## II. BACKGROUND

## A. Role of Chemistry in Society

Applications of chemical science have contributed significantly to the advancement of human civilization (1, 2, 3). With a growing understanding and ability to manipulate chemical molecules, the post-World War II chemist was considered a societal problem solver. They synthesized crop-enhancing agricultural chemicals to ensure a constant and viable food supply. They played a significant role in the eradication of deadly diseases by developing life-saving pharmaceuticals and chemical pesticides. Chemists also developed innovative plastics and synthetic fibers for use in a both industrial and consumer products (1, 2, 3).

The chemical industry has been a vital sector of the modern industrialized economy (2, 3). The chemical and allied manufacturing sectors in the United States employ over two million individuals. This accounts for approximately 11% of our nations manufacturing and industrial workers (4). The chemical manufacturing sector of the U.S. economy has maintained a positive foreign trade balance for the past several decades (3). Table 1 lists the high technology industries based on chemical science.

**TABLE 1: High-Technology Industries Based on Chemistry Science (3)**

| ***CHEMICALS*** | ***MATERIALS*** |
|---|---|
| **agricultural chemicals** | **ceramics** |
| **electronic reagents** | **glass** |
| **paints and solvents** | **metals and alloys** |
| **petrochemical feedstocks** | **paper** |
| **pharmaceuticals** | **plastics and rubbers** |
| **soaps and detergents** | **synthetic fibers** |

In 1994, the EPA estimated that between 60,000 and 70,000 different chemicals were used commercially in the United States (1). That same year, U.S. chemical manufacturers alone produced 729 billion pounds of the 50 most highly used industrial chemicals for global markets (1, 4).

## B. Chemistry and the Environment

In the past scientists concerned themselves with solving visible societal problems, such as easing poverty and disease, traveling faster, and making our lives more convenient (2). The environment was considered a source of natural resources which should be exploited to fuel societal development (6). Chemistry was viewed as a scientific tool which could harness natural resources to enhance our lives in these ways. This attitude was reflected by the following marketing slogan used by DuPont Chemical Company prior to 1970: "Better things for better living . . . through chemistry" (6). Unfortunately, in providing solutions to our immediate societal needs, scientists sometimes created more complex problems with large scale impacts (6, 7).

The production, processing, and use of chemicals in modern society has been accompanied by global-scale environmental pollution, natural resource depletion, and health impacts (8). In some cases the implications of such impacts were masked due to a superficial scientific understanding of and inability to measure the fate, transport, and toxicity of chemicals in the environment (9). Concerns regarding the safety of a chemical product were potentially addressed in terms of immediate and / or microscale impacts. However, long-term and / or global impacts of chemical use on environment and health were not necessarily of significant concern to scientists, regulators, and the public (9).

The depletion of the stratospheric ozone layer by chlorofluorocarbon chemicals (CFCs) and the bioaccumulation of chlorinated organic pesticides in the food chain demonstrate the need for more comprehensive consideration of the potential impacts of chemical use in society.

For almost 50 years CFCs were considered a "benign" class of chemicals due to their low acute toxicity and non-reactive nature (7, 10). Their competitive production cost made them an ideal candidate for numerous industrial and consumer applications, including refrigerants, propellants in aerosol cans, hospital sterilants, industrial solvents, and foam blowing agents (10). Worldwide use of CFCs increased from 400 million pounds in 1960 to 2.5 billion pounds in 1988 (7). In 1974 atmospheric chemists Mario Molina and Sherwood Rowland published data which suggested that CFCs could have a significant role in the depletion of the stratospheric ozone layer. These scientists encountered considerable skepticism from fellow chemists, government regulators, and the general public (8). However, their theory was confirmed in 1987 when other scientists definitively linked the chlorine component of CFC molecules to the destruction of ozone molecules in the stratosphere above Antarctica (7, 10).

