IV. EVALUATORY FRAMEWORK

A. Introduction

This framework for evaluating chemical reactions is based on P2 and LCD principles (16, 20). It incorporates the use of generic scientific and non-scientific criteria for identifying the “trade-offs” of utilizing alternative inputs and outputs for chemical reactions. Criteria are grouped into the following six general categories:

- Scope and Definition of System Boundaries
- Impacts of Production and Utilization.
- Quantification of Chemical / Reaction Inputs and Outputs
- Properties of Chemical / Reaction Inputs and Outputs
- Reaction Economics
- Regulatory Requirements

These criteria do not necessarily constitute a decision-making model. They are presented as a quantitative and qualitative analytical methodology to guide practitioners in the collection of information regarding the material resources and energy transformations associated with a chemical life cycle.

B. Scope and Definition of System Boundaries

Prior to initiating information gathering activities it is important to identify the scope of analysis; that is, defining the boundaries of a reaction system for the collection of qualitative and quantitative data (14). This is an important aspect of chemical life cycle analysis because it influences information collection activities in all the forthcoming categories. Ideally, the scope of analysis for design and evaluative activities should be equivalent if they occur simultaneously or are utilized in conjunction with one another (14).

Consideration of a chemical’s full life cycle provides most complete analysis of material and energy inputs and outputs for a chemical reaction (14). Scope of analysis may be limited to partial life cycle or (i.e., individual reaction steps) as a result of the following limitations: 1) cost and time to perform a full life cycle analysis may not coincide with the needs of practitioners, and 2) data regarding chemicals, reaction conditions, and production methodology is not available to the practitioner. However, less comprehensive analyses may allow practitioners to focus their efforts on improving chemical or reaction design, rather than collecting data.

When applying life cycle methodology to a chemical reaction it is important to recognize interactions between the chemical industry and other sectors of our economy (54). Indirect material and energy interactions may be important aspects of a chemical's life cycle (14, 17). Life cycle models generally limit the depth of analysis to primary inputs and outputs associated with a product. The environmental implications of secondary and tertiary inventory items, such as facilities and equipment, are often neglected in these analyses (17, 18). Experience in applying life cycle principles to product design models indicates that primary inputs and outputs account for the majority of environmental and health impacts (18). Although limiting of the depth of analysis may be necessary for practicality reasons, practitioners should be aware of the potential influence on overall products development of secondary and tertiary reaction inputs and outputs (54).

All life cycle studies, regardless of their complexity, should be motivated by a needs analysis. A needs analysis forces practitioners to ask, "What are we doing and why?" Answering this question allows a greater understanding of the motivation behind assessment and improvement activities. Such analyses identify the fundamental "needs" which a chemical or reaction pathway fulfills for internal and external stakeholders. They are useful in identifying situations where alteration of reaction pathways are circumvented by changes in downstream and/or upstream life cycle stages. A needs analysis therefore helps to determine the importance of life cycle stages to other chemical products and reactions and may avoid unnecessary data collection activities (14).

C. Impacts of Production and Utilization

The production and use of chemicals may result in specific health and ecological impacts throughout the various life cycle stages. Classification, characterization, and valuation of impacts associated with production and utilization is a value-laden and subjective activity, which may reflect practitioner bias (55). This aspect of life cycle analysis is not a part of the scope of this work. However, related concepts which affect other categories of this framework are discussed below.

The fundamental basis for life cycle and P2 principles is the concept of "ecology"; that is, the idea that environmental systems and subsystems are interrelated and interdependent (10). Decisions to alter aspects of a chemical life cycle not only affect other reaction inputs and outputs, but also have micro and macroscopic impacts on the larger ecosystem. Impacts on the Earth's physical and chemical environment may be described as primary and secondary (56). Primary impacts are the direct result of an action, while secondary actions are indirectly attributed to an action. Both have the potential to be positive and negative (56).

For example, the primary impacts of utilizing CFCs as a chemical refrigerant, versus a propane alternative, are increased energy efficiency and product safety. The secondary impacts are depletion of the ozone layer and subsequent destruction of aquatic phytoplankton. This example illustrates both a positive primary impact and a negative secondary impact, the importance of which are subjectively assessed by individual evaluators. Additional impact assessment criteria include magnitude and severity, duration, timing/season, scale, irreversibility, potential for mitigation, and overall significance (56).

