JETIR.ORG ISSN: 2349-5162 | ESTD Year : 2014 | Monthly Issue
JOURNAL OF EMERGING TECHNOLOGIES AND INNOVATIVE RESEARCH (JETIR)
An International Scholarly Open Access, Peer-reviewed, Refereed Journal

Future of the Chemical Sciences: Role of Chemists and the Landscape

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Abstract

These trends are changing the nature of chemistry as a discipline, the role of chemists and the landscape within which we work. The future of the chemical sciences is unclear. Our current response to changes may no longer be adequate. It is essential for organizations to look ahead, anticipate future developments and adapt to stay relevant. The Royal Society of Chemistry wanted to understand how the chemical sciences may evolve to improve the everyday lives of people in the next ten to twenty years. So in spring 2015 we launched the multi-stage Future of the Chemical Sciences initiative, involving leaders from across the chemical sciences.

We used scenario planning as a methodology to understand uncertainty and challenge conventional thinking. Scenario planning is based on the understanding that many factors can influence the future context. These different factors can interact and combine in complex and unpredictable ways to create surprising outcomes. These can be shifts that directly impact the immediate environment, for example the automatisation of chemical processes, or in developments in the wider context, such as an ageing population or changes in societal values. First, we identified seven key themes. We then considered how these themes might evolve and interact to create unexpected situations and challenges. In this way, we developed four plausible but unexpected scenarios for chemistry ten to twenty years from now. These scenarios are not designed to predict the future, make a case for a preferred outcome, or offer an exhaustive list of possibilities. Rather, they are tools to challenge assumptions and prompt strategic conversations about the future.

The aim of planning for the future is to transform the turbulent environment into one which can be managed. Strategic scenario planning has a unique role in this regard by considering multiple outcomes. Understanding how existing trends may develop and interact can help organizations manage and monitor

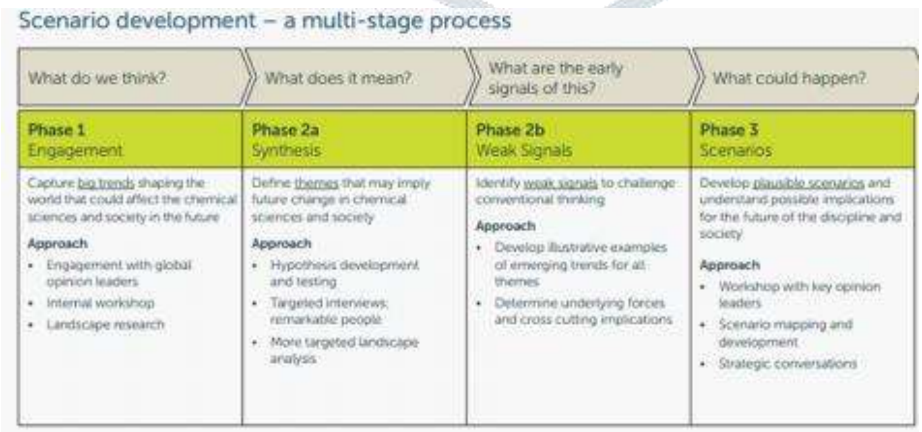
risk and make flexible long-term plans for the future. We hope this report, and our four scenarios, will stimulate dialogue within our field about how best to prepare for an uncertain future, so that we can shape the future of the chemical sciences for the benefit of people around the world.

Key words: *Trends are changing the nature of chemistry as a discipline, the role of chemists and the landscape within which we work.*

Introduction:

Future of the Chemical Sciences initiative brought together leading chemistry minds from around the world. Together, we challenged and tested emerging trends in the chemical sciences and beyond. Engaging thought leaders We engaged with thought leaders in the chemical sciences from industry, government and academia to gain insights into big trends that are shaping our field and the wider environment. These insights were complemented by comprehensive landscape research and analysis. Defining future themes of change in chemical sciences and society Based on our initial findings, we developed hypotheses and conducted targeted interviews with key leaders in our field, as well as further analysis of the landscape in which chemical scientists operate. This enabled us to identify seven key themes that may influence the future of the chemical sciences.

