A sustainable approach to nontargeted analysis using hydrogen as a carrier gas for GC×GC

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INTRODUCTION

Comprehensive two-dimensional gas chromatography (GC×GC) is a separation technique used to separate complex mixtures based on two different retention mechanisms, usually polarity and volatility. Below is a schematic of the GC×GC instrument used to analyze a 52-component Indoor Air standard.

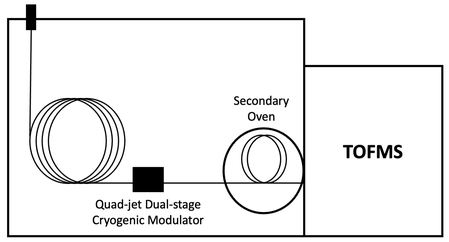

Figure 1: Comprehensive two-dimensional gas chromatography with time-of-flight mass spectrometry instrument schematic

A carrier gas carries the mixture through the columns before the components arrive at the detector. Common choices for carrier gas are helium, hydrogen, and nitrogen. Helium is the most common choice; however, hydrogen is a greener option.

Helium
- Non-flammable
- Obtained through fossil fuel mining
- Finite resource
- Cheaper
- Longer run time

Hydrogen
- Flammable
- Can be made through the electrolysis of water in the laboratory
- Renewable resource
- Expensive, but cost-efficient
- Shorter run time

One way to determine the sustainability of a method is to use the AGREEprep website: https://agreeprep.anvil.app/.[1] This website allows for the input of values for different criteria and in the end, provides a score from zero to one, with a score closer to one being greener.

A nontargeted approach is commonly used for a separation technique such as GC×GC. This type of approach means that instead of looking for one or two specific components and disregarding the rest of the sample, the whole sample can be viewed exhaustively. This approach is more applicable for forensic cases especially, where the identity or composition of the sample is unknown. It is also a more sustainable approach because only one run is needed to have the full characterization of a sample instead of needing to run a sample multiple times with a different target analyte each time.

PURPOSE

The purpose of this research was the quantify the sustainability of a method and compare the greenness of helium and hydrogen methods analyzing the same standard.

EXPERIMENTAL

LECO's Pegasus BT4D instrument was used for this project.

Hydrogen Translation

The Restek EZGC Method Translator was used to produce three different hydrogen methods.[2]

Translate Method
- Prioritizes making the hydrogen chromatography look as similar to the helium chromatogram as possible

Efficiency Method
- Takes into account peak shape and intensity while also prioritizing the speed of the hydrogen run in comparison to helium

Speed Method
- The fastest hydrogen method
- Does not take into account peak resolution

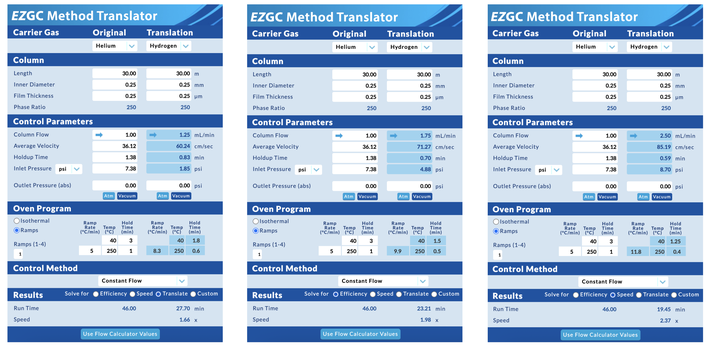

Figure 3: Restek Method Translator outputs for the three different hydrogen method options.

FINAL RESULTS

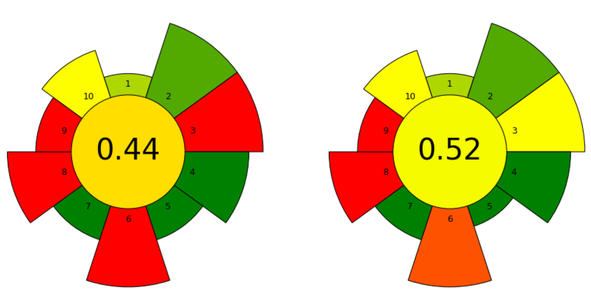

Figure 4: AGREEprep score outputs for helium (left) and hydrogen (right) methods.