Chlorinated hydrocarbon pesticides, such as dichlorodiphenyltrichloroethane (DDT), were first introduced for use in chemical pest management in the 1940s (11). Their effectiveness in eradicating pests and vector-born diseases, such as malaria, typhus, and yellow fever, made these chemicals a panacea for agricultural and public health programs (11, 12). Applications of DDT during World War II were responsible for making this conflict the first in history in which more combatants died from direct effects of war rather than epidemic and endemic diseases (13). In 1962, Rachel Carson published her controversial text, “Silent Spring,” which provided both scientific and anecdotal evidence of the negative effects of bioaccumulation of chlorinated organic chemicals in the food chain. As was the case with CFCs, scientists in government and industry initially discounted the hypothesis of Carson’s book . However, many of her observations were indeed valid. It was later discovered that DDT and other chlorinated organic chemicals bioaccumulate in the fatty tissue of non-target species at the head of the ecological food chain (11).

The development of CFCs and DDT exemplifies the dichotomy of beneficial and destructive impacts of chemical production and use in society (3). It also demonstrates the precarious position which all scientists hold in our society. Chemists are expected to fulfill our demands for innovative products. However, they also face sharp criticism for a perceived disregard of the environmental and health impacts of their work. The scientists who developed CFCs and DDT probably did not have the knowledge to predict the long range adverse impacts associated with these chemicals. Their research efforts focused on the development of less toxic chemical products with specific functional properties. However, the unexpected long-term impacts of their production and use demonstrates a clear need for scientists to develop a broader set of considerations in the initial design phase of chemically based products.

## C. Principles of Pollution Prevention

Most U.S. environmental regulations have been focused on the control and clean-up of pollution. The EPA estimated that capitol investment in pollution control technology to comply with these “end-of-pipe” regulations totaled more than $115 billion in 1992 (1). This figure did not include the additional regulatory compliance costs, such as obtaining permits for regulated air and water pollution releases. Despite this large expenditure, at least 3 billion pounds of chemicals listed on EPA’s Toxic Release Inventory (TRI) were released into the ambient environment by industry that same year. As of 1992, the TRI tracked the level of emissions of 300 high-priority chemicals in 20 categories, compared to the more than 70,000 chemicals used commercially in the United States alone[1] (1). Since the

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[1] On November 30, 1994, EPA added 286 more chemicals and chemical categories to the list of toxic chemicals subject to TRI reporting (1).

passage of the Comprehensive Environmental Response, Compensation, and Liability Act (CERCLA) in 1980, the public and private sectors have contributed over $15 Billion to the clean-up of sites contaminated with toxic chemicals. The regulated community has found itself caught in a costly, never-ending game of "catch-up," as they strive each year to comply with increasingly stringent environmental regulations (14). Pollution prevention (P2) has therefore developed as a concept of increasing importance for the chemical industry, manufacturing companies, and the public agencies responsible for regulating these companies (15).

There is a fundamental difference between P2 and traditional pollution control and waste management: prevention versus reaction. P2 emphasizes a proactive reduction or elimination of wastes and pollutants at the source of generation (16, 17). Such analyses consider traditional pollution forms (i.e., solid, liquid, gaseous) and less traditional ones i.e., energy consumption, multi-media pollutant transfers). Waste management and pollution control are reactive in nature and emphasize mitigating the effects of pollution generation. In making an analogy between P2 and preventative medicine, Hirschhorn and Oldenburg compare waste management and pollution control to treating the symptoms of disease, rather than the disease pathology (7).

Proactive chemical designs which prevent the generation of polluting waste products are often technically superior and cost less than reactive solutions developed as a result of a crisis or regulation. It is even more desirable to eliminate the use of potentially toxic and hazardous chemicals from the design process altogether. Such forethought in product and process design may increase resource utilization efficiency, decrease environmental liabilities, and increase the competitiveness of the product and manufacturer in the global economy (14). However, in some industrial processes pollution control and waste management are the only viable options. A thorough understanding of the various inputs and outputs associated with a chemical's life cycle is necessary to properly evaluate its P2 potential.

## D. Life Cycle Analysis and Chemical Stewardship

P2 becomes more preventative in nature as the scope of analysis expands to include the entire life cycle of a chemical or chemically based product. A product life cycle includes the following stages: raw material extraction, primary production and processing, secondary production and processing, product utilization, retirement and recovery, and final treatment and disposal (14, 18).

