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Application News

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Spectrophotometric Analysis

Introduction of a Search System for Contaminants in Tap Water

Various contaminants, both organic and inorganic, can be present in tap water. It is therefore necessary to identify not only contaminants that are organic, but also those that are inorganic in nature. Without information on both of these types of contaminants, adequate determination is not possible. Here, we present the determination of organic and inorganic contaminants in tap water using both infrared spectroscopy (FTIR) for analysis of organic substances, and X-ray fluorescence analysis (EDX) for inorganic elements.
This paper presents the analysis of these two types of contaminants in tap water and introduces how a tap water contaminant search system can be utilized for identification of the substances.

Contaminants Found in Tap Water

Contaminants due to foreign matter in tap water can originate from a variety of sources, including the tap water system materials themselves, minerals, and microorganisms. In particular, major sources of contamination include rubber and metallic components from seals that have degraded due to aging of the water supply equipment. These types of contaminants should be quickly identified to allay the concerns of users.
A combination of FTIR and EDX analysis can effectively provide useful information for elucidating the identity of a foreign substance. FTIR analysis can be used to identify organic compounds and some inorganic compounds, while EDX analysis can be used to obtain qualitative and quantitative information for such substances as iron rust and scale (calcium and magnesium deposits), which are difficult to identify from infrared spectra. In addition, this approach is effective in narrowing down and identifying the possible contaminant candidates when seals contain the same principal components (organic substances) but different additives. Another strong advantage is that the sample need only be about 1 mm in size for analysis by either FTIR or EDX.

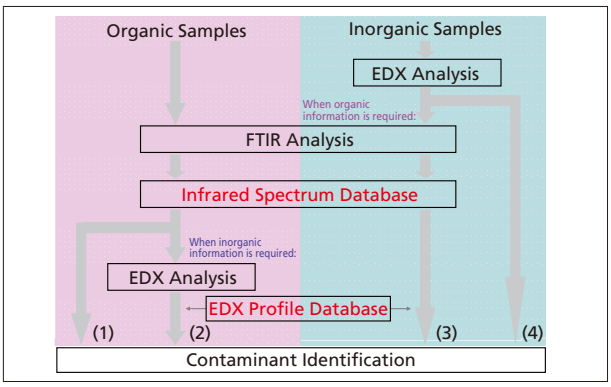


Fig. 1 Procedure of Contaminant Analysis by Tap Water Contaminant Search System

The Features of Tap Water Contaminant Search System

The tap water contaminant search system comprises two databases, an infrared spectrum database and an EDX profile database. The infrared spectrum database includes the infrared spectra of contaminants collected from tap water, in addition to the infrared spectra of commercially available tap water system maintenance parts. Since searches are conducted using a database created from actual contaminants found in tap water, the search suitability rate is quite good. In addition to qualitative results, the color, shape, hardness, presence or absence of metallic luster, and measurement technique pertaining to the contaminant materials are also recorded in the database. Furthermore, the elemental information obtained from EDX analysis results is also stored in this database, thereby permitting details to be viewed using the EDX profile database. In addition to the qualitative and quantitative information, the EDX profile database also includes photographs of the samples.
The procedure for identifying contaminants using the tap water contaminant search system is shown in Fig. 1. This sequence is used for analysis regardless of the category of the system where the contaminant was discovered. Here, we used the flow chart scheme to analyze contaminants in tap water.

Analysis of Organic Material

First, observation of contaminant A that was detected in tap water revealed a lusterless, black-colored material, suggesting that it was an organic substance. In the case of organic contaminants, following the procedure for "Organic Samples" shown in Fig. 1, FTIR analysis was conducted first. Contaminants found in tap water are typically visible, so it is simple to conduct measurement using a single reflection ATR accessory.
The analytical conditions are shown in Table 1, and a photograph of the instrument used is shown in Fig. 2. The search results obtained using the infrared spectrum database are shown in Fig. 3. From this, it is clear that components of the spectrum of the contaminant matches well to a "Discharge pipe packing" (principal component is SBS).

