2]. In this work, it was necessary to add some parameters to the equation, namely the percentage of the target in the target material, the target’s abundance, conversion number from Ampere unit to micro Ampere unit and the conversion number from Becquerel to mCi. The following is a description of the final equation to be used in this study, whereas the red texts are the additional parameters inserted in this study:

\[
Y = \left[ \frac{6.25 \times 10^{18}}{Z} \cdot (1 - e^{-\lambda \cdot t}) \cdot \frac{N_A}{M} \cdot \sum_{E_i} E_i \cdot \frac{\sigma(E_i)}{1 \cdot dE_i / dx} \Delta E \right] \cdot \text{P. R.} \cdot \frac{10^{-6}}{3.7 \cdot 10^7}
\]

\[
Y = \frac{6.25 \times 10^{18}}{Z} \cdot (1 - e^{-\lambda \cdot t}) \cdot \Delta E \cdot \sum_{E_i} E_i \cdot \frac{\sigma(E_i)}{1 \cdot dE_i / dx}
\]

\[
Y = \frac{1.017 \cdot I \cdot P \cdot R \cdot 10^{29}}{ZM} \cdot (1 - e^{-\lambda \cdot t}) \cdot \Delta E \cdot \sum_{E_i} E_i \cdot \frac{\sigma(E_i)}{1 \cdot dE_i / dx}
\]

(1)

Where:

- \( Y \) : yield radionuclide product (mCi)
- \( I \) : bombarding particles current (μA)
- \( P \) : percentage of the target element in the target material
- \( R \) : percentage of abundance of the target material
- \( M \) : The target’s atomic mass number
- \( Z \) : atomic number of bombarding particle
- \( \lambda \) : radioactive decay constant of radionuclide product
- \( t \) : duration of irradiation or bombardment
- \( \Delta E \) : increment of energy (MeV)
- \( E_{th} \) : threshold energy of nuclear reactions (MeV)
- \( E_i \) : energy of bombarding particle
- \( \sigma(E_i) \) : cross-section for the nuclear reaction at energy E (cm²)
- \( \frac{1 \cdot dE_i}{\rho \cdot dx} \) : stopping power or energy loss of bombarding particle on target material (MeV.cm²/gram)

The cross-section value was obtained from the TALYS-based evaluated data library (TENDL 2017) available online ([https://tendl_web.psi.ch/tendl_2017/tendl2017.html](https://tendl_web.psi.ch/tendl_2017/tendl2017.html)) [4]. In addition, the stopping power or energy loss of bombarding particle on target material was calculated from the SRIM software (SRIM 2013 version).
2.2 Programming Algorithm

In this work, the Java Programming language, which had been used elsewhere [5-8], was employed to build the algorithm. Since the equation used was a numerical integration operation, a special algorithm was required in the programming due to the fact that there was no function for numerical calculation in the Java language. In general, the calculation process was divided into 2 stages; the first stage was the calculation to get the numerical value and the second stage was the overall calculation. Details of the calculation process are shown in Figure 1.

![Figure 1](image1.png)  
**Figure 1.** Flowchart of the calculation process.

![Figure 2](image2.png)  
**Figure 2.** Flowchart of the numerical integration process.

The numerical integration is basically a discrete calculation so that it requires a looping process. The number of the looping processes depends on the interval (increment of energy) and the range of the numerical integration. In this research, the interval of 0.5 MeV was selected since the cross-sectional values obtained from the TALYS-evaluated nuclear data library and the stopping powers calculated from the SRIM software had an average energy increment of 0.5 MeV, though they could be interpolated to lower increments. The looping process was started at the threshold energy value of the bombarding particle in the material target and ended up at the energy level of the incoming particle. Thus, the number of the looping processes could be determined by equation (2) as follows:

\[
n = \frac{E_i - E_{th}}{\text{energy increment}} \tag{2}
\]

The description of the looping processes can be seen in Figure 2. The cross-section and stopping power databases were created using Microsoft Excel in the format as shown in Table 1. The whole developed program was then called the CalcuYield.
Table 1. Database format in MS Excel for storing cross-section (CS) and stopping power value (SP) as a function of incoming energy (E).

