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New Chemistry: Solutions for the 21st Century

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Abstract

Chemistry's linear model has led to incredible innovations, but also to unintended consequences, and contributed to the challenges we face in the 21st century. The environmental costs of traditional chemistry methods are being addressed by the Green Chemistry movement. Green Chemistry does not address the societal impacts of chemistry. It is in this absence that the evolution of chemistry continues and there is a need for chemists to ask: what does it mean to be chemists, members of society, and human? In response to these questions, a humanistic approach is taken and addressing the key components needed to help chemists rise to the challenges in the new era of chemistry. *New Chemistry* is a guide to allow society and chemists to prosper and grow sustainably, by acknowledging the human element and finding ways to cooperate with it rather than control it. New Chemistry. Twelve principles have been developed in this research that should be integrated at the undergraduate level thus, inspire the next generation of scientist, leaders, and innovators to be more than just chemist, and create a profitable industry, a sustainable environment, and ethical society. New Chemistry seeks the answers to new classes of problems, such as meta-information on the cell, climate instability, and dissipative systems.

Keywords: Sustainable Science, Undergraduate Curriculum, Chemistry Education

1. Introduction

The last century witnessed the increasing role that chemistry plays in society through its significant advancements. Global raw chemical sales reached over three billion (euros) in 2014, and over a trillion dollars in sales in pharmaceuticals alone.^{1,2} In America, almost a quarter of the population lives within a one-mile radius of an American Chemistry Council (ACC) or Societal of Chemical Manufacturing Affiliates (SCMA) facility, and it is estimated that nearly six million American jobs and over a quarter of the Gross Domestic Product (GDP) is tied to the developments in chemistry.^{3,4} There is major dependence on chemistry in our modern world, but this dependence cannot be sustained if the science itself is not sustainable. The industrial sector's standard focus has been on highyielding products, not the processes used to make them. This is due to the way chemistry is taught and practiced, which embraces a strictly utilitarian methodology.⁵ This limitation in our analysis has considerably contributed to our modern challenges of ozone depletion, climate change, ocean acidification, toxic waste, public health, limited resources, and increased use of nonrenewable energy. The awareness of these limitations provoked the urgency to adopt new practices and principles such as Green Chemistry as a way to practice high-level chemical experimentation without acting unsustainably.⁵ Green Chemistry has been an active catalyst in chemical innovation and has created awareness of the need for change, and begun to resolve some of the environmental issues that resulted from industrial practices, but a truly sustainable system consists of the interdependent relationship between economics, environmental, and social factors.^{6,39} The establishment of such social values in addition to Green Chemistry training is a more complete solution to the myriad of complex challenges humanity faces in the twenty-

first century.^{7,37}

New Chemistry proposes a comprehensive change in the way we think, teach, and learn about chemistry in order to fully address all three aspects of a truly sustainable science. New Chemistry harnesses Green Chemistry and systems thinking as its basis to develop a larger understanding of how we do chemistry, and it further expands by directly addressing the societal obligations and implications that must be faced.^{6,7} New Chemistry employs education about toxicology to demonstrate to future scientists facts about environmental persistence and the acute and chronic health issues related to our current known reagents, solvents, and products.^{5,6,36} New Chemistry seeks to eliminate chemical waste and phase out the use of unsustainable energy. In addition to obvious reasons of sustainability, an analysis of how we power our facilities, and the amount of energy used, needs to be transparent and accountable. Another dimension of New Chemistry is that, instead of focusing on accumulating massive quantities of information and not processing it, New Chemistry strives to educate students on efficient ways to use such vast amounts of data and apply them. Properly managing resources in a sustainable way is a concept that applies to chemical processes, and not just to solvents and reagents, beakers, and test tubes.^{5,39} Instead of teaching that product creation exists solely to satisfy the consumer demand for a product, and to create more profits, New Chemistry teaches that product creation stems from our obligation to solve the problems of society and humanity in general, and encompasses a new way of thinking about profits for the private sector: the triple bottom line of profit.^{6,8} Instead of focusing solely on profit in the monetary sense, New Chemistry also recognizes and accounts for the interim and perpetual profits and losses of products and services, both socially and environmentally. The undergraduate chemistry curriculum, not only educates future chemists but non-chemistry majors, as chemistry courses are required for all undergraduate curricula. Therefore the integration of New Chemistry introduces prospective CEOs, policymakers, and investors to the need for widely a adopted, safe, accountable, and ultimately beneficial science.^{5,6,36} Integration allows chemistry graduates to be uniquely suited to manage future challenges, and begin to expand the types of problems that chemistry can solve. Problems such as understanding dissipative systems (oceans, atmospheres, metabolism), creating rational drug design, and managing information and monitoring complex systems like public health and megacities. 5,7,9

