Consultant's Meeting on

Inter-comparison of PIGE analysis codes I: Bulk analysis

Minutes of the meeting held on 1-4 October 2018, IAEA, Vienna

1. Purpose

In IBA techniques such as RBS, EBS and NRA, inter-comparisons of available analysis codes have already been performed (see M. Mayer et al., NIMB 385, 65-73 (2016); N.P. Barradas et al., NIMB 268, 1829-1832 (2010); NIMB 262, 281-303 (2007); E. Rauhala et al., NIMB 244, 436-456 (2006); IAEA TECDOC-1342, Vienna 2003). These inter-comparisons have concluded that the widely used codes are compatible and provide consistent results.

For PIGE analysis, although the technique is well-established since the 60s, such an inter-comparison has been performed in a limited way only, with early versions of ERYA and of the NDF implementation (see N.P. Barradas et al., NIM B 268 (2010) 1829–18). As a consequence, the technique is normally applied by comparing with well-defined standards. The potential of standardless PIGE was already stressed by the IAEA CRP on PIGE (2013-2017) (IAEA TECDOC-1822, Vienna 2017), however, the lack of validated PIGE analysis codes has not allowed this potential to be fully exploited.

To address this gap in PIGE analysis software, the IAEA is coordinating a systematic inter-comparison of available IBA codes which aims at establishing the consistency of the codes and assessing their accuracy with respect to each other.

The purpose of this meeting was to present the results of the inter-comparison, establish the consistency of available PIGE analysis codes and make recommendations to the user community.

Participants: M. Mayer (MPI-Garching), J.D. Cruz (Univeristy of Lisbon), A. Lagoyannis (NCSR "Demokritos"), N.P. Barradas (Physics Section, NAPC), Dimitriou (Scientific Secretary, Nuclear Data section, NAPC).

PIGE analsyis codes: SIMNRA, ERYA-Bulk (no straggling), ERYA-Profiling (straggling), PIGRECO, NDF.

Participants presented a short description of their codes and then the results of the inter-comparison were presented by the coordinator of this project (P. Dimitriou). All the presentations are available from the meeting webpgae: https://int-nds.iaea.org/index-meeting-crp/PIGE-codes/. The meeting agenda as well as the list of participants are provided at the end of the Minutes.

2. Exercises

A set of four exercises was defined by participating code developers to test the performance of the codes on bulk analysis, starting from smooth cross sections and simple elemental compositions, and then extending to cross sections with structure and finally including effects such as beam energy spread and straggling.

The exercises are described in detail in the following:

General conditions applied to all exercises:

- Stopping powers are taken from SRIM-2013.
- Angular distributions are assumed to be isotropic.
- Absorption of gamma-rays are not considered.
- Yield units: N_γ/sr/ μC where μC is micro-Coulomb

Fundamental constants and other data to be used:

- Isotopic abundance of 10B: 19.9%
- Electron charge = $1.60217662 \times 10^{-19}$ Coulomb
- $N_A = 6.022140857 \times 10^{23}$

1. <u>Smooth cross sections known down to the threshold energy (no beam energy spread)</u>
   a) A target with only one element with a smooth cross section (without sharp resonances) and an energy step of around 200 keV that is measured down to the threshold energy at 3 MeV. Below 3 MeV cross sections are assumed to be zero and at 3 MeV the yield is assumed to be zero:
   $^{10}B(p,p'\gamma)^{10}B$

Beam Energy (keV)	E_γ (keV)	Theta	Target	Cross Section
5000-3000 200 keV step	718	165	B 100%	A. Lagoyannis et al., NIMB 342 (2015) 271-276

b) The same element B but in a matrix of three elements (B-O-Fe) where the concentration of Fe is known from some other experiment. Below 3 MeV cross sections are zero and at 3 MeV the yield is assumed to be zero.

Beam Energy (keV)	E_γ (keV)	Theta	Target	Cross Section
5000-3000 200 keV step	718	165	B 10% O 40% Fe 50%	A. Lagoyannis et al., NIMB 342 (2015) 271-276

2. <u>Smooth cross section known down to an energy (no beam energy spread)</u>

Cases 1a and 1b can be implemented for a smooth cross section of B that is known down to an energy of 3 MeV. An initial yield of 580000 N_γ/sr/μC exists from that energy down to the threshold energy.

Two reactions are considered and for each reaction, (a) and (b) of Exercise 1 are calculated: in the case of (a) the initial yield is 580000 N_γ/sr/μC, while in (b) the initial yield will have to be calculated by considering the scaling of the stopping powers as well

i) $^{10}B(p,\alpha\gamma)^{7}Be$ reaction :

Beam Energy (keV)	E_γ (keV)	Theta	Target	Cross Section
3800-3000 100 keV step	429	150	B 100%	A. Lagoyannis et al., NIMB 342 (2015) 271-276

ii) $^{10}B(p,p'\gamma)^{10}B$:

Beam Energy (keV)	E_γ (keV)	Theta	Target	Cross Section
3800-3000 100 keV step	718	150	B 100%	A. Lagoyannis et al., NIMB 342 (2015) 271-276

This dataset also has a small gap in energies.

