Gas Chromatography-Vacuum Ultraviolet spectroscopy (GC-VUV): a sustainable alternative measurement technology for volatile species. An early research application

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Introduction

Sources of pollution

- **Plastic waste** from **personal care products** (PCP) & **food packaging** (FP) are ubiquitous in the environment.
- Contain **primary plastic & additives** – latter can be **toxic to humans & environment**.
- **Leachate of additives – a cause for concern**.

Drivers for new monitoring methods

- Current methods offer **insufficient molecular selectivity** to understand **impact & risk**.
- International treaties & HMG policy for Enhanced Producer Responsibility requires better monitoring for enforcement.

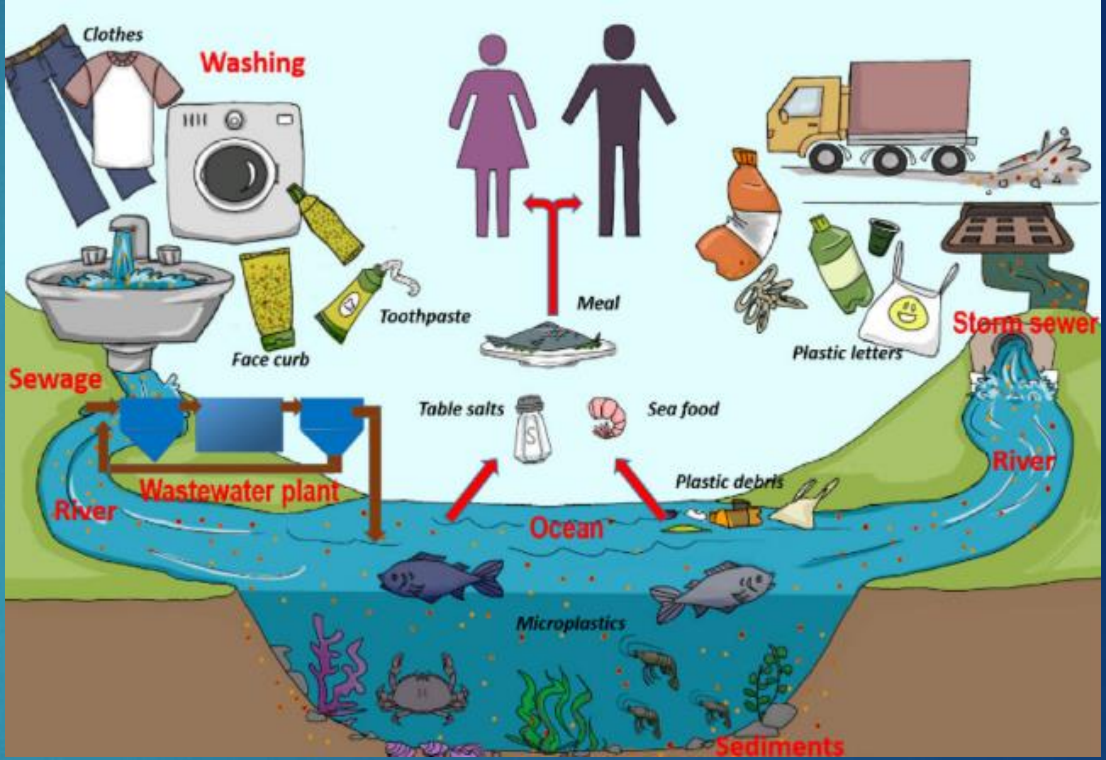

Figure 1. Microplastic pollution in aquatic environments and impacts on food chains. [1]

Multi-modal GC-VUV

- **<u>Optic-4</u>**: multi-modal inlet (**pyrolysis/TD, liquid injection**) to analyse solids & liquids.
- **<u>GC-VUV</u>**: Sensitive, 3D data (wavelength, time, absorbance) specific to chemical structure. Offers broader molecular detection & **structural isomer elucidation** (unlike standard GC-MS).
  - With backflush & N_2 gas for cleaner, **greener** (**<u>more sustainable</u>**) operation.

Research Aim

- Investigate utility of multi-modal inlet GC-VUV for plastics characterization.

Figure 2. Image of multi-modal GC-VUV, situated in Swansea University's School of Medicine (**<u>1st & only in UK!</u>**).

Method

Homogenisation of PCP & FP

1. Put 0.5 mg plastic in a stainless-steel milling jar.

2. Dry ice for 30 mins.

3. Homogenise for 5 mins. at 23 Hz (OMNI Bead Ruptor 96).

(Steps 2–3: x2)

4. Finished product (see results slide, fig 6b).

Pyrolysis (Pyr)/ Thermal Desorption (TD)

GC-VUV

- GC - ZB-1 (Restek) 30 m, 0.25 mm x 0.25 µm, 1.1 mL/min N_2 carrier gas, backflush flow 6.1 mL/min.
- VUV - make-up gas 0.35, system gas 3.0 psi, flow cell & transfer line @ 340 °C, 125-430 nm.