The life cycle perspective facilitates the analysis of chemical production and use impacts by facilitating classification in terms of applicable populations at risk. Human population categories include production facility workers (occupational chemical exposures), communities surrounding production facilities (daily and accidental chemical exposures), regional populations (production and chemical utilization), and global populations (production and chemical utilization). Impact on non-human flora and fauna populations applies in a similar manner, with the exception of the first category (10). One should strive to identify particularly vulnerable populations (females of child-bearing age, children, endangered species) within each category. Obtaining knowledge of the magnitude and nature of populations affected by various phases of a chemical life cycle is difficult. Impacts may not be realized for many years or may be masked by more predominant changes in species and habitats. It is also increasingly difficult to isolate single, causative agents of change as a result of multiple chemical exposures and physical intrusions into our environment. In addition, individual susceptibility of flora and fauna varies due to genetic disposition, age, sex, nutritional status, occupation, diet, and variations in personal behavior (i.e., smoking, alcohol consumption, and other lifestyle risk factors) (58). The assessment of impacts associated with any life cycle analysis is a complex and often ambiguous activity that is still in the initial stages of development by life cycle practitioners (18).

D. Quantification of Reaction Inputs and Outputs

Quantifying and defining the material and energy inputs and outputs of reactions is a fundamental aspect of chemical science. Stoichiometry can be utilized to determine the theoretical mass or volume of products and reactants given basic reaction information (i.e., temperature and pressure) (57). Feedstocks, desired products, and co-products are also quantified utilizing percent reaction yield, percent feedstock conversion, percent atom economy, and percent reaction selectivity (43, 57). Comparison of percent atom economy on the basis of theoretical yields is a rapid way to evaluate environmental impact of alternative reactions. However, all of these measurements tend to neglect solvent and catalyst utilization, as well as energy consumption (57). Appendix 2 contains additional discussion regarding measures of synthetic efficiency.

Reaction residuals (i.e solid and hazardous waste, air and water pollution, ambient energy loss) are not necessarily quantified in industrial scale chemical processes. Fugitive losses of reaction inputs and outputs occur at many points throughout a chemical life cycle and may result in unquantifiable errors in measurement. Mass balance procedures facilitated by computer programs have been developed to provide quantifiable estimates of reaction inputs and outputs. However, these data are no more precise than the methodology and measurements utilized by practitioners.

One of the challenges of interpreting quantified reaction inputs and outputs is drawing comparison between incompatible data units; that is, comparing energy versus matter (38). For example, one may be confronted with the following hypothetical alternative reaction pathways:

- Reaction A: 20 gallons of an aqueous heavy metal catalytic solution
- Reaction B: catalyst-free alternative requires 10,000 kJ of additional energy

In this example one must compare additional energy input with additional material input. Such comparisons are more easily facilitated if inputs and output data values are converted to equivalent units. Equivalent analysis of such trade-offs is not always possible given present level of development of life cycle principles (38).

Another challenge associated with life cycle analyses is the comparison of data aggregated into non-descriptive categories (38). For example, the category “hydrocarbon” may be utilized in a life cycle analysis without differentiation of the actual chemical composition. It may describe a mixture of benzene and benzo[a]pyrene or simply residuals oils and gasoline. Although data aggregation is useful in terms of simplifying analyses, it can lead to misrepresentations of the true nature of a particular chemical reaction (38).

E. Properties of Reaction Inputs and Outputs

The properties of chemicals and chemical reactions can be defined in the following manner: 1) physical and chemical characteristics, 2) quality and performance criteria, 3) recycled versus virgin resources, and 4) renewable versus non-renewable resources. Understanding these aspects of chemicals and reaction pathways provides chemists with additional criteria to analyze and improve chemical reaction systems.

(1) Physical and Chemical Characteristics

Table 4 contains selected physical and chemical properties associated with both chemicals and reaction pathways. The importance of these properties may vary depending on desired attributes of the chemical or reaction pathway. Table 5 contains a generic list of the physical and health hazards of chemicals as defined by the U.S. Occupational Safety and Health Administration's (OSHA) Hazard Communication Standard (29 CFR 1910.1200). Chemicals are designated as possessing a health or physical hazard if they meet the generic criteria specified in this regulation. The acute and chronic health hazards are somewhat more subjective designations based on toxicological data[1], epidemiological studies[2], and past case histories (10).