| i | E   | CS     | SP   |
|---|-----|--------|------|
| 1 | 16.5| 3.294  | 0.606|
| 2 | 17  | 5.610  | 0.195|
| 3 | 17.5| 21.562 | 0.165|
| 4 | 18  | 37.500 | 0.188|
| 5 | 18.5| 60.301 | 0.081|
| 6 | 19  | 83.100 | 0.065|
| 7 | 19.5| 109.228| 0.054|
| 8 | 20  | 135    | 0.175|
| 9 | 20.5| 169.275| 0.039|
|10 | 21  | 203.150| 0.035|
|11 | 21.5| 237.025| 0.032|
|12 | 22  | 271    | 0.029|
|13 | 22.5| 288.457| 0.161|
|14 | 23  | 306.053| 0.026|

| i | E   | CS     | SP   |
|---|-----|--------|------|
|15| 23.5| 323.648| 0.025|
|16| 24  | 341    | 0.024|
|17| 24.5| 346.043| 0.024|
|18| 25  | 350.835| 0.150|
|19| 25.5| 355.626| 0.024|
|20| 26  | 360    | 0.024|
|21| 26.5| 359.675| 0.024|
|22| 27  | 358.930| 0.024|
|23| 27.5| 358.186| 0.140|
|24| 28  | 357    | 0.024|
|25| 28.5| 344.145| 0.024|
|26| 29  | 330.827| 0.025|
|27| 29.5| 317.508| 0.026|
|28| 30  | 304    | 0.132|

2.3 Validation
To confirm the CalcuYield results, the values were then compared with the experimental results, while their relative errors were determined from equation (3):

\[
\text{% error} = \left( \frac{|y_c - y_e|}{y_e} \right) \times 100 \%
\]  
(3)

Where:

\( y_c \) = calculated yield
\( y_e \) = experimental yield

3. Results and Discussion
3.1 Application Testing
The results of the built application (CalcuYield) is depicted in Figure 3, which shows an example of radioactivity yield of \(^{18}\text{O}(p,n)^{18}\text{F}\) nuclear reaction for \(^{18}\text{F}\) radionuclide production at proton energy of 11 MeV, proton beam current of 30 µA and irradiation time of 30 minutes. In the target system, a havar window containing Fe, Co, Mn, Ni, Cr, W and Mo atoms is assumedly used in the production; thus several impurities are expected to be generated during the bombardment. As well, from Figure 3 it can be seen that the CalcuYield application can accept the input values which then display the calculated results.
Further tests were also conducted to determine the compatibility on some Android smartphones with different brands and versions ranging from Sony Xperia Z5 Compact to Samsung Galaxy Tab 2. The testing results are presented in Table 2, which can be concluded that the application is able to run properly for all types of Android-based smart-phones.

**Table 2.** The results of application compatibility testing on some Android smartphones

| No. | Android Device           | OS Version | Test Results  |
|-----|--------------------------|------------|---------------|
| 1   | Sony Xperia Z5 Compact   | 7.1.1      | Run very well |
| 2   | Samsung Galaxy J5       | 6.0.1      | Run very well |
| 3   | Sony Xperia Z3           | 6.0        | Run very well |
| 5   | Andromax A16C3H         | 5.1.1      | Run very well |
| 6   | Oppo Neo                 | 5.1        | Run very well |
| 7   | Xiaomi Redmi 3           | 5.0        | Run very well |
| 8   | Samsung Galaxy J1 Ace   | 4.4.4      | Run very well |
| 9   | Lenovo P780              | 4.2        | Run very well |
| 10  | Samsung Galaxy Tab 2     | 4.1.2      | Run very well |

**Figure 3.** The user interface of CalcuYield application
3.2 Comparisons with experimental data

Various experimental data were collected from several references to validate the CalcuYield calculated results as shown in Table 3 and Table 4. In Table 3, the CalcuYield results are compared with the experimental results from production of $^{18}$F using the Cyclone 18/9 Cyclotron in MRCCC Siloam Hospital Jakarta. During the production, 18-MeV protons were bombarded at 37-$\mu$A current for several irradiation times between 30 and 45 minutes. For 45-minute irradiation time, the yield difference between the experimental and CalcuYield calculation is 6.31%, whereas for 40, 35 and 30 minute irradiation the differences are 1.17%, 4.54% and 0.69% respectively. The average difference for the irradiation parameter is 3.18%.

| Duration of Irradiation (minutes) | EOB yield (mCi) | Difference (%) |
|----------------------------------|-----------------|----------------|
| 45                               | 2292.15         | 2147.54        |
| 40                               | 1960.92         | 1937.87        |
| 35                               | 1803.28         | 1721.48        |
| 30                               | 1508.56         | 1498.18        |
| **Average**                      | **15.31**       |                |