Developing plausible scenarios Following the research on themes and the associated weak signals, we held three workshops (two in London, UK and one in Boston, USA) to develop scenarios for the future of the chemical sciences. The workshops were attended by leading thinkers from academia, government and industry. Building on the seven themes, each group debated the drivers, consequences and likelihood of future changes. We developed four plausible but unexpected scenarios as a result of these discussions.



Based on our interviews with key stakeholders, landscape research and further focused-dialogue with the community, we identified seven major themes that may drive change in the chemical sciences. Three of these trends may directly impact the chemical sciences: Role of chemical sciences, Demand for chemical sciences, Funding structures, institutions and education

This is a world where chemists have become increasingly less influential and productive, and other disciplines have taken the lead on discovery. The pace of change in the past ten to twenty years was so fast that chemists did not have time to reinvent themselves. Advances in artificial intelligence have replaced many traditional jobs and creativity has not been embedded in the education of the next generation of chemists. The id entity of chemistry as a distinct discipline has disappeared and has emerged as part of other cross discipline subjects, such as the molecular sciences.

The critical mass of chemists is dispersed into sub- groups. These sub-groups nurture specific parts of chemistry. Some sub-groups produce lots of research, while others are neglected. There are overlaps between the chemistry research topics in different sub-groups. The general public does not understand what chemistry is and has no awareness of the impact that the discipline has made on the world. Celebrity biologists and physicists have attracted non-scientists to these fields, but there is no equivalent popular following for chemistry. Chemistry is still taught in schools, but most students choose to pursue their studies in areas that appear to be making more exciting discoveries and developments.

The role of chemical sciences

Chemistry may need to be increasingly interdisciplinary, which will result in opportunities for innovation. There is likely to be a shift from blue-skies to problem-driven research. There is a risk of chemistry turning into a "follower" discipline in discovery. Increasing interaction between chemistry and other sciences, most notably the biological sciences, but also fields such as mathematics, engineering, and computer and materials sciences, was identified as the single most important theme for the chemical sciences over the next ten to twenty years. It is recognized that, over the last two decades, innovation has most often arisen at the boundaries of traditional subjects.

Interdisciplinary is essential for tackling major challenges and driving new approaches to research. Advances in carbon capture and photovoltaic will involve further collaboration between chemistry and engineering, for example, while silicon technology is an exciting area at the interface of chemistry and technology. Engagement with arts and social science subjects may also play a role in changing attitudes to design and consumption, with implications for future manufacturing processes and use of natural resources. There is a shift from blue-skies to problem-driven research. Although already an important focus over the past decade, there is a sense that the future challenges posed by interdisciplinary must be addressed with greater urgency if chemistry is to remain an influential subject. The perception is that chemistry might turn into a "follower" discipline, whilst other sciences lead on discoveries. This implied threat demands changes in curricula, funding, culture and perhaps even the definition of the subject.

Chemistry for impact:

The chemical sciences will likely be increasingly required to solve challenges in health, energy and climate change, water and food production. Chemistry might have a greater role in biochemistry and the pharmaceutical industry, as well as in the maintenance and development of infrastructure. The world faces major challenges that demand a response from chemistry. Partnerships are needed between countries, disciplines - including social sciences - and the public and private sectors. There are a number of areas where there is likely to be an increased demand for chemistry.

Advances in personalized medicine, mutational drugs, sequencing, vaccines to deal with global health issues and treatments linked to an ageing population are important developments where chemistry will play a role. Chemistry is also expected to play a key role in tackling major challenges associated with energy and climate change, particularly in green solutions to generate and store energy. Carbon capture, renewable, energy storage, recycling (in materials and processes) and battery technology are research areas that will grow in importance in the future.

In the next ten to twenty years, the current infrastructure of the chemical industries could be unfit for purpose and, more widely, infrastructure may be degrading. Chemists can play an important role in developing processes and products to repair, replace and protect future equipment. They will be able to contribute through producing more durable and sustainable materials, for example.

The further development of the "Internet of Things" (IoT) is expected to affect local services, healthcare, communications and commerce. The IoT could make a difference in managing challenges linked to dense urban populations. There are opportunities for chemistry, for example, in the development and maintenance of sensors for air quality and safe sustainable lighting. For some of our participants, the role of chemistry in these sectors, and in interdisciplinary teams, is not yet well understood by the wider public, policymakers, funders and even some members of the chemistry community itself.