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[1] A working knowledge of the concepts related to chemical toxicity is an important for the following reasons: 1) widespread application to federal and state regulations, and 2) data limitations due to extrapolation of results between animal and human chemical exposures. Chemical toxicity tests measure the response of animal subjects exposed at specific doses to a chemical agent. These results are compared to a similar group of unexposed control animals. In vitro tests, such as the Ames mutagenicity test, are also utilized to determine potential chemical toxicity. These tests tend to be less expensive than acute and chronic toxicity testing. However, they are less reliable and inappropriate in some instances (10).

[2] The goal of human epidemiological studies is to investigate the incidence and cause of health-related outcomes in distinct populations (58). The information obtained in epidemiological investigations is utilized to forecast public health impacts and for devising strategies to prevent illness, disease, and premature death within a population (10). Types of epidemiological investigations include case control, cohort, clinical, intervention, and descriptive studies. An understanding of the analytical, data interpretations, and design limitations associated with each type of these studies is necessary for proper utilization of epidemiological evidence (58).

TABLE 4: Physical and Chemical Properties of Chemicals and Chemical Reactions

CHEMICALS	*CHEMICAL REACTIONS*
Form (solid/liquid/gas)	**Activation Energy (ΔH = exo/endothermic)**
Density	**Net Temperature**
Deactivation Rate (catalysts)	**Net Pressure**
Melting Point	**pH**
Boiling Point	**Reaction Time/Reactor Time**
Vapor Pressure	**Selectivity**
Lower Explosive Limit (LEL)	**Atom Economy**
Upper Explosive Limit (UEL)	**Percent Conversion of Reactants**
Speciation (ions, compounds, radicals)	**Reaction Yield**
Partition Coefficient (Log K_{OW})	**Batch/Continuous**
Persistence ($T_{1/2}$)	
Water Solubility	
Bioaccumulation Factor (chem. concentraion in biota or water)	
Freezing Point	

TABLE 5: Health and Physical Hazards Associated with Chemicals (60)

PHYSICAL HAZARDS	*HEALTH HAZARDS*[3]
Fire Hazards	**Acute**
combustible liquid	**irritantsG31**
flammable aerosols	**cutaneous hazards**
flammable gases	**toxic agents**
flammable liquids	**highly toxic agents**
flammable solids	**eye hazards**
oxidizers	**blood/hematopoietic agents**
pyrophoric materials	
	Chronic
Other Physical Hazards	**sensitizers**
water reactive materials	**carcinogens**
compressed gases	**reproductive toxins**
explosives	**hepatotoxins**
shock- sensitive chemicals	**nephrotoxins**
heat-sensitive chemicals	**neurotoxins**
unstable materials	**pulmonary toxins**

[3] Acute health effects are intense and short in duration, occurring relatively soon after an exposure. Acute exposures are those which occur for very short periods of time, such as a short term release of a chemical aerosol in a work place. Chronic health effects are characterized by a long latency period between exposure and the onset of the health-related outcome. They usually result in an incurable disease, such as cancer. Chronic exposures occur over long periods of time, such as drinking water contaminated by lead from the pipes of a house over a lifetime (10, 58, 60).

The EPA's Office of Pollution Prevention and Toxics (OPPT) has a four-tiered classification procedure for chemicals reviewed under its Synthetic Methodology Assessment for Reduction Technology (SMART) program[4]. Chemicals of highest concern are assigned a Tier I designation because they are extremely harmful to humans at part per billion levels. Tier II chemicals (moderate to high concern) are those found on the EPCRA[5] section 302 list of extremely hazardous substances, EPCRA section 313 list of toxic chemicals, or OPPT's categories of concern list. Tier III includes non-regulated, potentially harmful chemicals of low to moderate concern. Tier IV chemicals are of lowest concern due to their innocuous properties (59). Appendix 3 contains a list some of the chemicals contained in the four tier categories of this program.