Another comparison is conducted for $^{18}$F radionuclide production in Dharmais Cancer Hospital Jakarta which uses an 11-MeV cyclotron. In the experiment, the 11-MeV protons were bombarded in enriched water target at beam current 30 $\mu$A for 5 minutes. As can be seen in Table 3, the experimental and CalcuYield calculated radioactivity yields are in good agreement with a difference of 3.61%. Several radioactive impurities are identified from their (p,n) reactions, including $^{96}$Tc, $^{56}$Co, $^{52}$Mn, $^{184}$Re, and $^{65}$Zn, whereas other radionuclides such as $^{55}$Fe, $^{59}$Ni, and $^{58}$Cu are not detected. The identified radioactive impurities were also previously reported elsewhere [9-11]. While the experimental and calculated differences are mostly less than 10%, one experimental data shows 50% difference, e.g. for $^{184}$Re impurity. The huge difference could be due to the small radioactivity value which often corresponds to high deviation in radiation detection and measurement. Also, from Table 4, the calculated EOB yields for $^{55}$Fe and $^{59}$Ni indicates zero value, which is agreed by the experimental measurement. The two impurities are not detected experimentally.

In the EOB yield formula there is a function of $(1 - e^{-\lambda t})$, which is an exponential growth time factor, the longer the irradiation time used the greater the yield of the obtained radionuclide. However, the value of the radionuclide yield will be close to its saturation value (close to 1), which occurs when the term $e^{-\lambda t}$ is very small (close to zero), or the duration of irradiation ($t$) is long. Therefore there is a certain time limit (long irradiation) which causes radionuclide production no effective. The most effective yield increase is for any irradiation time up to one half-life of the corresponding radionuclides which has been discussed earlier [3].
Tabel 4. Calculated EOB yields compared to some selected experimental results from Eclipse Cyclotron in Dharmais Cancer Center Hospital Jakarta (Ep = 11 MeV, I = 30 μA, t = 5 minutes)

| Reaction Mode | Radionuclide Product | EOB yield (mCi) | Difference (%) |
|---------------|----------------------|-----------------|----------------|
| $^{18}$O(p,n)$^{18}$F | $^{18}$F | 156.510 | 162.156 | 3.61 |
| $^{96}$Mo(p,n)$^{96}$Tc | $^{96}$Tc | 0.410 | 0.425 | 3.65 |
| $^{55}$Mn(p,n)$^{55}$Fe | $^{55}$Fe | 0 | 0 | 0 |
| $^{59}$Co(p,n)$^{59}$Ni | $^{59}$Ni | 0 | 0 | 0 |
| $^{56}$Fe(p,n)$^{56}$Co | $^{56}$Co | 0.071 | 0.067 | 5.63 |
| $^{52}$Cr(p,n)$^{52}$Mn | $^{52}$Mn | 0.131 | 0.144 | 9.92 |
| $^{18}$W(p,n)$^{184}$Re | $^{184}$Re | 0.012 | 0.006 | 50 |
| $^{58}$Ni(p,n)$^{58}$Cu | $^{58}$Cu | - | 3.233 | - |
| $^{63}$Cu(p,n)$^{63}$Zn | $^{63}$Zn | 177.001 | 170.522 | 3.66 |

In the calculation of $^{58}$Cu, the yield value predicted by the Calcuyield application calculation is the yield value at the end time of irradiation (EOB) or when the irradiation process ends. According to the experimental measurement, there is no $^{58}$Cu detected. The undetected $^{58}$Cu impurity is due to the short half-life, which is 3.2 seconds. The post irradiated enriched water was measured nearly 2 hours after the EOB, thus it was impossible to detect $^{58}$Cu since the decay time was much greater than 3.2 seconds. As a result, the validation of the $^{58}$Cu calculated yield cannot be performed.

4. Conclusion
We have developed a novel Android-based software (called Calcuyield) for the End-Of-Bombardment (EOB) yield calculations relevant for cyclotron-based radionuclide production. Various nuclear reactions are listed and calculated using the Calcuyield and then the results are compared with the experimental data obtained from an 11-MeV proton accelerating cyclotron and an 18-MeV proton accelerating cyclotron in Jakarta, Indonesia. In the calculations, the cross-section values are calculated from the TALYS nuclear data library while the stopping power values are computed using the SRIM software. Based on the comparative results, the Calcuyield calculated results are in a good agreement with the experimental data, with a maximum difference of generally less than 10%, though one calculation error was 50% due to small measured radioactivity. Moreover, the same method can be applied to calculate other nuclear reactions.

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