

Development of a Screening Test for the Mobility of Polar and Ionisable Substances in the Environment

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Introduction

The OECD TG 121 screening method is often carried out as a simple, quick and cheap way of estimating organic carbon-water partition coefficients (K_{OC}) using high performance liquid chromatography (HPLC). The results reflect the interaction of the polar and non-polar groups of a test substance with the column material. However, other interactions, such as ion exchange interactions, are ignored, even though they may be influential in determining the adsorption properties of highly polar or ionisable substances in soils and sediments.

It may be possible to extend the general concept of the OECD TG 121 screening test to consider these additional interactions. This work investigates whether state-of-the-art mixed mode stationary phases using ion exchange combined with reversed phase material might have the potential to act as surrogates for surfaces in soils and sediments where the additional interactions may occur.

Method development

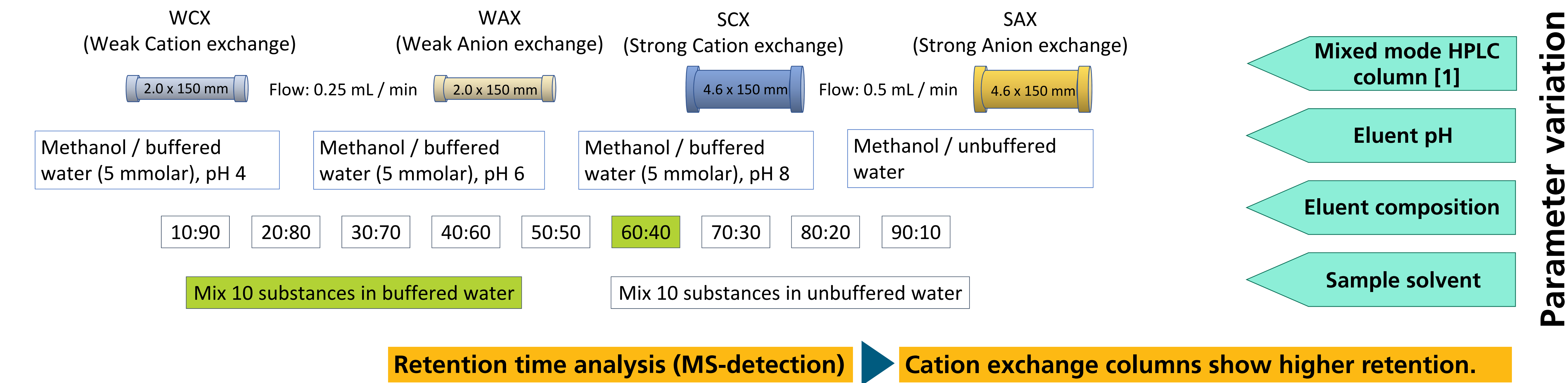


Figure 1: Schematic representation of method development for the OECD TG 121 extension.

Testing with a larger substance list

Nr.	Substance
1	3,3,4,4,5,5,6,6,7,7,8,8,8-Tridecafluorooctanesulfonic acid
2	Metam
3	Nicosulfuron
4	Sodium trichloroacetate
5	2,2'-(Benzylimino)diethanol
6	Benzyltrimethylammonium chloride
7	N-Butylbenzenesulfonamide
8	Tryptamine
9	Flumetsulam
10	Formamide (no MS-signal)
11	Melamine
13	Propoxycarbazone (sodium salt)
14	Clopyralyd
15	Gibberellic acid
16	Tribenuron-methyl
17	Florasulam
18	n-Butyric acid
19	2-Morpholinoethanol
20	Ammonium 2,3,3,3-tetrafluoro-2-(heptafluoropropoxy)propanoate
21	Serotonin
22	Methylephedrine
23	Acephate
24	Choline chloride
26	Acetanilide
27	Phenol
28	2-Nitrobenzamide
29	Benzamide
30	Hymexazol
33	1,4-Dioxane
34	Daminozide
35	Bis(4-hydroxyphenyl)sulfone
36	4-Nitrophenol
37	Methyl tert-butyl ether
38	Diclofenac
39	Ibuprofen
40	Ethylenediaminetetraacetic acid