TABLE 6: Statutory Terminology that Applies to Chemicals and Reaction Residuals

STATUTE	***TERMINOLOGY***
Resource Conservation and Recovery Act	**Hazardous Waste, Solid Waste**
Atomic Energy Act	**Nuclear Waste**
Comprehensive Environmental Response, Compensation, and Liability Act	**Hazardous Substance (reportable quantity chemicals, metals)**
Clean Air Act	**Hazardous Air Pollutants, Criteria Pollutants**
Clean Water Act	**Waste Water, Water Pollutants**

The terms "toxic" and "hazardous" are often utilized to describe chemicals that possess one or more health and / or physical hazards. Both these terms may inadvertently apply to regulatory definitions specified in federal and state environmental protection statutes. For example, the Resource Conservation and Recovery Act specifies a regulatory definition for "hazardous wastes." Therefore, it is important that use of these terms properly correlates with the specified regulatory implications. Table 6 contains a list of federal statutes that provide regulatory definitions for terms that describe chemicals and reaction residuals.

[4]The SMART program is operated in conjunction with EPA's review of Premanufacturing Notices for new chemicals, mandated by the Toxic Substances Control Act (48, 59).

[5] The Emergency Planning and Community Right to Know Act (EPCRA) is also known as the Superfund Amendments and Reauthorization Act (SARA), Title III.

(2) Quality and Performance Criteria

Absolute performance standards are defined by the laws of thermodynamics and physics. Theoretical reaction yield is an example of an absolute performance parameter. Actual reaction yield is an example of a technical performance standard, which is defined by the technological capabilities of equipment and one's knowledge and understanding of a process (14). Generic quality and performance criteria for reaction inputs and outputs include useful life and chemical purity grades. Other performance characteristics may be based on the physical and chemical parameters specified in Tables 4 and 5.

Useful life is the amount of time a chemical or other component of a reaction system can be safely utilized in order to meet specified performance standards (14). This applies most specifically to feedstocks, solvents, catalysts, and reaction products. Measures of useful life include the following: number of uses / duty cycle (electro-plating bath and solvent wash), shelf life (specialty chemicals such as picric acid), deactivation rate (catalysts), and degradation potential (environmental half-life) (14). Extending the useful life of chemical reactants and products may decrease the need for waste disposal of spent chemicals, as well as decreased resource utilization for production of new chemicals. For chemicals with health and physical hazards, a longer useful life is likely to result in fewer potential exposure situations. Inherently dangerous properties may therefore be tolerated in lieu of longer useful life for some reactants and products. Conversely, minimizing a chemical's "life," or persistence in the environment, is a design strategy of some chemical pesticides. Such products effectively degrade into less harmful chemical constituents in soils and water after short period of time (14).

Many chemicals are produced and utilized in accordance with purity grades specified by product manufacturers. Generally, higher purity is associated with greater production cost due to the increased post-reaction processing. Utilization of highly pure chemicals may result in higher reaction yields and production of less reaction residuals and undesirable co-products. However, the energy burden and reaction residuals associated with additional material processing may outweigh the benefits of greater feedstock purity in downstream reactions. Lowering feedstock purity may result in decreased reaction costs if there is no measurable impact on the quality of reaction products and residuals and co-products can be managed in an economical manner (14).

Useful life extension and higher chemical purity grades may require greater levels of material and energy inputs for all components of a chemical reaction system. Greater processing requirements result in the production of additional reaction residuals. Therefore, it is important to consider the overall impact on the entire reaction system prior to committing resources to these design strategies.

(3) Recycled vs. Virgin Resources

Reaction materials and fuels for energy production may be characterized as virgin or recycled resources[6]. In the past, products containing recycled materials were considered to be of inferior quality and performance compared to those produced with virgin inputs. This perception has now been altered dramatically. Product recyclability and recycled feedstock content are recognized as highly desirable features by both consumers and manufacturers. For example, the choice of utilizing recycled paper has obvious benefits to the environment and can enhance an organization's public image. The choice between recycled and virgin inputs in a chemical reaction system is not necessarily a straightforward decision for the chemists.

The ability for reaction inputs and outputs to be recycled and reused in same, similar, or external life cycles is a highly desirable quality. Recycling and reuse of chemicals and components of reaction pathways has the following potential advantages: 1) diversion of material from residual disposal streams, 2) reduced use of virgin resources, 3) cost avoidance associated with decreased residual disposal and more efficient use of feedstocks, and 4) equivalent or greater product performance (14).

