A Comprehensive Review of Green Metric Tools for Sustainable Analytical Method Development

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Abstract. The study on green metric tools for sustainable analytical method development is important because it critically assesses current approaches to improving environmental sustainability in analytical chemistry. This paper discusses the immediate need for thorough frameworks that evaluate the sustainability of analytical procedures in light of the growing need for environmentally friendly methods. The study emphasises the functions of tools like the Green Analytical Procedure Index (GAPI), Analytical Greenness Metric Method and Software (AGREE) and others in encouraging environmentally friendly practices, decreasing down on hazardous waste and enhancing safety in lab environment. In order to promote a comprehensive approach to sustainability, the study highlights the significance of taking into account each stage of the analytical process, from sample preparation to final analysis. It highlights the advantages and disadvantages of several green measures and offers information on how well they work in actual lab settings. This is especially important because a lot of the tools available now don't assess how well processes work in real-word settings, which is crucial for standard analytical labs. Furthermore, by supporting the creation of more reliable assessment frameworks that can measure the environmental effect of analytical processes, the study adds to the continuing conversation on green chemistry. In the end, this minimises the environmental impact of analytical chemistry by motivating researches to use more environmentally friendly techniques. This study promotes the importance of environmental consciousness in scientific research and is an essential resource for researchers and those working to enhance sustainable practice in the area.

Keywords: Green Analytical Chemistry, Green Metric Tools, Safety.

1. Introduction

The increased demand for ecologically friendly methods in analytical chemistry led to the development of Green method in analytical chemistry in 2000. It's fundamental objective is to preserve high-quality results while reducing the environmental effect of analytical techniques. Green chemistry, which promotes the reduction or removal of harmful chemicals in chemical processes, is the foundation of GAC. This strategy has attracted a lot of interest from chemists who want to improve the sustainability of experiments.

Notwithstanding its benefits, GAC has drawbacks, especially when it comes to evaluating the "greenness" of analytical processes. Several green metrics and tools have been developed as a result of the absence of standardised techniques for assessing

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the environmental effect of these operations. Each of them, such as the Green Analytical Procedure Index (GAPI) and the Analytical Greenness Metric Method and Software (AGREE), etc. has advantages and disadvantages. Although some methods offer a numerical evaluation of environmental performance, others could ignore important elements like energy usages or the king of waste produced.

Since, many of the current tools come short in capturing the complex nature of sustainability in analytical chemistry, there is a clear need for a comprehensive evaluation framework. From sample preparation to final analysis, GAC stresses the significance of taking into account every step of the analytical process and promotes the use of leading-edge materials and techniques that improve productivity and environmental friendliness. (1), (2),(3).

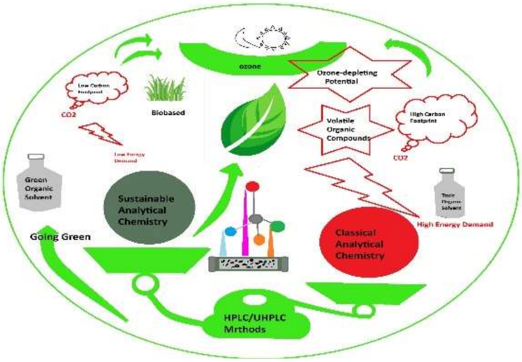

Fig. 1. Benefits of sustainable analytical chemistry

2. Method

A number of methods exist for evaluating the usefulness and sustainability of analytical procedures. The following important were mentioned.

2.1 Analytical Greenness Metric Method and Software (AGREE)

The Analytical Greenness Calculator (AGREE) is an innovative program that use an eye-catching and user-friendly picture to assess the environmental sustainability of analytical techniques. Fundamentally, AGREE uses a special RGB colour model, in which the three basic colors red, green and blue stands for important aspects of the analytical process, practical efficacy, analytical performance, and adherence to green chemistry principles. https://mostwiedzy.pl/en/wojciech-wojnowski,174235-1/AGREE.

2.1.1 Diagram Interpretation:

Colour Representation: The Vibrant colour spectrum in the AGREE graphic includes the following:

a. Red denotes analytical performance, emphasising the efficacy and dependability of the approach.
b. Green highlights the method's environmental friendliness and indicates adherence to green chemistry principles.
c. Blue denotes practical efficacy, demonstrating the method's viability and user-friendliness.

Composite Colour Output: These fundamental colours are additively synthesised to produce the final colour allocated to the assessed approach. This composite colour gives people a rapid visual indicator of the method's overall sustainability, making it simple to judge how green it is.
Scoring System: Accompanying the colour representation is a scoring system that quantifies the method's performance on a scale from **0 to 100%**. This score not only makes comparing various approaches easier, but it also identifies areas that need work.
User-Friendly Interface: The AGREE tool's simple interface, which enables researchers to enter data and get instant visual response, is part of its accessible design. (11), (12), (13)

2.2 Green analytical procedure index (GAPI)

An innovative tool that helps researchers select more environmental friendly solutions is the Green Analytical Procedure Index (GAPI), which graphically depicts the environmental sustainability of analytical techniques. Each point on the eye-catching pentagram diagram that forms the basis GAPI represents a crucial step in analytical process, ranging from sampling to final analysis. https://mostwiedzy.pl/pl/justyna-plotka-wasylka,647762-1/gapi.