Here's what some of the leading figures from the chemical science community had to say… "There will be pressure on chemists to supply the chemistry to address the serious problems facing humanity, particularly with climate change, more efficient ways of producing materials, chemicals for the rising population, as well as the more obvious health related issues. [To address this] there will be a focus on chemists being part of interdisciplinary teams working to address problems around the world." "I have some sympathy with the idea that chemistry needs to redefine itself, but this is an evolution not a revolution. In all areas [of the discussion], I could cite examples where change is already happening. It's really about shifting the centres of gravity. At the same time, we're probably all agreed that the organic, inorganic, physical split is less and less relevant."

Efficiency and innovation:

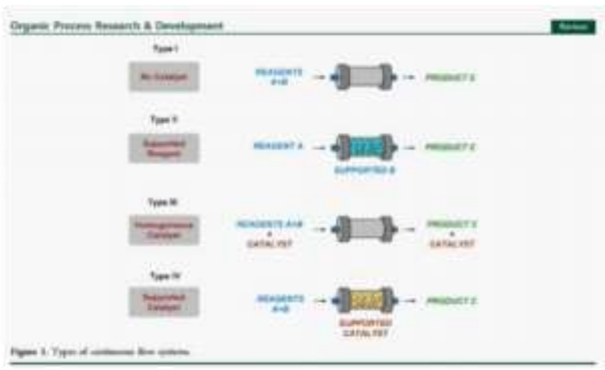
Advances in technology and the rapid adoption of innovation have far-reaching implications for the future of the chemical sciences. The nature of chemistry research, organisational forms and chemistry careers are likely to change. Technology is likely to drive radical improvements in efficiency, processes, computational modelling and metrology. This is likely to further impel interdisciplinary working and change the nature of research, the character of academic and professional careers, organisational forms and industrial structures. For example, there may be more start-ups, specialists and niche players. Experimentation is expected to become radically more efficient. This will impact research, who is able to conduct this work and the necessary infrastructure.

Computational developments, combined with advances in real -time and high -through put experimentation, may radically reduce the time required for modelling and to "get stuff out of the lab". Approaches to research on organic synthesis, general catalytic chemistry and testing the physical properties of models will see changes, and chemists are expected to become even more focused on thermodynamics.

The production of "molecules on demand" may follow, although this development probably sits beyond our ten to twenty year time horizon. Chemists may be able to produce models on demand for specific clients and to develop a product without extensive testing. New technologies are likely to enable an increasingly diverse audience to identify problems and take part remotely in experiments to develop solutions.

Flow Chemistry: Recent Developments in the Synthesis of Pharmaceutical Products

Recently, application of the flow technologies for the preparation of fine chemicals, such as natural products or Active Pharmaceutical Ingredients (APIs), has become very popular, especially in academia. Although pharma industry still relies on multipurpose batch or semibatch reactors, it is evident that interest is arising toward continuous flow manufacturing of organic molecules, including highly functionalized and chiral compounds.



This combination could allow the development of fully automated process with an increased efficiency and, in many cases, improved sustainability. It has been also demonstrated that a safer manufacturing of organic intermediates and APIs could be obtained under continuous flow conditions, where some synthetic steps that were not permitted for safety reasons can be performed with minimum risk.

In this review we focused our attention only on very recent advances in the continuous flow multistep synthesis of organic molecules which found application as APIs, especially highlighting the contributions described in the literature from 2013 to 2015, including very recent examples not reported in any published review. Without claiming to be complete, we will give a general overview of different approaches, technologies, and synthetic strategies used so far, thus hoping to contribute to minimize the gap between academic research and pharmaceutical manufacturing.

A general outlook about a quite young and relatively unexplored field of research, like stereo selective organ catalysis under flow conditions, will be also presented, and most significant examples will be described; our purpose is to illustrate all of the potentialities of continuous flow organ catalysis and offer a starting point to develop new methodologies for the synthesis of chiral drugs. Finally, some considerations on the perspectives and the possible, expected developments in the field are briefly discussed.

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