Similar to product useful life extension, recycled chemical feedstocks, solvents, and catalysts often must undergo extensive purification, cleaning, distillation, or other separation processes prior to utilization in any market. Such steps may involve additional energy consumption, additional operating and capitol costs, production of solid and hazardous waste, and air and water

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[6]Recycling may occur as a part of a reaction process (pre-consumer/closed loop) or after the final product is distributed to consumers (post-consumer/open loop method). Closed loop recycling recovers reaction inputs and outputs that may be a suitable substitute for virgin reaction materials. Solvent, catalyst and feedstock recycling are all examples of closed loop recycling processes. Open loop recycling occurs when recovered materials are recycled one or more times after the processing step prior to landfilling or incineration. Examples of materials that undergo open loop recycling include steel, plastic, and paper (14). Figure 2 designates closed and open loop recycling in the chemical life cycle.

pollution releases. In addition, recycling requires an existing or planned infrastructure to link raw material sources with end-use markets. Careful comparison is necessary to avoid misrepresentation of the true nature of recycled reaction inputs and outputs.

(4) Renewable vs. Non-renewable Resources

The fourth distinction regarding the properties of chemicals and reaction pathways is whether their associated inputs are derived from renewable or non-renewable resources. Table 7 contains a list of both categories of material and energy sources. The choice between these inputs is highly dependent on an adequate supply, existing infrastructure (i.e., pipelines, rail, truck, and cargo ship), transport costs, prevailing market prices, and regulatory intervention. Producers and consumers of energy are linked through extensive utility-owned power grids fed by both renewable and non-renewable energy sources. Most energy consumers do not choose their source of fuel energy. However, some large chemical production facilities have on-site energy production facilities, which enable them some flexibility in fuel energy selection.

TABLE 7: Renewable and Non-renewable Reaction Feedstock and Energy Sources (10)

	RENEWABLE	NON-RENEWABLE
FEEDSTOCKS	Biomass (agriculture-based, forests)	Petroleum, Minerals, Ores, & Metals
ENERGY	Solar	Fossil Fuels
	Wind	Nuclear
	Geothermal	
	Hydroelectric	
	Biomass (e.g., wood, crop/animal wastes, or glucose-based ethanol / methanol fuels)	
	Combustion of landfill methane	
	Combustion of solid and hazardous wastes	

Both renewable and non-renewable have inherent drawbacks which limit their P2 potential. Extensive ecological degradation and disruption of land, air, and marine ecosystems that occurs as the result of the extraction, transport, and processing of non-renewable and some renewable chemical and fuel feedstocks. For example, the oxidation and combustion steps associated with petroleum processing for chemical and energy production can be attributed to increased global warming, acid rain, and decreased urban air quality (10). Such ecological and human health impacts may seem to provide a clear incentive to utilize less non-renewable virgin resources in all sectors of the modern industrial economy. However, the secondary ecological impacts described in Table 8 may overshadow the immediate advantages associated with specific applications of renewable energy and chemical feedstocks. Such options should only be considered if responsible management is practiced to allow sustainable regeneration of supplies at a rate sufficient to support existing consumption (10).

TABLE 8: Ecological Impacts Associated with Renewable Feedstock and Energy Sources (10, 16)

CONSTRUCTION OF HYDROELECTRIC DAMS
- Loss of critical habitats and endangered flora and fauna, alteration of aquatic habitats
- Alteration in sediment and ground/surface water flows
- Displacement of human populations and loss of historical artifacts
BIO-BASED FUEL/FEEDSTOCK SOURCES
- Deforestation and land-clearing , topsoil erosion, loss of critical habitats & species diversity
- Surface and groundwater contamination from excessive pesticide and fertilizer applications
SOLAR POWER
- Hazardous materials (metals) utilized in batteries for long-term energy storage
HAZARDOUS AND SOLID WASTE COMBUSTION
- Air pollution associated with combustion and processing of fuels
- Ash and other residual solid wastes have concentrated toxicity
- Combustion and processing of inert materials may result in conversion to highly toxic species (i.e., ,dioxin and derivatives)

F. Reaction Economics

Most chemical manufacturers utilize financial and managerial accounting practices to track the costs and revenues associated with production. Traditional accounting methodologies are not compatible with P2 and life cycle principles due to the following limitations: (1) failure to account for externalities of chemical production and utilization, (2) misallocation of costs into overhead accounts, (3) inability to track costs over entire life cycle, and (4) inability to identify and quantify hidden costs and benefits necessary for strategic planning. The inherent “trade-offs” associated with chemical life cycle analyses require a costing structure which reflects the “true” costs and revenues associated a chemical reaction (14, 61).