**Figure 1: Generic View of a Product Life Cycle**

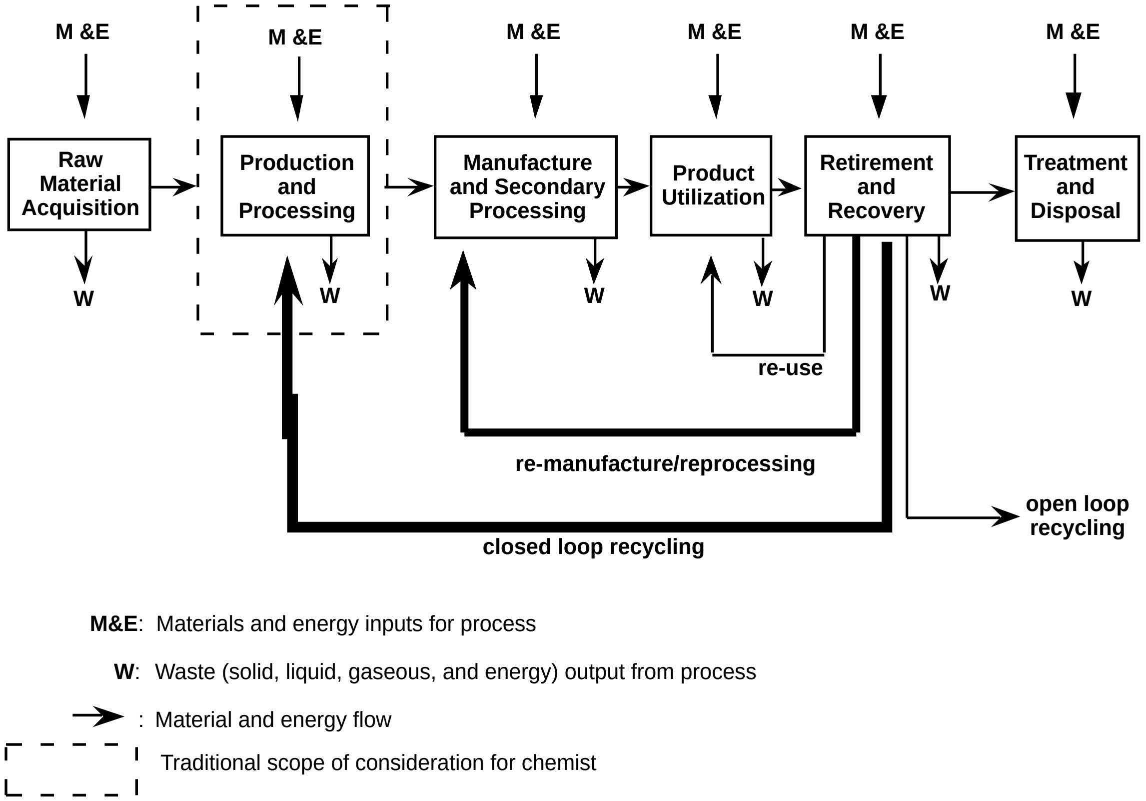
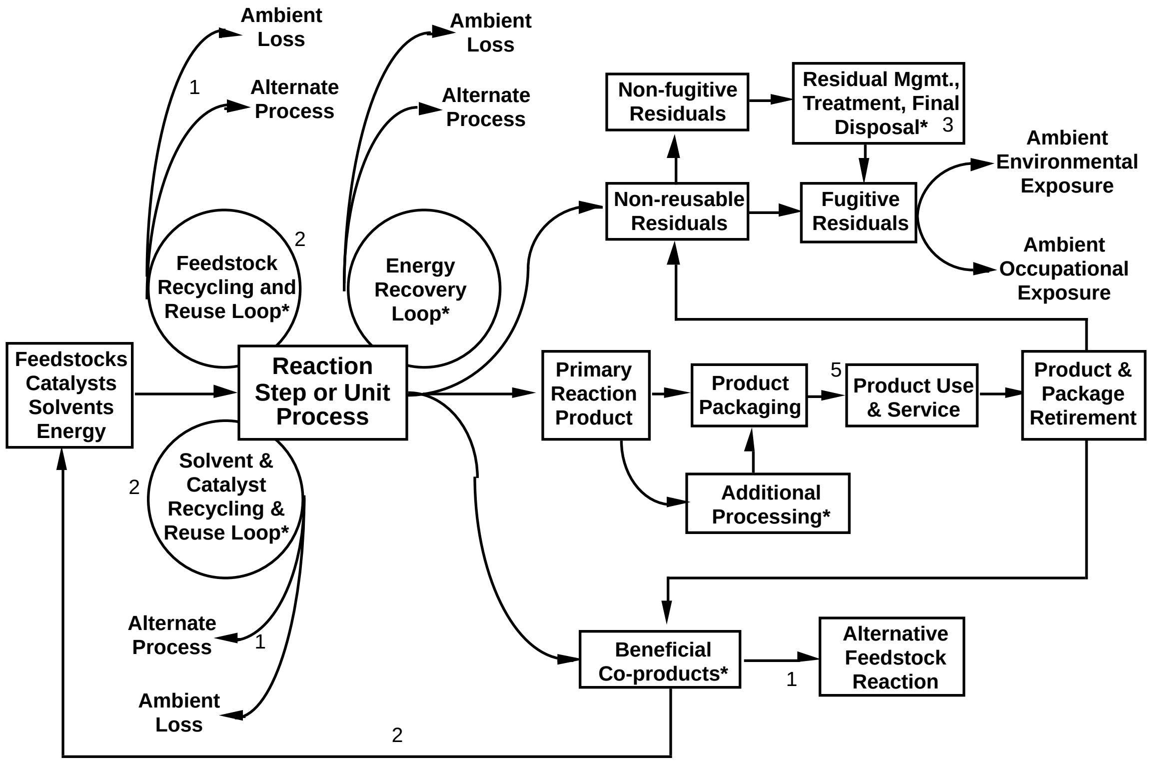


