Peering into the Shadows of Chemical Space.
Emerging Contaminants and Environmental Science: Is either being served by the other?

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A decade has passed since the term “emerging” was first formally used to describe the existence of water pollutants not previously recognized; a 1998 NRC workshop ("Identifying Future Drinking Water Contaminants") and several 1999 reports by USGS were among the first to feature the term "emerging contaminants." In the larger historical context, however, the issue of emerging contaminants evolved from concerns regarding unregulated trace organic pollutants, a topic of interest to the U.S. EPA beginning in the 1970s (e.g., see Donaldson, doi:10.1021/es60127a012).

This marks an excellent time to reflect on a number of questions surrounding this rather ill-defined but broadly used term. In describing various aspects of environmental science, has its use served us well? Is it leading us where we need to be in terms of a scientific discipline? What message does it convey to the public, legislators, and regulators? Do we share a common understanding as to what an "emerging" contaminant might be? Are we perhaps suffering from its overuse? Used as a modifier for a bewildering array of phenomena and activities,"emerging" and some of its allies such as "nano" have become frequently used in environmental science - - perhaps sometimes serving merely as obligatory but token adjectives adding little value.

The published literature on emerging contaminants began to escalate in 2001-2003 and became a bona-fide topic of active investigation and discussion in 2003-2005; the numbers of publications now total several thousand - - possibly obeying Moore's Law for exponential growth. Such a rapidly expanding literature challenges its in-depth examination even by experts, forcing narrower specialization and less synthesis of the field as a whole. Distilling the published literature into a useful body of knowledge is a daunting challenge, which unmet greatly increases the risk of duplication of work or failure to focus on the highest priority needs. Two recent but rare examples of valuable data mining and synthesis are the compilations of occurrence and waste treatment data for pharmaceuticals and personal care products by Miège et al. (doi:10.1016/j.envpol.2008.11.045) and Onesios et al. (doi:10.1007/s10532-008-9237-8).

In environmental science, the term "emerging" is often applied not just to chemical contaminants, but to any part of the risk paradigm continuum, spanning from stressor to exposure to effects. But is the term overused? It's certainly one whose banner is frequently raised in many fields of study - - from politics and economics to math, ecology, and epidemiology. In particular, emerging has a long-established, strong connotation associated with pathogens and infectious diseases - - long institutionalized at the CDC and FDA. Extended to environmental chemistry, does it faithfully convey our intended message - - whatever that might be? In current practice, is the term perhaps becoming misleading, given that it can pertain to issues that have persisted for quite some time but have simply eluded attention? In practice, but a small fraction of cases involve truly new issues that are just now developing. In its current usage, how do emerging contaminants differ from the universe of unregulated contaminants? After all, with millions of distinct, commercially available chemicals now inventoried by the CAS Registry (but fewer than 30 million), untold numbers have the potential to eventually come to our attention as contaminants, especially since the majority of all chemicals in any sample can evade current detection or identification methods. A large portion of potential chemical stressors lurk in hiding, ineligible to yet be termed emerging.

Regardless of whether we deem chemicals to have emerged, they can indeed be "revealed," largely as a result of the application of ever-more advanced methods of analysis, allowing us to peer into the shadows of chemical space with ever-greater magnification and clarity. Often asked is whether we are blindly following analytical chemists - - the Pied Pipers of ever-lower detection levels; Moore's Law might also apply to detection limits - - as these limits have been driven inexorably downward - - from the ppm range to ppb to ppt, and now ppq. Is there a genuine need to know as much as possible about minute concentrations? The need for ever-lower levels of detection is partly driven by the revelation of previously unrecognized subtle effects at exposure levels below purported no-effects levels (e.g., see De Lange et al. doi:10.1016/j.aquatox.2006.03.002) and by the properties that allow certain chemicals to bioaccumulate. At a certain exposure level, however, it may no longer be possible to deconvolute the occurrence of what might seem to be an induced effect in a certain population from its incidence as ambient (natural) background. And ever-lower detection limits pose increasingly greater challenges for assessing, communicating, and ameliorating ever-diminishing risks.

A certain irony haunts the research surrounding emerging chemicals - - those that could not be previously detected because they hid in the shadows of detection limits or because we did not know to look for them. Has an obsessive focus been cultivated on the targeted monitoring of chemicals selected primarily on the basis of the positive results of prior studies? From this can be borne highly biased data sets, populated predominantly by self-selected analytes - - all of which are distinguished from the universe of largely ignored chemicals solely by their amenability to analysis. Is greater emphasis needed on nontarget analysis and identification of unknowns? This could expand the known exposure universe and possibly highlight tomorrow's emerging contaminants before their presence grows.

Can selected representative contaminants (perhaps based on calculated properties) serve as surrogate proxies for the presence of many others? Other than serving to spotlight the fact that anthropogenic activities are closely connected with the environment, perhaps one of the most important outcomes of emerging chemicals research has been the focus applied to the challenge of understanding low-level long-term exposure to multiple chemical stressors. Given the countless potential chemical stressors to which any organism can be exposed (encompassing both anthropogenic and natural origins), questions immediately emerge regarding the long-established chemical-by-chemical approach to regulation. Is it sustainable, or will a paradigm shift be required to facilitate a more holistic approach to risk assessment, given the vast universe of chemicals for which monitoring has never been performed and for which toxicity studies do not exist? Should consideration be given to integrating biologically based detection methods (e.g., bioassays that translate to toxic endpoints) with instrument-based methods, using both to iteratively guide or direct the other - - moving beyond assay-directed sample fractionation and chemical identification to regulations based on biological endpoints (which serve to integrate the response from multitudes of stressors)?

Regardless of how "emerging" might be defined - or alternatives concocted - some key attributes might be critical to capture for a working framework. First, should the term impart clear meaning for the public and regulators while also facilitating the advancement of science in directions most useful to society? Second, how might progress be assessed with regard to emerging contaminants? Should today's emerging contaminants also be tomorrow's? Many chemicals still referred to as emerging are now well established as ubiquitous environmental pollutants. Is it useful to continue calling these "emerging," especially since they undoubtedly had an environmental presence long before their first detection? To continue referring to contaminants with well-established presence as emerging poses the eventuality of numerous unregulated contaminants all labeled with the same less-than helpful appellation. However the term might be defined, would a clear articulation of when a chemical has graduated from the domain of "emerging" be useful?

The current paradigm for emerging contaminant research still reflects a reactive (retrospective) approach to environmental protection. How might a truly proactive (prospective) system be designed - - one that could provide advance warning of new chemical stressors? Measure of such a program's success might be in eliminating the need for the term "emerging." A useful framework might ensure ready identification of “surprise” or "stealth" chemicals - - those newly revealed but whose occurrence is unexpected or could not have been anticipated or predicted by modeling or expert knowledge. For these, environmental monitoring could play a key role in revealing them. A standardized approach for prioritizing and evaluating newly revealed contaminants for regulatory consideration could be useful. To efficiently implement an emerging-chemicals framework, a fundamental need might be a central repository for all data derived from monitoring and effects studies; an important data quality objective would be to prevent further corruption of the published literature by ensuring that the structures of unknowns purportedly identified are appropriately verified (based upon defined quality objectives) or tagged as tentative. In the final analysis, however, a major objective of a chemocentric society focused on principles of sustainability and stewardship - - one that prevents new chemical stressors from reaching detectable or toxicologically meaningful levels in the environment - - might be to relegate "emerging" contaminants to the past.

NOTICE: Although this work was reviewed by EPA and approved for publication, it may not necessarily reflect official Agency policy.

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