Physicists Thomas Kuhn has argued that science has experienced paradigm shifts, a change in ways of thinking and the innate structure and framework.⁴⁰ For example, in the 19th century, the field of science became more complex and began to splinter into its current divisions.²² The organization and methodology of this era, such as publication of findings and works, are key components in the contemporary field of chemistry.^{7,22} During this era, there was a change in how the public perceived science and scientific authority was established. Although impactful, a relatively small amount of scientific developments were made. It was not until the World Wars that chemistry was called into play to help gain an upper hand in what seemed like a never-ending stalemate. Creating the chemicals and atrocities against humanity in the context of war, our mindset allowed us to accept irrevocable harm as a part of obtaining "just" ends. This mindset remained throughout the 20th century, affecting the drivers of the three pillars of chemistry advancement: academia, industry, and government.

The traditional triad of academia, industry, and government all began as individual silos with different drivers. Academia's driver of knowledge or intellectual capital has been one that has stimulated new ideas and theories that have proven to be beneficial in real world applications. Industry's goal of profits and developing markets have driven the consumer market to what it is today and has accumulated substantial wealth. Government's driver establishes missions for the betterment of society and institutes multidisciplinary collaborations to achieve such goals.^{10,11} This triad started in the 1900s with industry building the first research and development (R&D) laboratory, General Electric, in Schenectady New York.¹¹ Post WWII, industry and government began to collaborate, which led to the expansion of R&D facilities such as DuPont's Experimental Station, IBM's Watson Research Center, and AT&T's Bell Laboratories. Also, major government research facilities were established under the Department of Energy (DOE), the National Institute of Health (NIH), the National Science Foundation (NSF), and National Aeronautics and Space Administration (NASA).^{10,11} However, the established Western or laissez-faire model (Figure 1A) pits industry as the dominant focus and government and academia only as minor support.¹² When economic pressures rose in the late 1970's, this resulted in an almost complete collapse of industrial R&D facilities.¹¹ The modern balanced model (Figure 1B) creates an equal contribution among the three entities, distributes research responsibilities, and creates overlapping collaborative research among industry, government, and academia.10,12



Figure 1. A: Laissez-faire model established in the 20th century. B: Contemporary balanced model proposed by the Triple Helix Group at Stanford University.¹² The latter represents an equalized collaborative between the three major entities of research and development.

The change in industry, government, and academia's relationship is still in its adjustment period, and some sectors have progressed faster in their change than others. Both the government and the industrial sector have begun to create changes to their practices. In 2015 the chemical industrial giant, Dow Chemical Company, set new unprecedented 2025 sustainability targets including a 20% reduction in waste, two new products that will offset up to three times their carbon dioxide footprint within the product life, and created a business plan addressing and minimizing the company's impact on nature that is projected to save over a billion dollars.¹³ The director of the Green Chemistry Institute, David Constable, notes that even though there has been dramatic change when it comes to sustainability in industry and government, "the major research universities are not just blasé about it, they are actually ferociously antagonistic".¹⁷ If our learning and understanding have changed, then why are those who train and prepare our future scientist so hesitant to change as well?

