The Effect and Research of Environmental Analysis Software in Environmental Early Warning under the Background of Big Data

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Abstract. Enrichment of Pesticide Organic pollutants in Surface Water by solid Phase extraction, Analysis and characterization by Gas Chromatography - Mass Spectrometry and Total screening Software, semi-quantitative. At the same time, the semi-quantitative results were verified by SIM mode of gas chromatography - mass spectrometry. The results show that the recovery rate of acids, alcohols and ketones in water meets the requirements of monitoring index. The verification results show that, this screening method is based on the absence of external standard materials and targets. Can be used for early warning monitoring of most potential pesticide organic pollutants in water.

1. Introduction

In recent years, with the implementation of the national infrastructure for monitoring and early warning of rivers and lakes, the early warning ability of surface water environmental quality in China is greatly improved. But with the development of social economy, new types of organic pollutants are emerging. It is far from meeting the needs of management and scientific research to carry out early warning monitoring according to the 109 indexes required by the “Environmental quality standards for surface water” (GB3838-2002). Therefore, how to effectively early warn the potential organic pollutants in the environment and use the existing monitoring equipment to build an effective early warning network of organic pollutants, has become the focus of environmental protection industry.

This paper makes use of Compound Composer software and its database, through standard curves and retention time information for nearly a thousand compounds stored in its database, using specific method software, to establish a link between the database and the analytical methods currently used, so as to achieve in the absence of standard sample, implementation of specific target compounds semi-quantitative detection \cite{1,2,3}. Due to this kind of method can again in a short period of time, qualitative and semi-quantitative analysis of multiple chemicals, so this kind of screening method is especially suitable for early warning monitoring in the case of unknown pollutants and environmental emergency monitoring \cite{4,5}.

This paper makes use of Compound Composer software and its database, the surface water
environmental samples of typical sections in Heilongjiang Province were monitored. The main pesticides and organic pollutants in the water were screened, and carries on the quantitative calculation and analysis. In order to provide scientific basis for relevant departments to carry out urban water pollution prevention and control work. This article uses commercial software as a tool, Its application in environmental monitoring technology is extended.

2. Experimental part

2.1. Materials and reagents

Concentrated sulfuric acid, Sodium hydroxide, Anhydrous sodium sulfate as analytical purity; p,p’-DDT and n-alkane (C9–C33) are purchased from Beijing Bailingwei Company; Cypermethrin, standard, substance, Fenobucarb, Permethrin, Pirimphos-methyl, Fosthiazate, Parathion, 2-methylnaphthalene, Isopropcorn, Methidathion E.C, Chloroneb, Captan, Ip-Copinol, Dimethametryn, Cycloheptylether, Moli

2.2. Sample collection

The sample was collected in Heilongjiang, the local dry season was selected to collect surface water samples, the sampling amount was 2l, samples were collected and taken back to the laboratory immediately for pretreatment, and blank samples were tested in the control experiment and the recovery indicator standard solution was added. The recovery of the method is calculated.

2.3. Sample pretreatment

Water samples were extracted by solid phase extraction, and the target substance was extracted by C18 spe membrane. The solid phase extraction membranes were leached with 5 ml dichloromethane, 5 ml ethyl acetate and 15 ml pure water respectively. After soaking for 1 minute each time, the water sample is drained through the solid phase extraction tray for 3 minutes. The solid phase extraction plate was eluted with ethyl acetate three times, and the eluent was collected after soaking for 1 min each time. Using ethyl acetate to 1 ml.