Activity-based costing and management (ABC / M) and total cost assessment (TCA) are two innovative methodologies which chart the use and allocation of material, financial, and energy resources on the basis of process and product life cycles. These costing systems embrace some of the traditional cost and revenue factors associated with chemical production, such as feedstock and utility costs. They compliment a life cycle framework by allocating organizational costs and revenues to specific processes and activities, rather than to departmental accounts (14, 61). Embracing ABC / M and / or TCA results in consideration of reaction costs over an extended time scale. This allows broader consideration of hidden and intangible costs and benefits, as well as future liability costs. Table 9 contains a list of general components of ABC / M and TCA costing structures.

An important distinction when characterizing reaction costs is the difference between laboratory scale and industrial scale syntheses. Laboratory scale syntheses utilize minute quantities of feedstocks, catalysts, and solvents. Therefore pollution control equipment, reaction residual production, materials storage, employee training, and other capacity dependent aspects of chemical reaction pathways will differ significantly. Environmental emissions standards may be more lenient for laboratory-scale experiments, resulting in lower costs associated with environmental regulatory requirements. However, industrial production facilities may have lower feedstock and other raw material costs due to their ability to purchase and store bulk quantities. When portraying reaction costs in P2 and life cycle analyses it is important to recognize that magnitude and complexity of reaction costs will vary depending on production capacity.

It is not always clear how the various expenses and revenues presented in Table 10 will affect the overall cost associated with chemicals and reaction pathways. This is especially true of less tangible costs and benefits, as well as future liability costs. Proactive design, extensive testing, and strategic planning are important aspects of defining an accurate reaction cost picture. Accounting professionals are developing methodologies to integrate these important concepts into production costing schemes. Although these topics may be beyond the scope of an introductory chemistry students, an understanding of the relevant concepts of reaction costs may contribute to their understanding of life cycle analyses.

TABLE 9: Reaction Costing Framework Based on ABC/M and TCA Principles (14)

USUAL PRODUCTION COSTS

Capitol Costs	***Production Costs***	***Production Revenue***
• Buildings	• Residual Mgmt. / Disposal	• Desired Rxn Product
• Production Equip.	• Utilities	• Rxn Co-products
• Pollution Control Equip.	• Raw Materials	• Recycled Residuals
	• Misc. Supplies	• Managed Residuals
	• Labor	

HIDDEN & LESS-TANGIBLE COSTS & BENEFITS

Capitol Costs	***Expenses***	***Benefits***
• Emission-monitoring equip.	• Closure/post-closure care	• Green marketing
• Safety/control technology	• Reporting & recordkeeping	• Corporate image
• Personal protective equip.	• Monitoring/Testing	• Consumer loyalty
	• Planning/studies/modeling	
	• Medical surveillance	
	• Worker Training	
	• Insurance and material use taxes	
	• Facility and product labeling	
	• Research and Development	

LIABILITY COSTS[7]

- **Legal staff or consultants**
- **Penalties and fines**
- **Workplace injury**
- **Customer injury due to product malfunction (product liability lawsuits)**
- **Future liabilities from contamination of production and residual disposals**
  - **soil and waste removal , treatment**
  - **ground water removal and treatment**
  - **personal injury to surrounding community (health care, insurance ramifications)**
  - **economic loss, real property damage**
  - **natural resource damage**
- **Bans and taxes on chemicals and chemically based products**
  - **fines for non-compliance**
  - **capitol expenses for re-tooling of production equipment**
  - **research and development to identify alternatives**

[7]The Comprehensive Environmental Response, Compensation, and Liability Act (CERCLA), otherwise known as the Superfund Law, is forcing the private sector to account for potential liabilities associated with irresponsible disposal of hazardous chemical wastes. Another example is the costs associated with product liability lawsuits. Dow Corning spent nearly $800 million in litigation fees for supplying the raw materials used in the breast implant production, prior to going into bankruptcy in May 1995. Dow Chemical Company was responsible for product distribution and the initial toxicological testing on the silicon-based materials themselves. They are also in the process of civil litigation with women who believe the company did not properly inform them of the potential health risks associated with breast implants (62).