2.2.1 Diagram Description:

Pentagram Organisation: The pentagram's five points stands for the essential phases of an analytical process, enabling users to evaluate the environmental effect of each stage. A comprehensive picture of the whole workflow is offered by this structure.

a. Green denotes sustainable activities with little influence on the environment.
b. Yellow indicates areas that needs work and has a modest influence.
c. Red denotes strong impact, emphasising phases that need major adjustments to improve sustainability.

Visual Clarity: Capacity information is simplified into an understandable manner by the GAPI diagram. Researchers can rapidly determine which phases of their procedures require attention and which are ecologically favourable Essentially, GAPI turns the assessment of analytical techniques into an interesting visual tale, encouraging sustainability in analytical chemistry and aiding in well-informed decision-making. (15),(16),(17).

2.3 Complex Green Analytical Procedure Index (Complex GAPI)

The Complex GAPI is an advanced tool designed to provide a comprehensive evaluation of the environment sustainability of analytical methods. Building upon the original GAPI, Complex GAPI provides a comprehensive picture of sustainability by incorporating more dimensions to evaluate operations carried out prior to the analytical technique. https://mostwiedzy.pl/pl/justyna-plotka-wasylka,647762-1/complexgapi

2.3.1 Diagram Description:

Hexagonal Structure: Each side of the hexagon-shaped Complex GAPI diagram represents a distinct step in the analytical process, such as sample collection, transportation, preservation, preparation and final analysis. A comprehensive evaluation of the entire workflow is made possible by this arrangement.

a. Green denotes excellent practices and little environmental effect.
b. Yellow indicates areas that might use improved and has modest influence.
c. Red denotes significant impact, emphasising phases that need immediate attention in order to improve sustainability.
   Visual Clarity: By condensing complicated data into an understandable format, the hexagonal shape helps researchers swiftly pinpoint the steps that require improvement and the more environmentally friendly elements of their approaches. (18),(19),(20).

2.4 Blue Applicability Grade Index (BAGI)

A visual aid created to illustrate the assessment of analytical techniques use the BAGI statistic is the BAGI pictogram. Here is a thorough explanation of its elements. https://mostwiedzy.pl/pl/justyna-plotka-wasylka,647762-1/BAGI
Asteroid Form: The pictogram's asteroid-like form represent the analytical method's total score and adherence to predetermined standards. It is more captivating and memorable because to its distinctive form, which helps set it apart from conventional graphs or charts.
Central Score: A numerical score ranging from 25 to 100 is located at the asteroid's centre. This score represents the analytical method's overall effectiveness:

- A score of 25 denotes super performance from the approach.
- A perfect score of 100 denotes outstanding work.
- A technique is considered practical if it receives a score of 60 or above, indicating that it satisfies the requirements for successful implementation.

Hue Scale: A sequential blue colour scale determines the asteroid's colour and serves as a visual indicator of whether the procedure satisfies the following requirements:

- **Dark Blue:** Shows high compliance, indicating that the approach is highly successful and satisfies the majority of requirements.
- **Blue:** Indicates medium compliance, meaning that while the approach satisfies certain requirements, it does not fulfil all of them.
- **Light Blue:** Indicates low compliance, implying that the approach finds it difficult to satisfy the requirements.
- **White:** Shows no compliance, indicating that the procedure completely fails to adhere to the necessary requirements.

Divisions: The asteroid is divided into 10 sections, each of which stands for different one of the 10 characteristics that the BAGI metric assesses. The section enables a thorough evaluation of particular elements of the analytical process:

- The inner sections match characteristics associated with the phases of sample preparation and analytical determination.
- The outer section provide a thorough understanding of method's performance by encompassing attributes related to both processes.

Visual Visualisation: The asteroid form and colour coding allow for a rapid visual evaluation of the method's advantages and disadvantages. This design improves the tool's usability and efficacy by making it simpler for users to quickly compare various analytical techniques. (21),(22),(23).

3.Discussion

A variety of test for evaluation, such as the Green Analytical Procedure Index (GAPI), Complex Green Analytical Procedure Index (Complex GAPI), Analytical Green Chemistry Evaluation (AGREE), and the Blue Analytical Grade Index (BAGI), have been developed as a result of the growing emphasis on sustainability in analytical chemistry. Using a colour-coded approach for rapid evaluations, GAPI provides a visual pentagram diagram to analyse the environmental effect of each step in an analytical process. By integrating preparation procedures into a hexagonal framework, Complex GAPI improves this and offers a more thorough assessment of sustainability.

