

Analysis of emerging contaminants in environmental systems

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22c. Applications of emerging geochemical and isotopic analytical techniques for integrated water resource management and environmental monitoring

Innovative mass spectrometry techniques make it possible to detect emerging contaminants, including pharmaceutical compounds and explosives, at concentrations that are environmentally relevant. Applications of these techniques are challenging because of the very low concentrations of these compounds and because of the complex matrices often encountered in the environment. Sample collection methods and analytical procedures must be refined to provide representative samples and analyses that can be used to assess the potential impacts of emerging contaminants.

Two case studies are used to illustrate steps required for the application of tandem mass spectrometry techniques. These studies involved refinement of sample collection techniques, analyte separation methods, analyte quantification, and modifications of instrument configurations.

A large nation-wide survey of explosives was conducted which initially involved the application of HPLC-MS/MS methods. The HPLC-MS/MS technique required inclusion of several isotope-labelled internal standards at multiple concentrations. Modification of the analytical procedure to an IC-MS/MS procedure resulted in decreased matrix suppression effects and improved analyte quantification. These modifications were particularly important for the analysis of groundwater and saline waters.

On-site wastewater disposal systems represent one of the largest volumes of contaminated water discharged to the subsurface. This wastewater contains elevated concentrations of dissolved organic matter, and nitrogen and phosphorus species. Interaction of this water with natural aquifer materials also can result in the presence of elevated concentrations of dissolved metals. The quantification of trace pharmaceutical compounds within this setting requires consideration of sample acquisition methods, sampling equipment materials, the interaction of these materials with the target compounds, and sample matrix effects. Analyses of a suite of pharmaceutical compounds in the low ng L⁻¹ were made for samples collected from wastewater discharge areas, groundwater and DOC-rich surface water. These studies required diligent use of isotope-labelled internal standards to optimize analytical results. Based on these results, mechanisms controlling transport of these compounds can be better delineated.

Early Earth: an insight from the combined Os-Nd-Hf isotope systematics of Barberton komatiites

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We report ¹⁹⁰Pt-¹⁸⁶Os, ¹⁸⁷Re-¹⁸⁷Os, ^{146,147}Sm-^{142,143}Nd, and ¹⁷⁶Lu-¹⁷⁶Hf isotopic, trace lithophile, and highly siderophile element (HSE) abundance data for remarkably well preserved komatiites from the Komati and Weltevreden Formations of the Barberton Greenstone Belt (BGB). These data provide new insights into the chemical evolution of the early Earth. The 3.48 Ga Komati lavas are mildly depleted in LREE and Th and show strong depletions in HREE, whereas the 3.26 Ga Weltevreden lavas are strongly depleted in LREE and Th and are enriched in HREE; both systems show positive Nb and Ta anomalies. The two komatiite systems are characterized by initial $\gamma^{187}\text{Os}$ of $+0.34\pm 0.10$ and -0.14 ± 0.03 and $\epsilon^{143}\text{Nd}$ of $+0.30\pm 0.13$ and $+0.41\pm 0.11$, respectively ($2\sigma_{\text{mean}}$), indicating evolution of their sources with time-integrated near-chondritic Re/Os and slightly suprachondritic ¹⁴⁷Sm/¹⁴⁴Nd. The initial $\epsilon^{142}\text{Nd}$ in both systems are not resolvable from that in the terrestrial standard. At the same time, these systems have radiogenic initial $\epsilon^{176}\text{Hf}$ of $+1.9\pm 0.3$ and $+4.7\pm 0.8$, respectively, implying long-term evolution to the times of melting with suprachondritic ¹⁷⁶Lu/¹⁷⁷Hf. The Weltevreden system is also characterized by an initial ¹⁸⁶Os/¹⁸⁸Os of $+0.22\pm 0.03$, indicating evolution of its source with a time-integrated suprachondritic Pt/Os (3.3 ± 0.2 vs. 1.8 in chondrites). Finally, the sources of the two komatiite systems are calculated to have had distinct absolute HSE abundances, containing ~50% (Komati) and ~80% (Weltevreden) of the total HSE estimated for the modern Primitive Mantle. The combined data require early formation and long-term isolation of deep mantle domains enriched in majorite and/or perovskite; these domains served as the melting source regions for the BGB lavas. The isolation must have occurred after ¹⁴⁶Sm was no longer extant, but before the mantle accumulated the full complement of the HSE as a result of the late accretion. Our combined data also require deep-sourced formation for the BGB komatiites, most probably *via* dry melting in starting mantle plumes. The potential mantle temperatures calculated from the emplaced lava compositions are in excess of 1800°C, thus providing evidence for extremely hot conditions that existed in the early Archean mantle.