Trends in Chemistry

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Big Questions in Chemistry

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Beyond Reductionist Thinking in Chemistry for Sustainability

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Great breakthroughs in chemistry over the past two centuries have been accomplished largely through reductionist methods. However, the incredible sustainability challenges that we face as a civilization are systems challenges, requiring careful combination of knowledge gained from reductionist approaches with integrative-systems thinking to inform designs for a sustainable future.

Beyond Reductionism Toward Integrative-Systems Thinking

There exists a seemingly insurmountable challenge of pursuing improved design for sustainability in complex systems using the traditional reductionist approach; that is, finding sufficient simplifications to describe complex systems [1]. While reductionism has resulted in tremendous advances across many sectors, this approach has also brought about significant and deleterious unintended consequences. These consequences are perhaps most evident in human health and the environment where the singular (reductionist) focus on function or efficiency has resulted in the disruption of the climate system, the use of depleting feedstocks, the generation of hazardous waste streams, and the commercialization of products with undesirable bioactivity and ecotoxicity. There are numerous examples with some the most egregious: for example, the horrific chemical disaster of Bhopal, India; the tragic birth defects from thalidomide; and the sinking millions of shallow tube wells into arsenic-laced groundwater for Bangladeshi drinking water supplies.

While the aforementioned examples are mainly historic, we continue to apply this reductionist framework to address the current sustainability challenges. That is, new solutions are implemented with the necessary but incomplete knowledge generated through the reductionist framework. When the scientific community mobilizes collectively to protect the environment and human health – to do the right things – we have too often found that we are doing the right things wrong. Several contemporary examples include:

- Disinfecting our water supply from pathogens that kill millions of people every year using acutely lethal substances that create disinfection ‘byproducts’ that are persistent, toxic, and often carcinogenic.
- Facilitating greater crop production to improve available food supplies using fertilizers that contaminate drinking water and lead to eutrophication, as well as persistent, toxic pesticides that damage biodiversity and ecosystem function.
- Replacing bisphenol A (BPA; a plasticizer with significant data and public concern about its role as an endocrine disruptor) with bisphenol S (BPS) because it was functionally equivalent and ‘not BPA’, although recent studies have identified similar toxicological concerns [2].
- Developing life-saving drugs that increase both quality and length of life by using pharmaceuticals that contaminate our drinking water supply to biologically active levels.
- Developing photovoltaics to capture the power of the sun to move toward more renewable fuels while relying on toxic, depleting, and/or rare/scarce metals.
- Pursuing biofuels that reduce reliance on fossil carbon but in the first incarnation compete with food, feed, and land use options.

While the knowledge gained from the reductionist approach is critical, it is incomplete. We must combine this knowledge with integrative-systems thinking to inform future designs for a sustainable future (Figure 1). For example, knowledge of the functional performance of a molecule is a minimal requirement. However, we must also understand the potential hazards of the molecule. Ideally, we would know what properties or structures dictate the functional performance and potential hazards. This knowledge of property–function and property–hazard must then be used to inform enhanced design of future solutions where performance includes not only function and cost but also environmental, social, and human health considerations. To be successful in this approach, we must combine knowledge from the reductionist framework with insight from integrative-systems thinking to realize intentional design for sustainability. This is the intention behind the ‘Twelve Principles of Green Chemistry’ [3]. The following represent foundational criteria toward the design of the right things right.

Design for Inherency

Functional performance and cost are often the exclusive considerations in design. As such, the inherent ability to cause adverse consequence to humans and the environment is often overlooked. Green Chemistry Principle 4 states that chemical products should be designed to preserve efficacy of function while reducing or eliminating hazard. In recent years, this has been the focus of extensive research to elucidate not only the elements that contribute to molecular and material toxicity but also inform design guidelines such that the next generation of molecules and materials are inherently less hazardous. Although designing molecules and materials from first principles to have predictable biological activity is still viewed as an immense challenge (e.g., efforts in pharmaceutical and pesticide design), the intersection of recent