3. <u>Cross section with sharp resonances (no beam energy spread)</u>

   a) A target with only one element with sharp resonances: the 197 keV gamma ray from the $^{19}F(p,p\gamma_{2\text{-}0})^{19}F$ reaction. The energy threshold is considered at 1 MeV, so below 1 MeV the cross sections are assumed to be zero, and at 1 MeV the yield is assumed to be zero:

Beam Energy (keV)	E_γ (keV)	Theta	Target	Cross Section
2700-1000 1 keV step	197	130	F 100%	A.P. Jesus et al., Nucl. Instr. Meth. B 161-163 (2000) 186

   b) The same as a) but with 3 elements in the matrix:

Beam Energy (keV)	E_γ (keV)	Theta	Target	Cross Section
2700-1000 1 keV step	197	130	F 10% O 30% Cr 60%	A.P. Jesus et al., Nucl. Instr. Meth. B 161-163 (2000) 186

4. <u>Add straggling calculations to exercises (1) to (3) using **Bohr's model** with a beam energy spread of 3 keV.</u>

3. Results and discussions

The first results of exercise 1 that were provided by code developers prior to the meeting showed differences of the order of 20%.
To investigate the reasons for these large differences, 4 additional tests were performed:

TEST 1

For the conditions of 1a:
- use a flat cross section, 0 up to 3 MeV, 1 mb/sr above that.
- use SRIM stopping

TEST 2

For the conditions of 1a:
- use the given experimental cross section.
- use constant stopping power (at the value of 1.2 in units of eV/1e^{15}at/cm^2)

TEST 3

For the conditions of 1a:
- use a flat cross section, 0 up to 3 MeV, 1 mb/sr above that.
- use constant stopping power (at the value of 1.2 in units of eV/1e^{15}at/cm^2)

Tests 1-3 look at possible origin of the differences due to way of treating either cross section or stopping.

A fourth test was to test internal consistency of the calculations:

TEST 4

For the exact conditions of 1a:
- Use different calculation steps.

The comparison of the results for Tests 1-4 showed that the main reasons for the large deviations found originally were:

1) Large integration bin used by ERYA and PIGRECO
2) Small differences in the abundance of B-10 used in ERYA

Once the codes PIGRECO and ERYA introduced a smaller integration bin of 1 keV and the same abundance was adopted by all codes, the results for Exercise 1 were found to be in agreement within <1%.

The final results for all four exercises were compared at the meeting and a summary of the discussion and recommendations is given in the following:

Exercise 1

The handling of the sharp cut-off of the excitation function and yield at the threshold energy is done differently by the different codes. In the case of ERYA and PIGRECO, this resulted in discrepancies of the order of 0.3-0.5%. This was solved by adding an interpolated cross section value at the threshold energy in the R33 files used as input.

After this improvement, the results of the inter-comparison are:

(1a) ^{10}B(p,pγ)^{10}B, 100% B:

All the codes agree within 0.01% in the given energy range, with the exception of the ERYA code which has a maximum deviation of 0.2% at 4200 keV.

(1b) $^{10}B(p,p\gamma)^{10}B$, 10%B:

All the codes agree within 0.025% in the given energy range, with the exception of ERYA code which has a maximum deviation of 0.7% at 5000 keV.

A possible reason for the discrepancies in the ERYA code is the use of an analytical formula for the stopping power which is fitted to the values taken from SRIM-2013. The fitted stopping powers deviate as much as 1% from the SRIM values.

Exercise 2

I. $^{10}B(p,a\gamma)^{7}Be$: all the codes agree within 0.05% for the 100% B and 0.04% for the 10% B target. In the case of ERYA, the agreement is within 0.1% for both 100% and 10% B target.
This difference observed in the ERYA results is due to the same reason mentioned in Exercise 1.

II. $^{10}B(p,p\gamma)^{10}B$: all the codes agree within 0.03% for 100% B except for ERYA which agrees within 0.6%. For the 10% B target all codes agree within 0.06%.
Part of the above discrepancies can be attributed to the differences in the initial yields which are calculated based on the stopping power ratios used when going from a 100% to a 10% B target.

Exercise 3

In the case of the $^{19}F(p,p\gamma_{2\text{-}0})^{19}F$ cross sections with sharp resonances, overall, NDF and SIMNRA show excellent agreement within 0.02%. Within this precision, there are very small differences in the ratio between the two calculations. This needs to be further investigated.

The results show that ERYA and PIGRECO become less accurate in the vicinity of narrow resonances. This is partly attributed to the integration method used in these two codes which is not sufficiently accurate to deal with the fine structure of the excitation function. This is indicated by the dependence of the yield on the energy step of the integration.

For example, in the case of ERYA, the discrepancy at the 1090 keV resonance was 7% with respect to NDF and SIMNRA when an energy step of 1 keV was used. The discrepancy dropped to 0.9% when an energy step of 0.1 keV was used.

In the case of PIGRECO, the discrepancy with respect to NDF and SIMNRA dropped from 23% to 0.1% by changing the integration method from the simple trapezoidal to 3-point Simpson and decreasing the energy step in the integration from 1 to 0.5 keV.