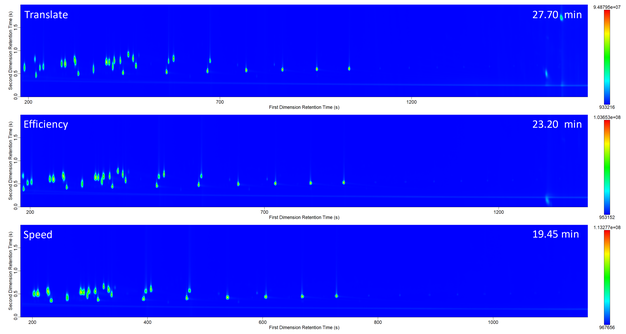

Figure 5: Total Ion Current (TIC) chromatograms for each of the three hydrogen methods.

#	Criterion		Score	Weight
1.	Sample preparation placement:	On-line/In situ	0.66	1
2.	Hazardous materials:	0.03 [g or mL]	0.84	5
3.	Sustainability, renewability, and reusability of materials:	< 25% of reagents and materials are sustainable or renewable, but can only be used ONCE	0.00	5
4.	Waste:	0.035 [g or mL]	1.00	4
5.	Size economy of the sample	Mass or volume of the sample: 0.001 [g or mL]	1.00	2
6.	Sample throughput:	1 [samples/h]	0.00	5
7.	Integration and automation	Sample prep. steps: 2 steps or fewer, Fully automated systems	1.00	2
8.	Energy consumption:	5273.23 [W]	0.00	4
9.	Post-sample preparation configuration for analysis:	Advanced MS with high energy and/or noble gas consumption: ICP-OES, ICP-MS, etc.	0.00	2
10.	Operator's safety:	2 hazards	0.50	3

#	Criterion		Score	Weight
1.	Sample preparation placement:	On-line/In situ	0.66	1
2.	Hazardous materials:	0.03 [g or mL]	0.84	5
3.	Sustainability, renewability, and reusability of materials:	50-75% of reagents and materials are sustainable or renewable, but can only be used ONCE	0.50	5
4.	Waste:	0.035 [g or mL]	1.00	4
5.	Size economy of the sample	Mass or volume of the sample: 0.001 [g or mL]	1.00	1
6.	Sample throughput:	2 [samples/h]	0.16	5
7.	Integration and automation	Sample prep. steps: 2 steps or fewer, Fully automated systems	1.00	2
8.	Energy consumption:	2636.61 [W]	0.00	4
9.	Post-sample preparation configuration for analysis:	Advanced MS with high energy and/or noble gas consumption: ICP-OES, ICP-MS, etc.	0.00	2
10.	Operator's safety:	2 hazards	0.50	3

Figure 6: AGREEprep score breakdown comparison for helium (left) and hydrogen (right) methods.

AGREEprep Comparisons:

The overall scores for the two methods were 0.44 and 0.52 for helium and hydrogen, respectively. This means that the hydrogen method is more sustainable than the helium method. The criteria breakdown in Figure 6 shows the 10 different criteria used to score the methods, including sample throughput, sample preparation steps, and sustainable material usage, namely carrier gas choice.

CONCLUSIONS

The Restek EZGZ Method Translator can be used to provide three possible hydrogen methods for any given helium method. After inputting the values of a helium method, the respective hydrogen values are given for three possible methods, each prioritizing something different: translate, efficiency, and speed. The translate method was chosen as the best choice.

The hydrogen method achieved a higher score on the AGREEprep metric, meaning that this method is more sustainable that the helium method. This better score is solely due to the carrier gas change – everything else in the methods stayed constant.

Hydrogen as a carrier gas allows for higher sample throughput and faster run times. It can also be a renewable resource, made through the electrolysis of water in a laboratory using a generator.

A nontargeted approach is inherently greener than a targeted approach because instead of re-running a sample multiple times to analyze a different component each time, the whole picture was captured from the beginning and can be looked at through a different lens to analyze a new component.

FUTURE RESEARCH

- Use the AGREEprep metric to score different methods that we use in our laboratory.
- Translate more helium methods into hydrogen methods.
- Quantitatively analyze the differences between helium and hydrogen methods analyzing the same sample.

REFERENCES

1. Wojnowski, W.; Tobiszewski, M.; Pena-Pereira, F.; Psillakis, E. AGREEprep – Analytical Greenness Metric for Sample Preparation. *TrAC Trends Anal. Chem.* **2022**, *149*, 116553. https://doi.org/10.1016/j.trac.2022.116553.
2. Restek. *EZGC Method Translator and Flow Calculator Help*. EZGC Method Translator. https://www.restek.com/articles/ezgc-method-translator-and-flow-calculator-help (accessed 2025-12-08).

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