G. Regulatory Requirements

It is important for the chemist to understand the legal framework which affects their design and production activities. All phases of a chemical's life cycle, from raw material extraction to product end disposal, are regulated by a complex structure of federal, state, and local regulations. Table 10 contains a list of federal statutes with regulatory jurisdiction over aspects of chemical production activities. Regulations may influence the following aspects of chemical production operations: construction of production facilities, air and water pollution control, management and disposal of reaction residuals and spent products, storage of feedstocks and other reaction inputs, transportation and distribution of chemicals, worker protection and safety, product packaging and labeling requirements, new product testing requirements, and emergency planning and preparedness.

In some instances, compliance with a Federal statute may be delegated to an applicable state agency. For example, the EPA has designated a number of state environmental regulatory agencies with the authority to implement the Resource Conservation and Recovery Act (RCRA). Non-compliance with federal, state, and local regulations may result in production shut-downs, fines, and jail sentences for the responsible individuals. In addition, international agreements, such as the 1992 Montreal Protocols, may place specific limitations on sale, production, and residual disposal activities in the U.S. (10).

The statutes in Table 10 are predominantly involuntary mandates. The EPA and other regulatory bodies have also initiated a number of voluntary P2 programs (17). The EPA's SMART program allows the Agency to review new chemical production processes and recommend P2 opportunities to manufacturers (47, 59). Formal partnerships between government and industry, such as EPA's 33/50 program, promote substitution of hazardous materials from operations and reduction of process pollution. EPA and the National Science Foundation (NSF) have allocated joint funding of grants for applicable research under the Design for Environment (DfE) program (26, 59). In addition, the Environmental Defense Fund has announced the unprecedented formation of the Alliance for Environmental Innovation. This non-profit research and consulting organization will be working with private industry to promote incorporation of P2 principles directly in their business and production activities (65).

TABLE 10: Federal Laws for Consideration in Chemical Production and Utilization (10, 14, 63)

STATUTE	***MEDIA/AREA OF REGULATION***
Clean Air Act[8]	**Air pollution discharges(point/non-point source; mobile/stationary sources)**
Clean Water Act	**Water pollution discharges (industrial, agricultural, municipal sources; stationary/mobile sources)**
Safe Drinking Water Act	**Sets health based standards for levels of contaminants in water delivered to users of public water supplies**
Comprehensive Environmental Response, Compensation, and Liability Act	**Allocates federal and state authority to clean up industrial sites contaminated with chemicals**
Federal Insecticide, Fungicide, and Rodenticide Act	**Regulates sale, labeling, and testing of pesticides, herbicides, fungicides, and rodenticides**
Occupational Safety and Health Act	**Regulates safety and health of workers in the occupational environment**
Resource Conservation and Recovery Act	**Generation, storage and disposal of solid and hazardous waste**
Toxic Substances Control Act	**Production, use, distribution of new chemicals into industrial and consumer markets**
Mining Safety and Health Act	**Regulates all aspects of mining activities in U.S.**
Pollution Prevention Act	**Establishes a national policy for P2**
National Environmental Policy Act	**Requires all applicable federally funded projects to undergo an environmental impact assessment prior to initiation**

[8]The Clean Air Act Amendments of 1990 list 189 volatile organic compounds used in common solvents as hazardous air pollutants (HAP). In March 1994 the EPA issued its final Chemical Manufacturing Rule, which requires existing chemical manufacturing operations to reduce use of 112 of the 189 hazardous organic air pollutants by 88% of 1990 levels over three years. New plants must comply immediately with these operating restrictions. EPA estimates that compliance will reduce use of the 112 hazardous organic air pollutants by over 500,000 tons per year. The Agency also expects a reduction in emissions of smog producing VOCs by over one million tons per year, which is equivalent of removing over 38 million gasoline powered vehicles from the road. At least 370 chemical facilities in 38 states, most of which are located in Texas, New Jersey, and Louisiana, will have to upgrade their control technology to prevent evaporation and leaks from process vents, wastewater and transfer operations, storage tanks, and equipment. The expected cost to the chemical industry is $450 million in capital expenditures and will increase annual operating expenses by $230 million (30, 64).