In recent years, chemists began to ask questions about the established approach to chemistry, and if some of the current practices are still beneficial and relevant. These inquiries have led to significant changes in industry, yet the majority of academia remains stagnant in curriculum progression. With the growing integration of Green Chemistry and engineering in industry, objective measurements of progress such as metrics have become vital. While metrics are beneficial tools, Paul Anastas' talk at the 2015 Green Chemistry and Engineering Conference highlighted the lingering issue of "preventing getting stuck in a metric driven loop."¹⁸ This loop often blinds people from the bigger picture, much like industry's focus on percent yield of the past century.

To better understand the history of the field of chemistry as well as current issues facing the field, a thorough literature review was conducted.²¹ In addition; the field of Green Chemistry was researched, as my study builds upon some of the key areas of sustainability that it does not address. My main research questions were:

- How can we make chemistry more sustainable, both for undergraduates studying and practicing chemistry, and for the larger chemistry industry?
- What key components are foundational to develop sustainable chemistry practices?

In response to these driving questions, a framework was developed that can begin to address critical components required to help all chemistry students rise to the challenges in the new era of chemistry, and this framework recognized 12 fundamental principles of the New Chemistry.

2. The Principles

Analysis of the need for sustainability in the field of chemistry, and re-imagining the field of chemistry has resulted in the development of 12 principles of New Chemistry, explained in this section. Figure 2 demonstrates the interconnected relationships between the 12 principles of New Chemistry.

2.1 Think Systemically

In all stages, from the development of ideas to the finished goods, an insight of where the products and byproducts fit into the total system and their subsequent impacts are needed. Traditionally, the linear based problem-solving accesses challenges by focusing on isolated components. Today when encompassing a systems view, it is not enough to only identify the current components, but it is also necessary to successfully identify new or emerging components in order to understand their relationships and impacts. Systems thinking helps increase competitiveness while supporting more efficient, effective and sustainable practices as the needs of humanity evolve.¹⁰

2.2 Develop And Deepen Communications

Communication is with society, most of whom are not experts, and with other scientists, both those intellectually familiar and unfamiliar with the topic. The form of communication can be oral and/or written. These may be one-on-one encounters, broad audiences, a variety of written forms (journal article, book, report, notes), and the use of social media. Of note is the recent development of Open Access and Open Notebook. It is important to know one's audience, and in most cases it is important for the communication to result in receiving constructive feedback – telling, and listening. Scientists have an obligation to provide scientific information and also to share the thinking that is involved. This is important for decision makers with political, economic, and social agendas. Misinformation is to be avoided and addressed. The challenge is communicating something that is most complicated in a way that is truthful and understandable.

2.3 Reshape The Use Of Information

We need to transform our use of information from knowing to learning, and answering to understanding. Often the use of memorization requires little thinking and bypasses the real conceptual learning. It is the connections and associations of information that is important. As scientists we need to know how to analyze, collect, classify, utilize, store, retrieve, disseminate, and protect information. Communications need to be accurate, complete, and objective with scientific information. The challenge is to understand the problem, know what information is needed, where to obtain that information, and how to best use the information.

2.4 Realize Diversity

Socially responsible solutions that chemists create cannot be fully realized without the input, perspective, and concerns of all individuals in a society. To better create a more diverse scientific field, chemists should not only increase the number of underrepresented minorities in the field, but chemists must also welcome and understand the diversity of the ideas and perceptions of the individuals, rather than create a field of homogenized ideas or perpetuated methodologies. It is important to support diverse mindsets that, due to experiences, environment, and interests, can create a myriad of solutions and even new questions to explore.

2.5 Incorporate Green Chemistry

Always seek to incorporate the 12 Principles of Green Chemistry into chemical education and design, as these principles successfully address many environmental and economic challenges chemists face. True sustainability consists of the interdependent relationship between economic, environmental, and social factors.

2.6 Develop Timeless Products

What is a timeless product, if not sheer innovation? A timeless product is something that we can easily take for granted but is necessary to heighten our awareness of the absurdities of the current system. A timeless product must be environmentally, economically, and socially just. To create a timeless product, one must envision not only something new but something that simplifies complexity, is influenced by the diverse ideas that are present in a society, is accountable to the environment in which it is present, and fuels future solutions by exploring humankind's curiosity.