An additional factor in the case of ERYA is the issue with the stopping power calculation mentioned above. This issue needs further investigation.

Exercise 4

The introduction of a beam energy spread of 3 keV and straggling effects using the Bohr model, overall led to larger differences between the codes.

For exercises 1 and 2, NDF, SIMNRA and PIGRECO have differences within 0.3%, except for the lowest energy where PIGRECO deviates by up to 40%. It should be noted however, that at this energy the yield is extremely low, so large relative differences correspond to very small absolute differences.

The discrepancy observed in the PIGRECO results at the threshold energy can be attributed to the handling of straggling near the threshold energy.

The same holds for ERYA which shows differences of about 30% at the threshold energy, which however drop to 0.5% at higher energies.

For exercise 3, the results of the codes show some additional interesting features:

NDF and SIMNRA agree typically within 0.05%, except for energies in the vicinity of resonances where the difference is 0.2%. In the energy range from 1100 keV to approx. 1900 keV, a saw-like pattern of the order of 0.02% is observed in the ratio between SIMNRA and NDF. This requires further investigation.

ERYA exhibits differences of the order of 40% near the threshold energy and up to 30% at the resonances, while PIGRECO shows a similar trend with differences of about 20% at threshold energy and 22% at the resonances. A sizeable part of this effect may be due to a shift in the energy axis less than 0.3 keV. Off the resonances PIGRECO has deviations of the order of 0.3% with respect to NDF and SIMNRA while ERYA deviates by 0.1-7%.

The problem at threshold energy again is attributed to the handling of straggling near threshold. A further exercise that could possibly clarify the situation is to calculate the yield at threshold energy by considering the cross-section data below threshold energy. This will be done by both code developers after the meeting.

For the differences at and near the resonances, the integration method plays an important role and will be further investigated for both the ERYA and PIGRECO codes.

To summarize this bulk target exercise, in the absence of sharp resonances overall agreement between the codes is better by 1-2 orders of magnitude than the accuracy of available experimental cross-section and stopping-power data. Near resonances NDF and SIMNRA agree within 0.2%.

Further work needs to be done in ERYA and PIGRECO as detailed above. The final results of these codes will be submitted by the end of November 2018.

4. Publication

The meeting participants agreed that the outstanding issues regarding the codes need to be resolved to a satisfactory point before the results of the inter-comparison are submitted for publication.

It was agreed that the results should be published in a peer-reviewed journal (NIMB).

The preparation of the manuscript will be coordinated by N.P. Barradas. The following assignments were made:

-Introduction by P. Dimitriou

-Main text by N.P. Barradas:

It will include short descriptions of the different codes which will be provided by all the code developers. A table with the main specifications of the codes will also be prepared.

The discussion section will include a list of improvements/modifications that were made in the course of the inter-comparison exercise.

-Figures by A. Lagoyannis:

The figures will include plots of average values of the codes that are in good agreement and deviations from this average.

The order of authors in the authors list was decided to be alphabetical.

5. Dissemination

Once the final results are collected and all the issues mentioned in the previous sections have been addressed satisfactorily, the results (numerical tables and figures) and conclusions of the inter-comparison will be made available online on a dedicated webpage along with links to the different codes. This webpage will be accessible to the user community from the IBANDL interface.

Meeting participants recommended that the results of the IAEA Inter-comparison of IBA software (published by N.P. Barradas et al., NIMB 268, 1829-1832 (2010)) are also made available on this dedicated webpage.

Consultants' Meeting on
Inter-comparison of PIGE Analysis Codes

IAEA, Vienna, Austria
1 to 4 October 2018
Meeting Room VIC C0219

PRELIMINARY AGENDA

Monday, 1 October

09:00 – 09:30	**Registration (IAEA Registration Desk, Gate 1)**
09:30 – 10:00	**Opening Session** Welcoming address (P. Dimitriou) Administrative matters Election of Chairman and Rapporteur Adoption of the Agenda
10:00 – 17:30	**Presentations by participants** (~30 min. each) 1) *ERYA code*, J.D. Cruz, Istituto Superior Tecnico 2) *PIGRECO code*, A. Lagoyannis, NCSR "Demokritos" 3) *SMNRA code*, M. Mayer, Max Planck Institute 4) *NDF code*, N. Barradas, IAEA 5) Results of Exercises 1-4: coordinator P. Dimitriou Results of comparisons will be presented for each exercise followed by discussions and conclusions *Coffee break(s) as needed* ***(12:30 – 14:00 Lunch break)***

Tuesday, 2 October

09:30 – 17:30 **Round Table Discussions**

- Results of Exercises 1-4 (cont'd)
- What needs to be done next
- Publication of results
- Dissemination – web interface

Coffee break(s) as needed

(12:30 – 14:00 Lunch break)

19:00 ***Dinner at a restaurant (see separate information)***

Wednesday, 3 October

09:30 – 17:30 **Round Table Discussions** (cont'd)

Coffee break(s) as needed

(12:30 – 14:00 Lunch break)

Thursday, 4 October

09:30 – 12:00 **Drafting of the Summary Report**

Closing of the Meeting

Coffee break as needed

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List of Participants

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