Table 1 Instrument and Analytical Conditions

Instrument	: IRAffinity-1, MIRacle10 Ge, Diamond
Resolution	: 4.0 cm^{-1}
Accumulation	: 40
Apodization	: Happ-Genzel
Detector	: DLATGS

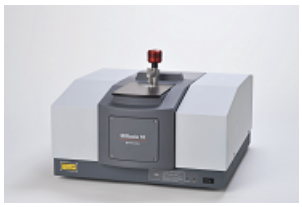
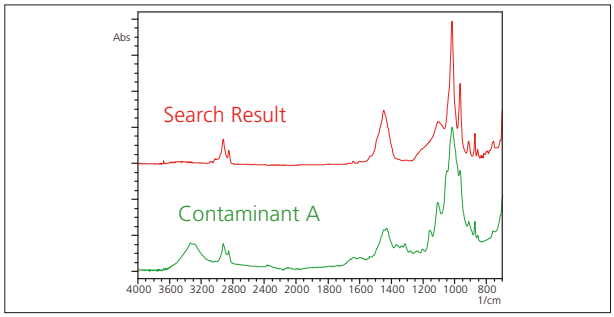


Fig. 2 Photograph of IRAffinity-1 with MIRacle 10 ATR Accessory Attached



Details of infrared spectrum database search result:
"Discharge pipe 32 packing_Gray_Inside"
Materials: Styrene butadiene styrene (SBS),Calcium carbonate ($CaCO_3$), Magnesium silicate (TALC, $3Mg_4SiO_2H_2O$)
Major elements: Cl, Ca, Si, Mg, S, Zn, Ti
Color: Gray Shape: Resin/Ring-shaped Hardness: Soft
Metallic luster: No Technique: ATR (Diamond)

Fig. 3 Infrared Spectra and Search Results for Contaminant A

Next, as indicated in procedure (2) of Fig. 1, EDX analysis was conducted to obtain element information, and the "Discharge pipe packing " determined in the FTIR analysis result was matched against the EDX profile database. The profile used for matching is shown in Fig. 4. Primarily, the elements Ca, Si, and Mg were clearly detected. These results clearly support the presence of calcium carbonate and magnesium silicate (talc), as shown in details of infrared spectrum database search result-Fig.3.
Here, when the main component is an organic substance (in this case SBS) as identified in a search of the infrared spectra, the quantitative results obtained from the EDX profile database are calculated using the FP method.

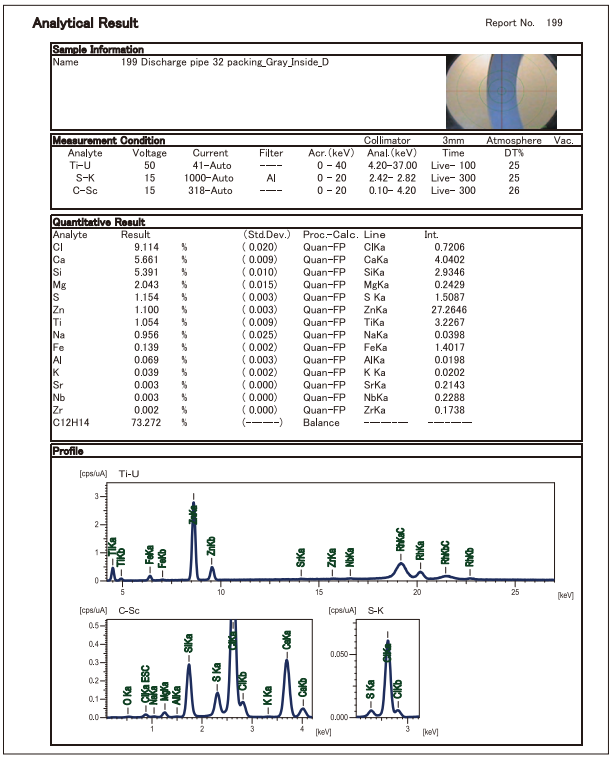


Fig. 4 Qualitative and Quantitative Results for "Drain Fitting Seal" by EDX

Analysis of Inorganic Materials

Next, observation of contaminant B in tap water revealed a powder sample with metallic luster, suggesting that contaminant B was an inorganic material. Inorganic contaminants are first analyzed by EDX, as indicted in the procedure of Fig. 1 for Inorganic Samples.
The analytical conditions are shown in Table 2, and a photograph of the instrument used is shown in Fig. 5. The EDX analysis results are shown in Fig. 6. The principal component of this contaminant was detected as Fe, and is assumed to consist of iron rust based on the quantitative results.
In addition, contaminant B was measured by the FTIR single reflection ATR method, and the infrared spectrum database was used to conduct a search, as outlined in procedure (3) of Fig. 1. The infrared spectrum search results are shown in Fig. 7. These results indicated a similarity of the contaminant to iron rust. Also, this similarity is supported by the "Iron Rust_3" hit in the FTIR search result using the EDX profile database.
This analysis shows that tap water contaminants can be identified more accurately using the EDX profile database together with the infrared spectrum database.