2.7 Use Design Thinking

Designing new chemical products and processes is more than providing a problem solving approach, but provides long-term solutions through the combination of analysis and imagination. A major component is sustainable design, which incorporates full life cycle, elimination of waste, and environmental impact evaluations. Included in design thinking is using a combination of logic, imagination, intuition, and systems reasoning. Design thinking addresses the human interaction dimension with the designed products and also establishes a process of listening, designing, and delivering.

2.8 Be Social Stewards

Society and chemistry are irrevocably intertwined and therefore the public needs and requires the chemical community's products, activities, and vision to reflect responsible leadership and to be attuned to society's needs.

2.9 Engage In Ethics

Academic chemistry departments, along with industry and government, are responsible for ethics being fully integrated into their respective communities. Academic communities should provide students with a full understanding of ethical reasoning and processing. Throughout the chemistry community, well-defined policies and guidelines should be established, which are widely communicated and supported. It is not only "what can chemists do," but also more importantly, "what should they do." While it is important for chemistry to provide needed materials and solve many of society's challenges, it is most important that the total system is understood in both near-term implications, and also what may happen in the future. The chemistry community has the responsibility of intentional consideration and infusion of ethics in every step of chemistry, which will show that they have earned the public's trust, credibility, and accountability.

2.10 Monitor And Review With Metrics

The primary metric that has been used in chemistry for a chemical reaction has been the product yield, but now for a much broader understanding of the impacts of chemicals and their reactions on the environment and society, more meaningful assessments are necessary. Metrics that have been developed recently include: Reaction Mass Efficiency (RME), Atomic Economy (AE), E-Factor (E), Process Mass Intensity (RMI), and Carbon Efficiency (CE).^{6,39} Each of these has a different emphasis as related to waste, energy usage, toxicity, economic costs, environmental impact, and other factors. No one of these metrics is favored in New Chemistry, and other metrics will be developed in the future. One or more metrics should be used in comparing different chemical reactions, based on the defined objective for a particular chemical product. Also to be taken into consideration are various quantitative and qualitative metrics, which includes Life Cycle Analysis (LCA) and EcoScale.³⁹

2.11 Cultivate Curiosity

Curiosity-driven research is synonymous with basic/fundamental research, but it is also important in the discovery of chemicals for the use by humans. Breakthroughs in chemistry are often the result of curiosity.

2.12 Advocate For Accountability

An action that is not being monitored still has consequences, and the validity of the tools we use to report current figures, findings, and ideas is proportional to the number of participants. Supporting and practicing accountability and transparency creates an environment where information is shared and widely available.



Figure 2. New Chemistry Principles and their overlapping integration.

3. Discussion

Through the literature review, as well as discussions among leaders in many disciplines at the university, and among the emerging sustainability leaders, I have identified the 12 principles of New Chemistry. Embraced at the undergraduate level, these principles give a greater understanding of the bigger picture, sustainability, and chemistry's role in the new century. Further in-depth explanation of a few principles are provided in this section.

3.1 Incorporate Green Chemistry

The integration of Green Chemistry in the undergraduate curriculum is quintessential to changing chemistry as we know it. Education and understanding of the Green Chemistry principles is a base through which environmental and economic challenges are successfully being addressed. John Warner and Paul Anastas's novel approach to chemistry addresses toxic waste production, synthesis efficiency, and safer reagents and solvents, while focusing on the environmental and economic costs of chemistry.¹⁹ Green Chemistry's compliment, Green Engineering, focuses on product design and strives for the elimination of waste, over-dependence on toxic product sources, and an increase in material and energy efficiency from beginning to end of the product life.²⁰