2.4. Experimental analysis

2.4.1. Mass spectrum parameters

The sample was determined by GCMS-QP2010 of Jinda company in Japan, and the chromatographic column was DA-5MS (30m × 0.25mm × 0.25µm); the carrier gas is 99.999 % pure helium; the column flow is 40 cm.s⁻¹; the temperature rising program of column temperature box is 50°C (hold for 2 min) to 10°C·min⁻¹ to 300°C (hold for 5 min); inlet temperature: 280°C; detector temperature: 200°C Interface temperature: 290°C; the injection method was no shunt injection and the injection volume was 1 ml. The scanning mode of mass spectrometry is SCAN, and the scanning range is 50 ~ 600 mass-charge ratio (m/z).
2.4.2. Full screening software preparation

There are two ways of screening software qualitative, one is to use gc-ms with spectral library qualitative, the relative retention time of n-alkanes (C9 ~ C33) with the target was used for qualitative analysis. Therefore, the relative retention time of the corresponding compounds in the database needs to be corrected by normal alkane (C9 ~ C33) before the actual sample analysis and testing. The response values of 8 internal standards in the internal standard mixture were confirmed to be within the specified range.

2.5. Quality control and quality assurance

Before the determination of chromatographic column should be aging, to prevent the impact of column loss in the process of determination, use p, p'-DDT to check the pollution level of liner regularly; the tuning parameters required by EPA625 are used to reduce the discrimination effect of mass spectrometry in full scan mode.

The standard recovery of 11 kinds of recovery indicators by solid phase extraction was obtained by adding compounds with known concentration (indicator standard solution) to the sample before the test. According to the data, the recoveries of the other nine compounds were all between 78% and 120%, except for some phenol and alcohol compounds whose recoveries were less than 60%. The results show that the software has good qualitative and quantitative effects. the recovery rate is shown in figure 1.

![Figure 1](image1.png)

Figure 1. The standardized recovery rate of eleven recovery indicators

3. Result and discussion

3.1. Semi-quantitative analysis of real water samples

Using shimadzu company of japan and composite composer software the full scanning total ion current maps of five sections in heilongjiang, including huma, luogucun, heihexia, donggang and fuyuan, were obtained. See figure 2. From the figure, it can be seen that there are more overlapping peaks in each section, indicating the existence of the same pollutants.

![Figure 2](image2.png)

Figure 2. Total ion flow diagram of pesticide compounds
The results of pesticide screening showed that 29 kinds of pesticides were detected, including 14 kinds in Huma section and 14 kinds in Luogu Village section. There were 14 species in Heihe river, 11 species in Jiangdong section and 15 species in Fuyuan section. In general, herbicides and fungicides were detected in all sections.