Optic

- Pyr - 0.1 mg plastic, heated 35-600 °C at 60 °C/sec.
- TD - 0.1 mg plastic, heated 35-350 °C or 400 °C at 60 °C/sec.

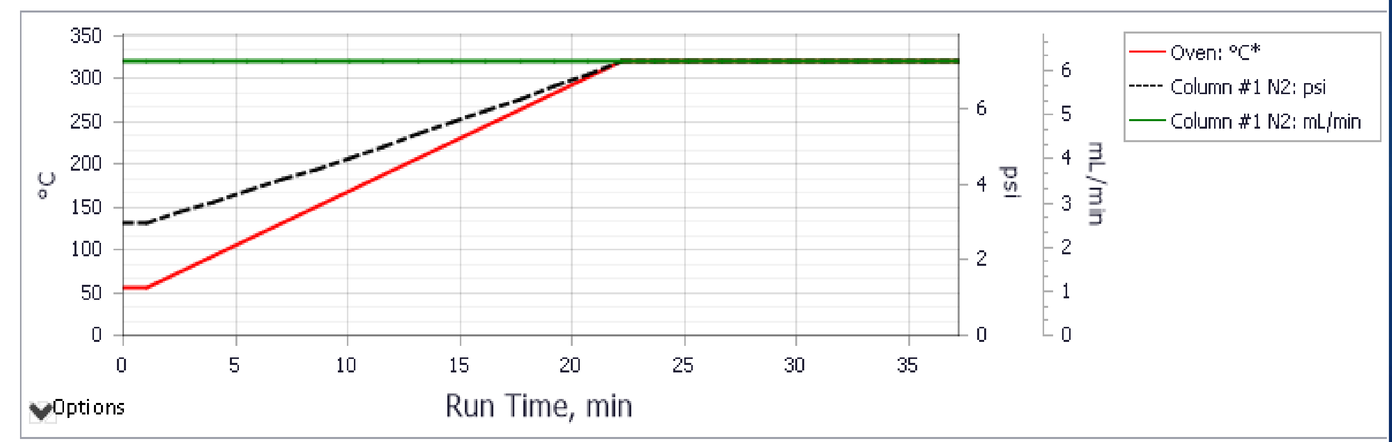

Figure 3. Gradient program for GC.