The 1997 integration of the Green Chemistry Institute (GCI) into the American Chemical Society (ACS) has been the root of stimulating the resounding response to Green Chemistry and Engineering in the industrial world.⁵ Pharmaceutical companies such as Eli Lilly and Pfizer have embraced Green Chemistry since the early 2000s and have called for a "Green Chemistry Round Table" that includes the input of industry leaders and the experts at the American Chemical Society to develop greener synthesis of pharmaceuticals.^{5,38} This has led to the creation of greener, more efficient synthesis such as the proposed benign K60 silica as a catalyst for amide bond formation.¹⁴ Traditionally, amide binding required the use of inefficient reagents like carbodiimides and phosphonium uranium salts, which in turn led to unnecessary toxic by-products.¹⁵ Successful improvements on synthesis processes like this have given rise to similar roundtables for formulators, chemical manufacturers, and hydraulic fracturing businesses.³⁸ Government-sponsored initiatives such as the Presidential Green Chemistry Challenge Awards (PGCCA) have resulted in the elimination of over 800 million pounds of toxic chemicals and solvents, 7.8 billion pounds of carbon dioxide, and 21 billion gallons of water annually in the United States.¹⁶

Teaching Green Chemistry principles to undergraduate students, and applying them to undergraduate laboratories, will provide the tools to create more economical and environmentally safe syntheses. These principles

address the need to integrate and expand knowledge of bioavailability, kinetics/dynamics, and activity relationship in order to allow for the greatest number of design options and to reduce risk by addressing the intrinsic hazards of chemical schemes.^{5,6,36}

3.2 Think Systemically

The outlook of industry is changing from the antiquated industrial model to a complete systems review of the industrial process. From the mid-20th century to present, industry has adapted to understand that the consumer side of production can be an influential power in determining what goods are to be produced, or to gain pressure on how they are produced.^{39,10} Risk analysis has become a key element in the chemical industry.⁶ Shown in Figure 3, the current system of production is only pushed by the resource input and only pulled by the consumption (bottom line profit).¹⁰



Figure 3. The linear production and consumption model of the industrial age, 1950-present.¹⁰

The proposed, evolving new industrial model focuses not only on what is going on in the immediate areas of industry but looks at the entirety of the system. As demonstrated in Figure 4, industry is now progressing towards including waste, social systems, and ecological systems to push and pull production.¹⁰ It also embraces analysis of the individual parts and their reciprocal effects upon each other.¹⁰ The adaptations of Green Chemistry in industry address economic and ecological factors. Further training and awareness of the full system at the undergraduate level will enable future scientists to innately and intentionally incorporate cyclic logic into their practices.



Figure 4. The systems model of industrial production. Ecological and social systems are integrated and are considered regenerative resources.¹⁰

3.3 Cultivate Curiosity

Curiosity is fundamental to the use and further development of chemistry and drives us to learn the whys and the hows of the chemical universe that enable us to gain knowledge and understand chemistry. The intuitive dimension of learning is necessary in the curiosity approach.²³ Fundamental advances in chemistry result from basic research, or sometimes noted as curiosity-driven research.⁷ Without this form of experimentation, applied research (production of improved products) would be stymied.

The cornerstones of the scientific world were not thought of and then sought, but rather were byproducts of curiosity. Targeted research seeks to find the answer, rather than ask the question.²⁴ More often than not, pursuing curiosity, questions are asked that lead to unimagined answers. For example, Rosenberg's research on the potential effects of electric fields on cell division led to the discovery of an important cancer drug; Kendall's work on the hormones of the adrenal gland led to an anti-inflammatory substance; Bloch and Purcell's fundamental work in the absorption of radio frequency by atomic nuclei in a magnetic field led to MRI, and the discovery of the laser - initially a laboratory curiosity - is used in such diverse applications as the reattachment of a detached retina and the reading of barcodes in supermarkets.²⁴

The products of fundamental research are often not instantaneous, but are drawn out over decades, like the 10 years for Nylon, or even 80 years in the case of liquid crystals.²⁴ Whitesides notes that basic research is used to gain knowledge, and that gaining knowledge is almost inevitably linked to applied "problem solving" research.⁷ In recent years, Staudinger's century-old curiosity-driven research helped create the new field of Bioorthogonal chemistry that studies chemical processes solely *in vivo*, in order to create better pharmaceutical therapeutics.²⁵ Though, being a curious individual is not enough, rather the entire culture of education and research must recognize the immediate and non-immediate value of curiosity. Once this environment is cultivated, the effects of increasing fundamental research can reach decades and maybe even centuries into the future.