Figure 1 provides a generic view of a product life cycle, and Figure 2 provides a more comprehensive description of the theoretical inputs and outputs of a chemical life cycle. Chemical production and processing activities may encompass one or more reaction step, depending on the desired end product. Note that material, energy, and residuals flow into and out of all steps of the chemical life cycle. Figure 2 is useful for describing individual reaction steps, as well as entire reaction pathways. The production and processing step noted in Figure 1 is the traditional area of focus for synthetic chemists. However, it is only one of six major steps in the life cycle of a chemical.

Life cycle design (LCD) is the integration of environmental considerations into the product development process (14). Similar to LCD, design for environment (DfE) is the practice by which environmental considerations are integrated into product and process design procedures. DfE is an evolution of the engineering concept of DfX or designing for “X.” In terms of traditional engineering disciplines “X” may stand for manufacturability, testability, reliability, or downstream design considerations (14, 17).

**Figure 2: Life Cycle of a Chemical Product**

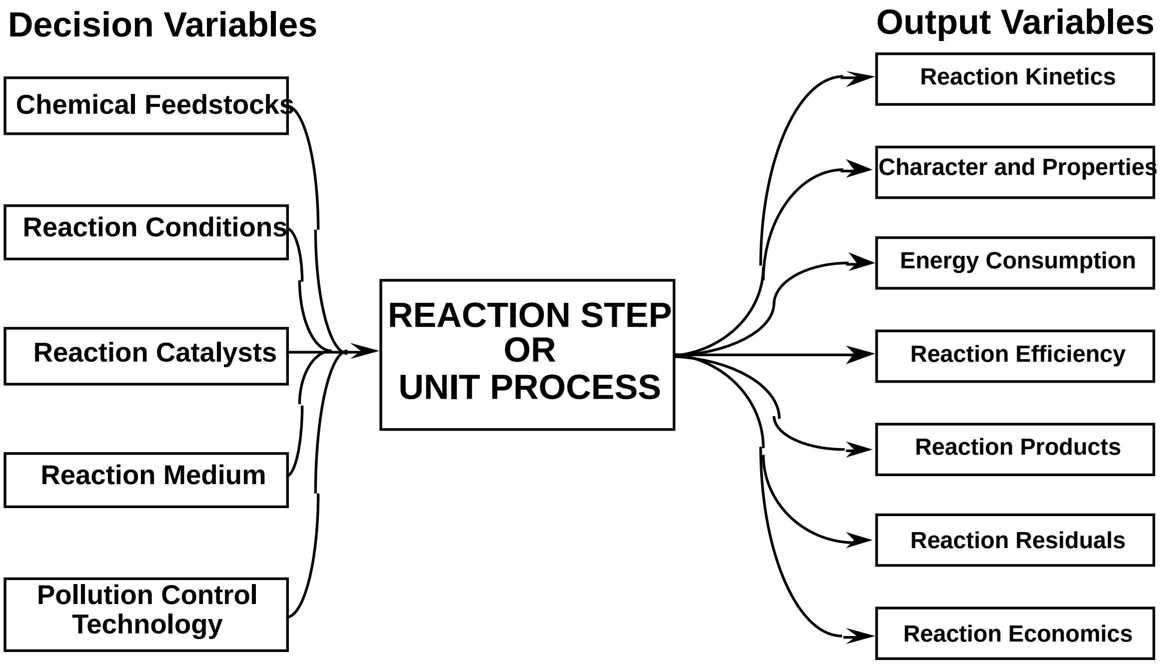


* Separate reaction and/or processing may be required for use in external reaction step or process (additional energy use, residual production, and potential occupational exposures)
** Given reaction conditions such as temperature, pressure, reactor
1 Open-loop recycling to external process
2 Closed-loop recycling to same process
3 Treatment through combustion (incineration, pyrolysis) and landfill gas harvesting may involve energy recovery
4 Non-fugitive, non-reusable residuals may be separated and/or collected by pollution control/treatment equipment
5 Product packaging materials will have their own life cycle

In terms of chemical science, life cycle models are a useful generic framework for the assessment of inputs and outputs of chemical reaction pathways. Incorporation of LCD methodology into the underlying thought process of the chemist facilitates a more complete assessment of the environmental requirements, product performance, production cost, regulatory requirements, and social factors associated with chemical production and use (17, 18). Life cycle assessment (LCA) is an analytical tool utilized to identify and evaluate the upstream and downstream environmental effects associated with a product or activity (14). A LCA examines the environmental impacts and resource usage which occurs at the major stages of a product's life cycle (17). Appendix 1 contains additional information regarding LCAs and their applicability to LCD methodology.

Figure 3 identifies proposed life cycle parameters relevant for evaluating the P2 potential of chemicals and reaction pathways. These reaction parameters are