Table 1. The surface water samples of pesticide screening results

| Number | CAS          | Pesticide                    | Huma (µg•L⁻¹) | Luogu Village (µg•L⁻¹) | Heihe River (µg•L⁻¹) | Tongjiang (µg•L⁻¹) | Fuyuan (µg•L⁻¹) |
|--------|--------------|-------------------------------|---------------|------------------------|---------------------|--------------------|-----------------|
| 1      | 29232-93-7   | Pirimiphos-methyl             | 0.091         | 0.084                  | 0.038               | 0.067              | —               |
| 2      | 3766-81-2    | Fenobucarb                    | 0.041         | 0.063                  | —                   | 0.064              | 0.087           |
| 3      | 71697-59-1   | Theta-Cypermethrin            | —             | —                      | 0.067               | —                  | 0.057           |
| 4      | 52645-53-1   | Permethrin                    | 0.085         | 0.111                  | 0.039               | 0.071              | —               |
| 5      | 98886-44-3   | Fosthiazate                   | 0.036         | —                      | —                   | —                  | 0.039           |
| 6      | 56-38-2      | Parathion                     | 0.124         | 0.069                  | 0.114               | 0.124              | 0.087           |
| 7      | 91-57-6      | 2-Methylphenylalanine         | —             | —                      | —                   | —                  | 0.025           |
| 8      | 2631-40-5    | Isoprocarb                    | —             | 0.036                  | 0.068               | —                  | —               |
| 9      | 950-37-8     | Methidathion                  | 0.091         | —                      | —                   | 0.017              | —               |
| 10     | 2675-77-6    | Demosan                       | 0.119         | 0.109                  | 0.073               | 0.068              | 0.077           |
| 11     | 133-06-2     | Captan                        | —             | 0.096                  | 0.077               | —                  | 0.031           |
| 12     | 26087-47-8   | Iprobenfos                    | —             | 0.029                  | —                   | —                  | 0.024           |
| 13     | 625-28-5     | 3-Methylbutenitrile           | 0.085         | 0.213                  | —                   | —                  | —               |
| 14     | 87818-31-3   | Cinmethylin                   | —             | —                      | 0.088               | 0.041              | 0.154           |
| 15     | 2212-67-1    | Molinate                      | 0.047         | —                      | —                   | —                  | —               |
| 16     | 1114-71-2    | Pebulate                      | 0.051         | —                      | 0.021               | —                  | —               |
| 17     | 74712-19-9   | Bromobutide                   | —             | 0.113                  | —                   | 0.039              | 0.078           |
| 18     | 42609-52-9   | Dydron                        | —             | 0.066                  | 0.079               | 0.102              | —               |
| 19     | 608-31-1     | 2,6-Dichloroaniline           | 0.052         | 0.087                  | —                   | —                  | —               |
| 20     | 122-39-4     | Diphenylamine                 | —             | —                      | —                   | —                  | 0.049           |
| 21     | 98-60-2      | 4-Chlorobenzenesulfonyl chloride | —        | 0.074                  | —                   | —                  | —               |
| 22     | 120-12-7     | Anthracene                    | 0.068         | —                      | 0.023               | —                  | 0.066           |
| 23     | 85-01-8      | Phenanthrene                  | —             | —                      | 0.051               | 0.088              | 0.069           |
| 24     | 132-64-9     | Dibenzofuran                  | —             | —                      | —                   | —                  | 0.013           |
| 25     | 86-73-7      | Fluorene                      | 0.044         | —                      | —                   | —                  | —               |
| 26     | 25321-14-6   | Dintrotoluene                 | —             | —                      | 0.102               | 0.038              | —               |
| 27     | 150-76-5     | 4-Methoxyphenol               | —             | —                      | 0.085               | —                  | —               |
| 28     | 14938-35-3   | 4-Pentylphenol                | —             | 0.044                  | —                   | —                  | 0.072           |
| 29     | 95-16-9      | Benzothiazole                 | 0.111         | —                      | —                   | —                  | —               |

3.2. The level of pesticide pollutants in water samples

The total concentration of pollutants detected in five sections was 1.044 µg•L⁻¹, 1.194 µg•L⁻¹, 0.925 µg•L⁻¹, 0.719 µg•L⁻¹ and 0.955 µg•L⁻¹. The concentration range of 14 kinds of organic compounds detected in huma section is 0.036~0.124 µg•L⁻¹, and the concentration range of 14 kinds of organic compounds detected in luogucun section is 0.029~0.213 µg•L⁻¹, the concentration range of 14 organic compounds was 0.021~0.114 µg•L⁻¹ under heihe river and 11 organic compounds were 0.017~0.124
µg•L⁻¹ at donggang section of tongjiang river, the concentration range of 15 kinds of organic compounds detected in fuyuan section is 0.013~0.154 µg•L⁻¹. The literature shows that the yellow river, herbicides were detected in haihe and liaohe rivers and in the middle and lower reaches of the yellow river. The concentration of pesticides detected in this paper was much lower than that in haihe and liaohe. Anthracene and phenanthrene were detected in high concentrations and frequencies in pahs, which may be related to the combustion of biomass fuel in cruise ships during local tourism development.

The highest concentration of the pesticide compound in the five sections was cycloheptyl ether, which belonged to eucalyptus brain herbicides and inhibited meristem growth. Rice planting can effectively control most grass weeds, such as barnyard grass, duck tongue grass, etc. Japan in the "food residue agricultural chemicals positive list system" in the clear compound may not be detected in imported food and agricultural products. China's commodity inspection authorities have also made fairly strict regulations on the detection of this substance in grain for export, but there is no relevant limit standard in the water environment.

4. Conclusion

Compound composer software database can be used to screen pesticide compounds in water quickly and efficiently. A total of 29 pesticides were detected in five monitoring sections in Heilongjiang province. Semi-quantitative results showed that most of the detected pesticides were pesticides and fungicides, although the concentration was not high. But the situation of pesticide pollution in water body needs urgent attention.

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