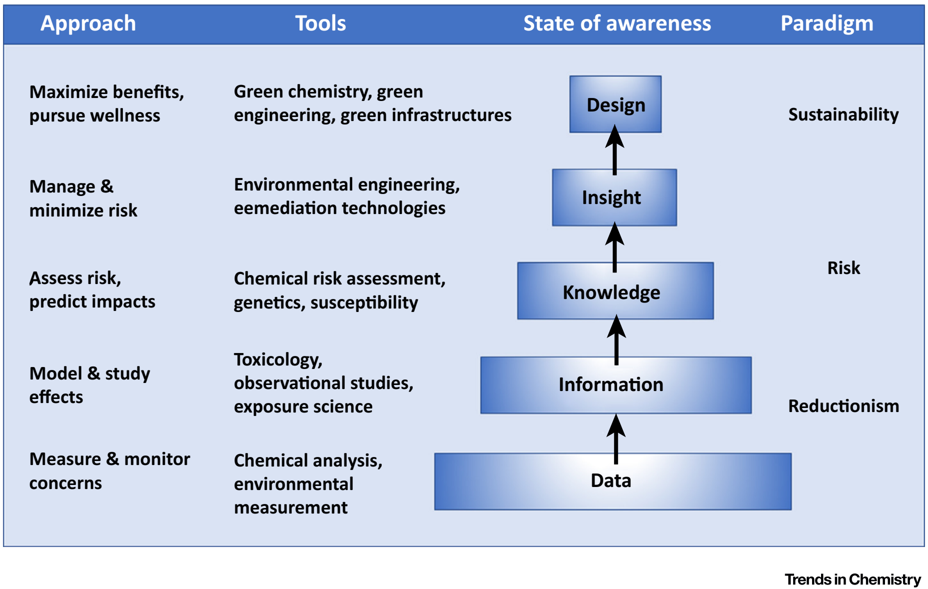

Figure 1. Expanding the Data–Information–Knowledge–Wisdom Hierarchy (or Pyramid) to Realize Design as the Pinnacle. Adapted, with permission, from [14].

advances in mechanistic toxicology and computational chemistry provides the foundation necessary to identify the essential desirable properties for minimizing adverse biological effects. Significant contributions have been made to advance rational design of safer chemicals [4] as demonstrated by the first set of property-based guidelines for distinguishing toxic chemicals from those in general commerce [5–7]. These important efforts in the development of safer molecules and materials must 'preserve efficacy of function'.

Design for Life Cycle

Life-cycle thinking endorses a holistic perspective where a design is evaluated from the acquisition of feedstocks through transforming the feedstocks to use and end of life. Considering the entire life cycle is vitally important because different impacts (i.e., energy use, carbon emissions, water use, eutrophication, waste generation, and toxicity) can occur at different life stages. For example, some materials may have adverse impacts when they are extracted or processed, but may be relatively benign in use and easy to recycle. However, other designs will have the majority of their impacts during the use phase. With this knowledge, enhanced designs can be pursued to minimize 'hot spots' or to understand the consequences of implementing a new design *a priori*. Further, and potentially more importantly, life-cycle thinking will minimize the possibility of shifting impacts from one life-cycle stage to another by considering the entire system.

Design for Function

Nobody ever 'bought' a chemical. Instead, it is the function or service of that chemical that is actually being purchased. Setting functional performance goals rather than specifying a solution enables the most degrees of design freedom for innovation to realize sustainable solutions. In this way, life-cycle benefits can be realized by meeting functional requirements, possibly with the ideal solution of not having to deliver a physical product at all. In the same way the lotus flower demonstrates self-cleaning properties through microscopic and nanoscopic architecture, the functional performance of water repellency (hydrophobicity) can be realized without using the chemical intensity of traditional man-made systems. This encourages innovation in novel 'solution' space that would not be realized by incrementally improving existing designs or realizing acceptability by controlling the circumstances under which the design is used.

Design for a Dynamic World

While we have designed systems with fixed operating conditions assuming that our world is static, virtually all reviews of the state of our environment [8,9] reveal that we are living in a dynamic world; that there is exponential change in human impacts at the global scale ranging from population to carbon dioxide emissions to water and fertilizer consumption in this time deemed the 'Anthropocene' [10]. The stressors and impacts of this 'dynamic world' have come to suggest that there is a need to expand our design considerations to acknowledge that the conditions in which the design will function over its lifetime will exist in a world of rapid and increasing change. Our designs must be dynamic as well. As such, functional performance cannot be evaluated merely at the outset with resource- and energy-intensive efforts to slow the decline over time. Enhancing performance over the lifetime of the system will require the system to have the ability to adapt and evolve, to demonstrate emergent properties, and to maintain resilient performance.

Design for Resiliency

Achieving sustainability will arguably require the development of resilient engineered systems that mirror the dynamic attributes of ecological systems. Resilience can be defined as the capacity of a system to tolerate disturbances while retaining its structure and function [11], and has emerged as a critical characteristic of complex, dynamic systems in a range of disciplines including economics, ecology, pedology, psychology, sociology, risk management, and network theory [12]. Engineering research has emphasized resilience as recovery from perturbations, but ecological resilience also emphasizes adaptive capacity, which may lead to new equilibria [13]. Resilient systems are able to survive, adapt, and grow in the face of uncertainty and unforeseen disruptions, particularly relevant given the 'dynamic world' discussion earlier. While resiliency tends to increase if a system has diversity, redundancy, efficiency, autonomy, adaptability, cohesion, and strength in its critical components, a rigorous definition is difficult to find and system parameters that can be used as design specifications remain even more elusive.

The Path Forward

We can no longer deny that the unintended consequences that society is enduring are due partly to the way that we, as chemists, have pursued our craft, focusing on knowledge generated in a reductionist-only framework. 'Unintended' is not the same as unknown or unknowable. Knowledge is not the same as insight or wisdom informing improved future design. As Einstein said, 'The right to search for truth implies also a duty; one must not conceal any part of what one has recognized to be true.' If we recognize that the knowledge we are imparting is limited – and that those limitations have consequences – then are we fulfilling our duty? If the knowledge is precisely right for the reduced system but generally wrong for the integrated one, are we honoring what Einstein called our 'right'?

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