**Figure 3: Decision and Output Variables Associated With a Chemical Reaction**



either *decision variables* or *outcome variables.* Decision (independent) variables are reaction inputs which the chemist can physically manipulate. For example, the choice of chemical feedstock, reaction conditions, catalysts, reaction media, and pollution control technology are all decision variables. Outcome (dependent) variables are characteristics of chemical reactions which are dictated by decision variables. Examples of output variables include reaction efficiency, kinetics, energy consumption, products, residuals, and production cost.

Outcome variables are only manipulated as a result of changes in decision variables. Manipulation of decision variables may be motivated by desired characteristics in outcome variables, decision variables, or both. For example, an alternative chemical feedstock may be chosen to reduce reaction residuals (outcome variable) or because it does not require input of a previously used heavy metal catalyst (decision variable). Such changes ultimately result in “trade-offs”; that is, the choice between two or more less desirable production and use characteristics. For example, in order to produce a certain chemical product a chemist may choose to utilize either a heavy metal catalyst or increase energy consumption to raise reaction temperatures and/or pressure. Table 2 contains a generic list of trade-offs associated with manipulation of decision and outcome variables.

**TABLE 2: Trade-offs Associated With Decision and Output Variables of Chemical Reactions**

| | | |
|---|---|---|
| Less | Input/Output Toxicity/hazardous properties | More |
| Less | Reaction Residuals | More |
| Less | Feedstock conversion/selectivity/yield | More |
| Less | Energy Burden | More |
| Less | Dangerous Reaction Conditions | More |
| Less | Product Durability/Resource Intensity/Useful Life | More |
| Less | Reaction Costs | More |

Thus, a valuable application of LCD principles is their use in identifying alternative choices when comparing chemicals and/or aspects of reaction pathways. A definitive choice may not necessarily be evident as a result of applying LCD methodology for making such comparisons. Looking at the various “trade-offs” associated with alternative reaction pathways using a life cycle perspective, however, provides chemists with the level of knowledge necessary to make potentially educated decisions. In addition, application of LCD principles in evaluating alternative reaction pathways may help practitioners identify areas for incremental improvement as specific stages in the chemical life cycle. In such cases, addressing incremental improvements throughout a chemical life cycle may be the most effective way to address the trade-offs associated with the entire system. (19).