BAGI primarily addresses the sustainability of biogenic amine analysis, whereas AGREE concentrates on a score system that assesses the greenness of analytical techniques based on number of parameters. Every instrument has its own advantages and disadvantages, ranging from AGREE comprehensive score to GAPI's simple visual depiction. In order to promote more sustainable practices in analytical chemistry, this comparative study emphasises the significance of choosing the appropriate equipment depending on particular research objectives. When selecting from these useful resources, researches are urged to take their work's requirements and context into account.

4. Conclusion

In conclusion, future researchers will greatly benefit from the wide range of green analytical tools like GAPI, Complex GAPI, AGREE and BAGI that will support sustainability in analytical chemistry. These technologies enable scientists to make well-informed judgements regarding their methods by offering thorough evaluations of environmental effect, which eventually reduces waste and improves eco-friendliness. These tools will support the creation of creative, sustainable analytical techniques, promoting an environmentally conscious culture as the need for greener practices grows. These materials can be used by researchers to further the larger objective of sustainable scientific development in addition enhancing their individual procedures.

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6. Conflict of interest:

The authors declare no conflict of interest relevant to this article.

Reference:

1. L. Novakova, Advances in sample preparation for biological fluids, LCGC Int. 29,9–15(2016).
2. G.M. dela S. A, Green analytical chemistry: theory & practice, in: B. Dami`a (Ed.), Compr. Anal. Chem. Ser., Elsevier, 2011.
3. A. Gałuszka, Z. Migaszewski, J. Namie´snik, The 12 principles of green analytical chemistry and the SIGNIFICANCE mnemonic of green analytical practices, TrAC Trends Anal. Chem. 50,78–84(2013).
4. P.M. Nowak, R. Wietecha-Posłuszny, J. Pawliszyn, White analytical chemistry: an approach to reconcile the principles of green analytical chemistry and functionality, TrAC Trends Anal. Chem. 2021 138.
5. V. Sivasankar, R.N. El-Shaheny (Eds.), Green Chem. Anal. Sample Prep. Proced. Instrumentation, Data Metrics, Sustain, Springer International Publishing, Cham, pp. 29–99(2022).
6. M. Shi, X. Zheng, N. Zhang, Y. Guo, M. Liu, L. Yin, Overview of sixteen green analytical chemistry metrics for evaluation of the greenness of analytical methods, TrAC Trends Anal. Chem. 166 (2023).
7. M. Sajid, J. Płotka-Wasylka, Green analytical chemistry metrics: a review, Talanta 2022 238.
8. M.B. Swanson, G.A. Davis, L.E. Kincaid, T.W. Schultz, J.E. Bartmess, S.L. Jones, E. L. George, A screening method for ranking and scoring chemicals by potential human health and environmental impacts, Environ. Toxicol. Chem. 16,372–383(1997).
9. L.H. Keith, L.U. Gron, J.L. Young, Green analytical methodologies, Chem. Rev. 107, 2695–2708(2007).
10. R. Hartman, R. Helmy, M. Al-Sayah, C.J. Welch, Analytical method volume intensity (AMVI): a green chemistry metric for HPLC methodology in the pharmaceutical industry, Green Chem. 13,934–939 (2011).
11. Armenta, S.; Garrigues, S.; de la Guardia, M. TrAC, Trends Anal. Chem. 27, 497−511(2008).
12. Tobiszewski, M.; Marc, M.; Gałuszka, A.; Namiesnik, J. Molecules. 20, 10928−10946(2015).

13. Pena-Pereira, F. From Conventional to Miniaturized Analytical Systems. pp 1−28(2014).
14. Poole, C. F. J. Chromatogr. A (2013). 1296, 1.
15. M. K. Parr, A. H. Schmidt, Life Cycle Management of Analytical Methods, J. Pharm. Biomed. Anal. 17, 31221-31229(2017).
16. Life Cycle Assessment: Principle and Practice, National Service Center for Environmental Publications, Reston (2006).
17. R. McDowall, Life cycle and quality by design for chromatographic methods, LCGC Europe, 27, 91–97(2014).
18. L.H. Keith, L.U. Gron, J.L. Young, Green Analytical Methodologies, Chem. Rev. 107, 2695–2708(2007).
19. D. Raynie, J. Driver, Green Assessment of Chemical Methods, In: 13th Annual Green Chemistry and Engineering Conference, Maryland (2009).
20. M. Poliakoff, P. Licence and M. W. George, Curr. Opin. Green Sustainable Chem., 2018, 13, 146
21. M. K. Parr and A. H. Schmidt, J. Pharm. Biomed. Anal.17, 31221(2017).
22. J. Pryshlakivsky and C. Searcy, J. Cleaner Prod.309(2021).
23. J. P. Hutchinson, L. Setkova and J. Pawliszyn, J. Chromatogr. A, 1149, 127–137(2007).
24. J. D. Hunter, Comput. Sci. Eng. 9, 90–95(2007).
25. K. D. Moreland, Diverging Color Maps for Scientific Visualization (2009).