Results: GC-VUV

Pyrolysis

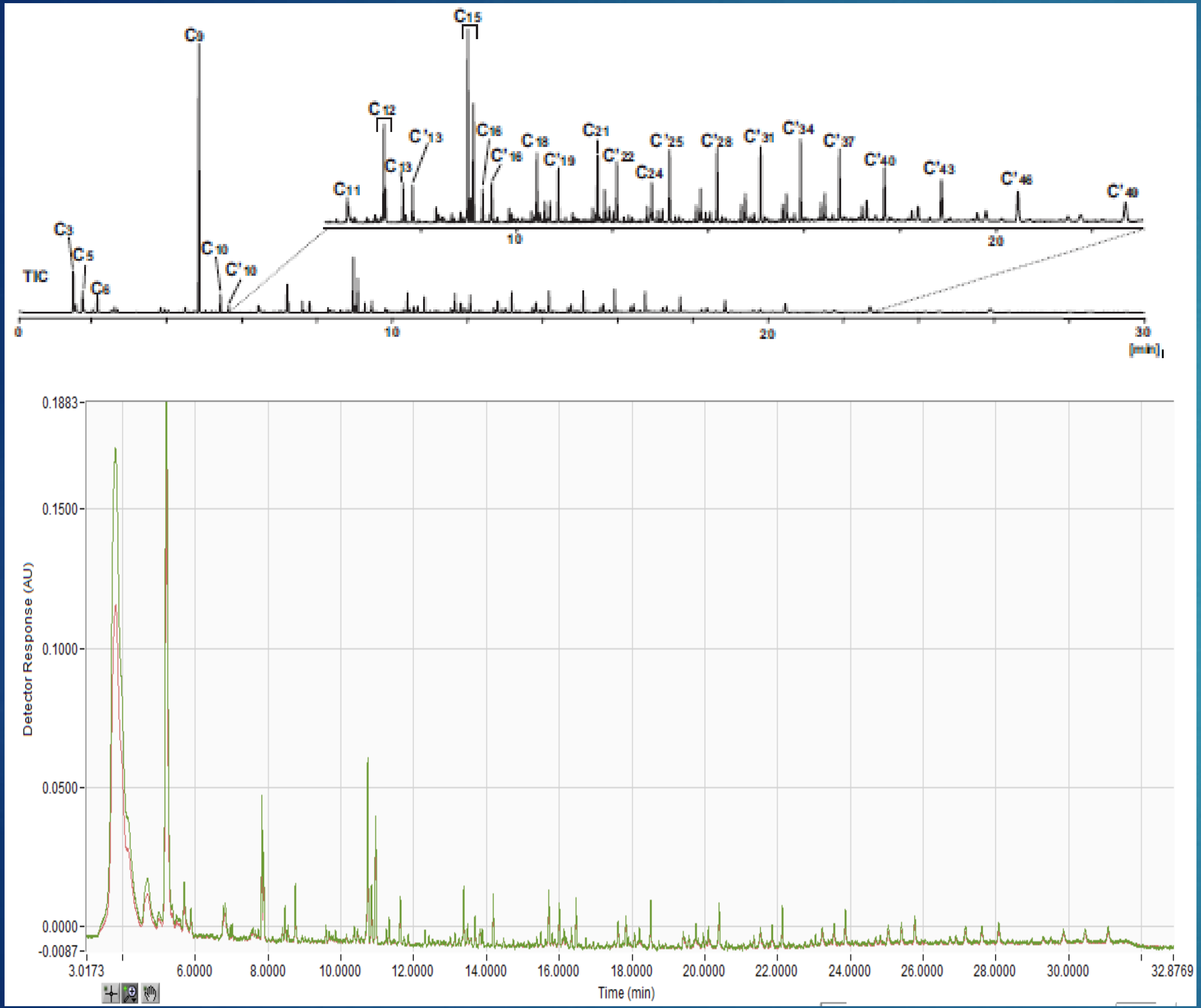

Figure 4. Pyrograms of PP via GC-MS & GC-VUV. Top – GC-MS using similar DB-1 column (25 m, 0.53 µm) showing C3-34 & additives taken from Shin et al. [6]. Bottom – using GC-VUV with ZB -1 column (25 m 0.25 µm).

Benefits of running with GC-VUV rather than GC-MS

- ✓ **More peaks** identification with PP, PE, PET and PS, providing further information on each plastic.
- ✓ Different pyrogram with **oxygenated species (PP & PE) – alternative chemistries formed?**

Table 1. Pyr-GC-MS data (from literature) comparison with Pyr-GC-VUV

Temperature 600°C		
	Number of peaks	
Plastic	GC-MS	GC-VUV
PP	61	83
PE	26	64
PET	28	44
PS	29	35

Results: Homogenisation

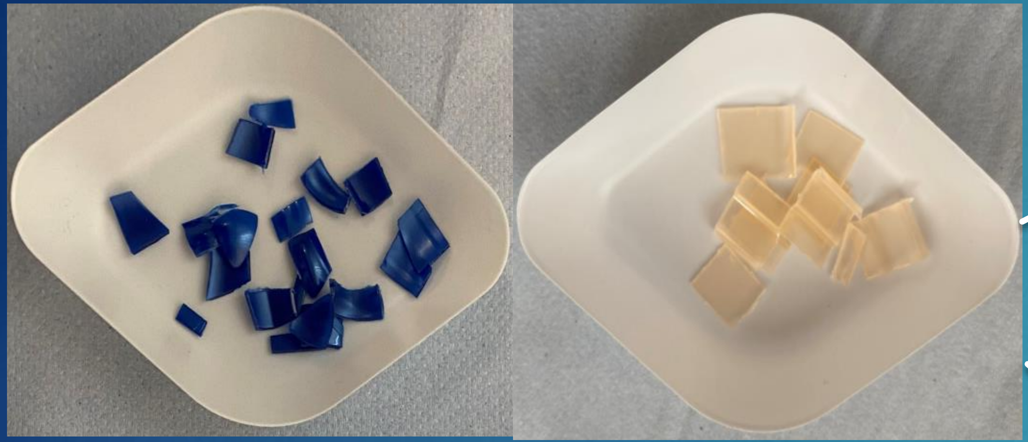

Figure 5. 0.5 g of PCP (left) & food packaging (right) before dry ice & **automated** homogenization.

Figure 6a. Particles of PCP & food packaging unable to be broken down

Figure 6b. Particles of PCP & food packaging broken down to smaller particles

Table 2. Particle sizes of PCP and FP using a digital caliper.

Unsuccessful		Successful	
PCP	FP	PCP	FP
5.47 mm	6.05 mm	0.54 mm	0.91 mm
1.97 mm	2.87 mm	0.29 mm	0.64 mm
2.93 mm	3.62 mm	0.25 mm	0.52 mm

Conclusion and future work

Developed GC-VUV plastics analysis method & established new plastics spectral database.

1. Will compare data with GC(xGC)-MS coupled with Optic-4 inlet to elucidate unknowns.

2. Develop GC-VUV method for plastic additives & expand plastics VUV library for additives.

3. Characterise leachate using homogenisation & GC-VUV method – compare with standard plastics analysis (e.g. FT-IR & AFM.)

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