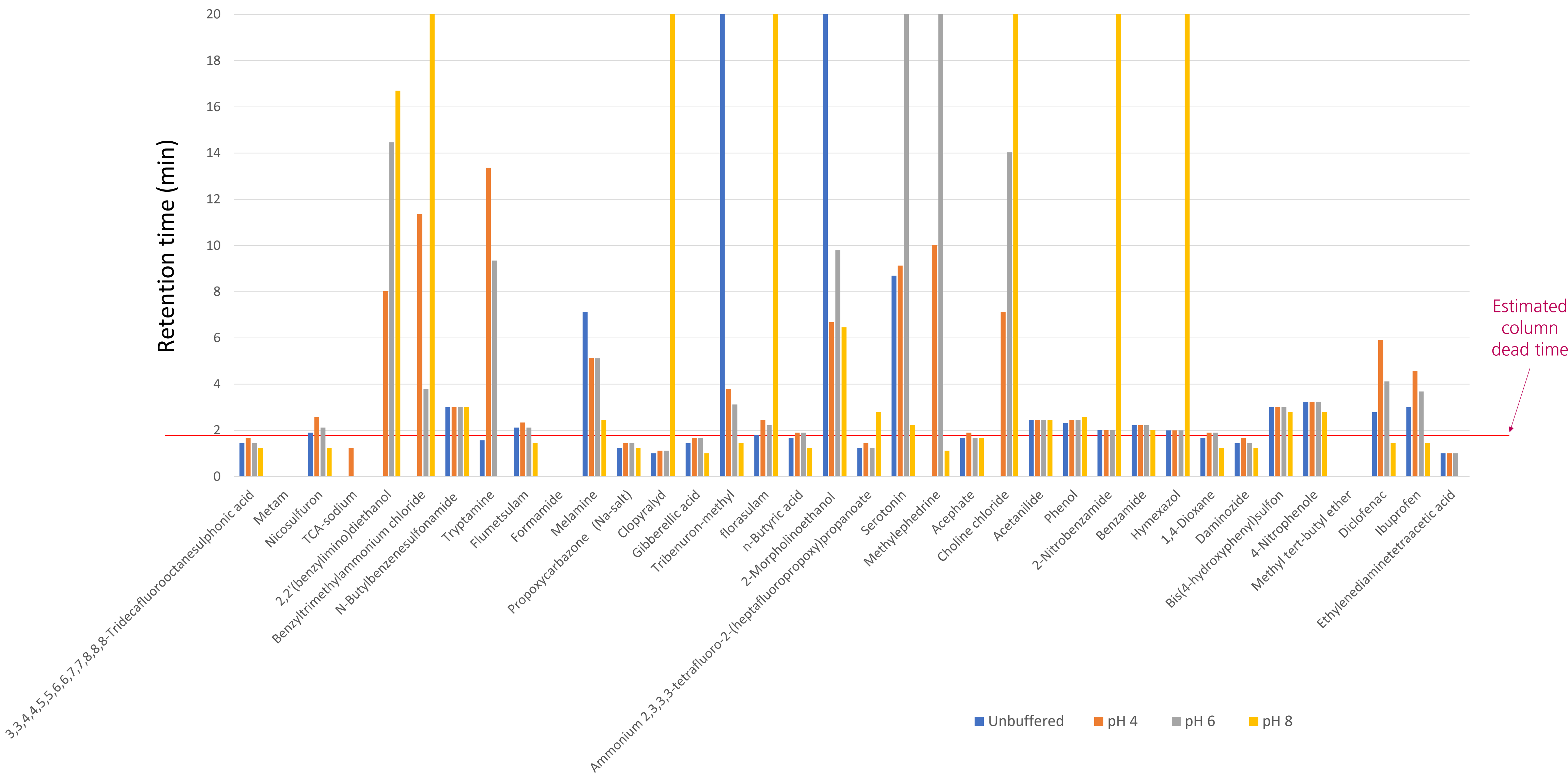


Figure 2: Retention time (R_t) in min on the WCX column at different pH with 60:40 eluent composition.

The evaluation is ongoing, but at least some substances show considerable retention on the cationic mixed phase HPLC-columns. The results demonstrate the expected pH dependency for many substances.

Outlook

- Testing of another set of 25 to 40 substances is planned.
- Detailed evaluation of the results will be performed, and connections made with related projects (e.g. CEFIC LRI ECO 62).
- Further discussion will take place at an expert workshop later in 2025 (if you are interested in attending please email steph.jones@environment-agency.gov.uk)

Acknowledgement

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References

[1] Environment Agency (2025). A review of the applicability of the screening test for soil adsorption potential, and recommendations for expansion. Environment Agency, Bristol, England.