Table 2 Instrument and Analytical Conditions

Instrument	: EDX-800HS
X-Ray Tube	: Rh target
Filter	: #1 (for Cl)
Tube Voltage	: 15 [kV] (C - Sc), 50 [kV] (Ti - U)
Tube Current	: Auto
Atmosphere	: Vacuum
Measurement Diameter	: 1 [mmϕ]
Measurement Time	: 100 [sec] (Ti-U), 300 [sec] (C-Sc), 300 [sec] (Cl)
Dead Time	: Max 25 [%]

Fig. 5 Photograph of EDX-800HS Energy Dispersive X-Ray Fluorescence Spectrometer

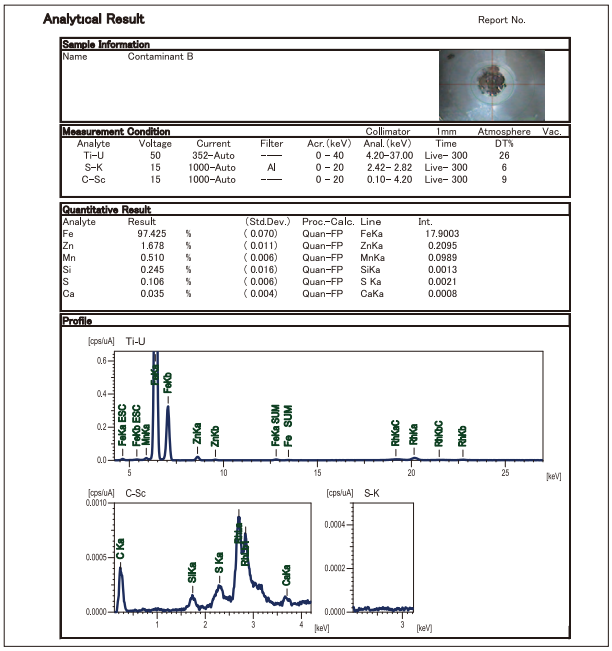
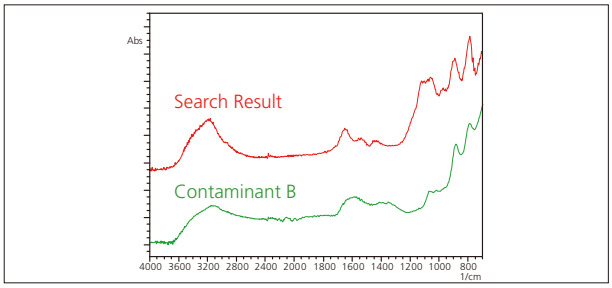


Fig. 6 Qualitative and Quantitative Results for Contaminant B by EDX



Details of infrared spectrum database search result: "Iron rust_3"
Materials: Iron (Ⅲ) oxide hydroxide($Fe(OH)_3$) Major elements: Fe, S, Si, P
Color: Yellow Shape: Sand-shaped Hardness: Soft Metallic luster: No
Technique: ATR(Ge)

Fig. 7 Infrared Spectra and Search Results for Contaminant B

Conclusion

Here, we introduced a tap water contaminant search system using FTIR analysis and EDX analysis. Even when a commercially available product is provided with information about materials that are included, information related to additives is often not known, making it difficult to identify such materials as rubber and plastics.
However, the infrared spectrum database prepared here includes qualitative information related not only to principal components but also to additives, in addition to elemental information detected by EDX. Also included is a sample database containing information collected from actual contaminants, as well as cross-section and surface measurements of seals, which have a relatively high detection rate in tap water. Thus, this system can be utilized as a contaminant analysis tool not only for tap water-related utilities, but across a wide range of fields, such as environmental (including contract analysis), petrochemical, and food fields.

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