3.4 Realize Diversity

The word diversity can conjure many meanings. One prevailing sense of diversity is the physical manifestation. It is no secret that science has struggled with creating more inclusion in the field among female, Hispanic and African American populations. The numbers show the discrepancy. Hispanics and African Americans made up a total of 12% in the U.S. science and engineering workforce in 2010, whereas they comprise a total of 28% in the general work-age population (ages 18-64).²⁸ Women are more than half (50.4%) of the general work-force population, yet only 28% are represented in science and engineering.²⁸

One well-meaning attempt to address this issue is by funding, such as the 1.5 million GlaxoSmithKline grant to UNC Asheville that was announced in 2016, and more notoriously the numerous multi-million dollar NSF grants and government initiatives over the past few decades. Even with these efforts, the numbers of under-represented groups in science have not changed significantly.^{26,27} Diversity is not just physical characteristics, rather diversity is different perspectives, expectations, types of creativity and intelligence. Without this awareness, those whose mindsets are different from the traditional European scientific mindset may either assimilate, adding to the homogeneity, or are discouraged to leave or not even attempt to enter the sciences. The expectation of one cultural dominance in science is what led to the almost century-long delay in international recognition of the discovery of the fifth taste, Umami, and glutamates such as mono-sodium glutamate (MSG), in 1908 by Japanese scientist Ikdea.^{29,30}

To fully realize our best science, we must address the core issue of diversity. The issue is the conventional rigid construct of what constitutes a "good" chemist. This construct needs to bend and flex to appreciate the different talents, interest and mindsets that must be achieved for science to create comprehensive resolutions.

One example of limiting diversity can be through teaching to only one or two types of intelligence, as explained through Howard Gardner's theory of multiple intelligences. This theory breaks from the traditional education that only recognizes verbal-linguistic and logical-mathematical skills, and offers six other types of intelligences through which people learn and problem solve.³¹ These types of intelligences include musical, visual/spatial, bodily/kinesthetic, interpersonal, intrapersonal, and naturalistic.³¹ In a recent study of school children, students who demonstrated preferences for kinesthetic, logical-mathematical, visual-spatial and naturalistic intelligences, demonstrated strongest science problem-solving and processing skills. The highest correlation with scientific learning was between kinesthetic and visual-spatial intelligences.³² Inclusion of all the diverse types of intelligence in the sciences can further learning for all students and improve their attitudes about the sciences, and possibly increase success in further science education beyond high school and at the undergraduate level.^{33,34}

4. Conclusion

When beginning this research, the large strides in altering chemical practices were evident in industry and government, yet the outlook of changing the status quo in chemistry education seemed dismal. When change was introduced to academia, the primary target was graduate schools, leaving the undergraduate curriculum neglected. However, after presenting at the 2015 Green Chemistry & Engineering conference, the probability of change at the undergraduate level is more hopeful, due to developments such as the ACS GCI's development in 2016 of a Green Chemistry education roadmap vision and core competencies.³⁵

The idea of change is taking hold, but in order for chemistry to truly evolve into a more sustainable science, we must include more than just Green Chemistry education. The drivers in the field of chemistry must consider human, technological, and environmental aspects. The 12 principles of New Chemistry are fundamental ideas that attempt to address all three aspects (human, technology, and environment). Integration at the undergraduate level is vital, as the effects of science practices will resonate for generations, proliferating throughout the field of chemistry. As of now the 12 principles of New Chemistry are just words, and in order to be proven viable, these words must be implemented in practice. The next steps in the research include identifying the necessary steps to apply these principles widely in undergraduate chemistry courses and laboratories.

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