## E. Evaluation of Chemical Reactions

Chemists and chemistry students are trained to design, optimize, and evaluate chemical synthetic pathways based on the selectivity and/or yield of a reaction step (1, 20, 21). Yield is the percentage of actual products obtained versus the theoretical amount which could be obtained from a given amount of reactants at specified conditions (1, 21). It is an important indicator of how efficiently chemical feedstocks and other reaction inputs can be utilized in a reaction step. Efficient use of chemical feedstocks inevitably increases the cost effectiveness of a reaction or synthetic pathway. Coupled with the cost of feedstock materials and energy consumption, reaction yield is one of the fundamental performance criterion for chemists to evaluate the industrial-scale feasibility of chemical reaction pathways (1).

Until recently chemists focused very little on the toxicity of feedstocks or the by-products of production used in commercial syntheses (21). In addition, chemists’ concerns about reaction media and reaction pathways were narrowly focused on use of traditional organic solvents and reducing the number of steps in a particular pathway, respectively. Similarly, when chemistry students are taught to synthesize and / or isolate chemical substances, their thought process must be structured toward consideration health and environmental consequences of reaction pathways (20, 21). Students need to be aware that decisions to utilize, generate, and dispose of hazardous substances are made intrinsically through selection of specific reaction inputs. In addition, they must learn to evaluate the upstream and downstream impacts of design decisions related to chemical synthetic pathways (1).

## F. Importance to the Field

How will chemists of the future balance competing concerns of environmental stewardship and innovative, cost-effective product development? For chemists to accept the idea that environmental quality and economic prosperity can be intertwined, P2 ideals must first be integrated into their underlying thought process. Chemistry students need to understand the complexities that health and environmental concerns bring to a particular chemical synthetic pathway. They must consider them no different than traditional concerns of yield, reaction selectivity, and stereo-specificity (6).

Such knowledge is just as critical for introductory chemistry students as it is for those enrolled in more advanced chemistry classes. Nearly 80% of all students enrolled in college-level chemistry courses do not enter science or engineering professions (22). However, these courses have a significant and lasting effect on a student's approach to and understanding of the discipline (6). Their knowledge of chemical science is reflected in their daily decisions as consumers in our society.

A meaningful question to ask is what should chemistry educators be teaching their students to enable them to understand and form appropriate responses to global-scale impacts of chemical production and use (22). Steinfeld and other faculty at the Massachusetts Institute of Technology suggest that chemistry students should have a basic understanding of the following subject areas in order to adequately address environmental and health considerations in their own field of study: biology and biochemistry, risk assessment and statistical modeling, economics and management, politics and sociology, media and communications, and ethical perspectives (22).

Ethical and philosophical questions are a part of the foundation of all scientific study. Chemical science principles are applied by scientists to define the physical and biological outcomes that occur as a result of chemical production and use in our society. However, chemists are not necessarily trained to weigh the “value” of a chemical to society versus its inherent impact on the biosphere. Chemistry professors, as both scientists and educators, have an obligation to impart both ethics and knowledge through their teaching. As Vellaccio states, to teach chemistry any other way is like, “teaching someone to use a gun without teaching them responsibilities that go with that knowledge,” (6).

Traditional chemistry curricula currently fail to train students with the appropriate multi-disciplinary background and skills necessary for them to make such decisions in an unbiased and educated manner (21). Educational institutions must therefore make changes in the methodology in which they educate chemists (15). Such monumental changes are not made by simply telling students to avoid using hazardous reagents, solvents, or reaction conditions. Analyzing the P2 potential of a chemical reaction requires the utilization of scientific and non-scientific parameters to balance societal costs and benefits (7). Such analyses are complex, uncertain, and subjective. However, government regulators, employers, and the public will expect innovative chemists to incorporate life cycle and P2 principles directly into their decision-making processes in the future (21). It is the responsibility of the academic establishment to provide chemistry students with an appropriate educational background, which incorporates these concepts into their training and fosters the development of multi-disciplinary, informed decision-makers (22).