# THE INTEGRATION OF PROCESS AND PRODUCT DESIGN

James Wei
Princeton University
Princeton, NJ 08544

*Abstract*

The current chemical engineering curriculum emphasizes product engineering, which was appropriate in an era when we had many large-volume and long-lived products, which needed a continuous process of cost reduction.  Today, in the rapidly growing products of polymers, biomedical devices, and information material, the products tend to be small-volume and short-lived, which needed continuous improvements in product properties and customer appeal.  The study of molecular structure property relations is the principal intellectual tools in product design. In principle, product design is concerned with the question "what would have the desired properties", and product design is concerned with the question "how to make it".  In practice, there should be a strong integration between the two in creating a new or improved product.  Traditional process design concentrated on the meter scale of process equipments, and the hundred-meter scale of plants.  In the future, chemical engineering design must also integrate the complexities involved from the nanometer scale of molecules to the ten thousand kilometer scale of global environment and sustainability.

*Keywords*
Product design, Process design, Integration of complexities

## Introduction

A dynamic profession such as chemical engineering must keep on evolving and changing to adapt to the most important needs of the world. There was the time when we had a parade of exciting new products sold in large volumes at healthy profit margins, and remained dominant in the marketplace for many decades, such as nylon and chlorofluorocarbons. The chemical engineering curriculum concentrated on process engineering, based on the assumption that we already know what products to make, and the assignment is how to make these commodity products with increasing efficiency and safety. The world today presents a dual impact to the process engineers: a slow down of the introduction of exciting new commodity products to enchant the consumers, and a diminished opportunity for improving process efficiencies after many years of effort for the mature commodities.

In the meantime, the most innovative chemical engineering researchers have enlarged the menu by investigating the science and invention of new products, particularly in the polymers, the biomedical devices, and the informational materials. In these new fields, both the risk and the reward are much greater than in traditional mature areas. These new products tend to be made in small quantities, and tend to have short product life cycles, as the rate of new product introduction is prodigious. Success in these new fields depends more on the immediate need of designing the product to improve its properties and consumer acceptance, and less on the long term need of making the product at ever-lower cost over many years.

The concept of Product Life Cycle suggests that there is a spring time when the product is not yet proven and the creative pioneers stand to generate much excitement and to make great gains; followed by a summer time when a successful product generates many fast followers coming out with improved or me-to products; followed by an autumn time when the innovation pace has slowed down and the main competitive tool for a stable product is in continuous cost-cutting; and ended with a winter time when the main challenge is to be a competent care taker to keep things going as long as possible. This is shown schematically in Figure 1.

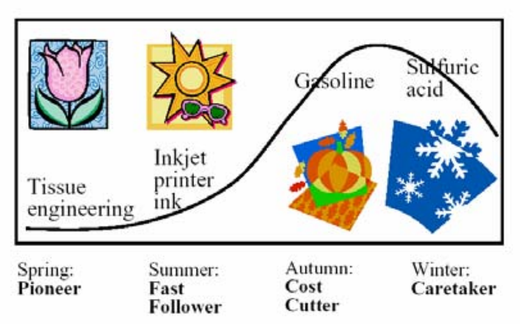

*Figure 1 Product Life Cycle*

The products of the chemical industry occupy all four seasons in the life cycle, and the chemical engineering community needs to service all four phases by teaching both product and process engineering, and how they are integrated.

There was a time when a commercial transaction was mainly a two party affair: the manufacturer sells a product and receives payment, and the customers receive a product that satisfies their needs. Then came the discovery of the hazard of vinyl chloride in cancer, the Exxon Valdez oil spill, and the demise of the chlorofluorocarbons due to the ozone hole. Therefore today, besides the seller and the buyer, every commercial transaction also has a third party - the public and the environment. The design of a product and its process must consider factors far beyond the factory and the customer, to include complexities and scales ranging from the nanometer of molecules to the ten thousand kilometer of global environment.

## The Case of Nylon: integration of product and process design

An often-mentioned folklore states that at the beginning, a chemist invents a new product, and then the chemical engineers are summoned to the office of the vice president to design a process, to make the product with economy and safety. In reality, there is a great deal of integration between these two investigations and designs. It would be instructive to follow the story of the development of nylon, as the steps involved were well documented. (Hounshell and Smith 1988, Hermes 1996)

Wallace Carothers jointed DuPont in 1928 to investigate a number of scientific questions in the nature of polymers. He was able to make a condensation polymer with a 3-carbon dihydric alcohol with a 16-carbon dicarboxylic acid, in a molecular still to remove the byproduct water and shift the equilibrium to a material with the molecular weight of 12,000. This polymer has sufficient tensile strength when cold stretched, and a handsome appearance; but it also has a melting point below 100 C, is partially soluble in dry cleaning fluid, and swells in water. What should DuPont do with this discovery? The first totally synthetic polymer was bakelite, made from the low cost materials of phenol and formaldehyde, which was widely used to make low cost electrical appliances. For this more elegant material, the problem of manufacturing would be much more difficult and expensive, so that the product must command a high price per pound as well as a large volume of sale. DuPont has been in the business of rayon manufacturing and marketing, and thought about a synthetic polymer to replace silk for stockings, which had a very large volume of sale and a price of \$2 per pound. A pair of knit stockings consumes only 10 grams of polymer. But stockings need to be washed and ironed, so this material would not be suitable.

Carothers and his coworkers needed to find a polymer that has all the good qualities of the first material, but should not dissolve in dry cleaning fluid or swell in water, should have a high enough melting point, and can be manufactured from readily available raw material to make profit at a price below \$2. They turned to the condensation of diamines and diacids to make polyamides, which have much higher melting points than polyesters. By 1934, they made a polyamide with a 5-carbon diamine and a 10-carbon diacid, with a melting point of 190 C. The problem of swelling in water is related to the ratio of the number of polar groups to the length of the hydrocarbon chains, so that there would be more swelling when the carbon chains are shorter in the monomers. The other problem is the lack of a ready source of supply of 10-carbon straight chain material, such as decane as raw material. By 1935, they made a polyamide with the 6-carbon diamine and the 6-carbon diacid, which will be called nylon 66 with a melting point of 250 C. This seems to be the right material at last, as benzene can be the raw material with six carbons, readily extracted from coal tar or crude oil.

Nylon 66 was still not ready for manufacturing, and parallel efforts were launched in product and process investigations. The first target was to make nylon at $0.80 per pound, with a plant capacity of 8 million pounds per year. Benzene extracted from coal tar or crude oil required the development of a process to hydrogenate into cyclohexane, which is oxidized to make cyclohexanol and then adipic acid. Half of the adipic acid is converted to adiponitrile and then to hexamethylene diamine. A new fiber spinning method needed to be developed, and a prototype is the existing technology of rayon, which is spun from solution into fibers, as it does not melt. They tried to dissolve nylon in hot phenol or formamide, and to pump the hot syrupy solution through spinnerets into fibers, then to evaporate the solvent. Melt spinning makes more sense for nylon, but it has to be done at 260 C with heat resistant spinnerets. Silk stockings are sized and dyed before they are knitted into stockings, and similar processes must be worked out for nylon fibers. The first knitting test at a textile mill at Maryland was a disaster, as the fibers snagged at knitting machines and the product had the color of gunmetal. After numerous product and process problems were solved, DuPont finally authorized in 1938 $8.5 million to build a 4 million pound a year plant at Seaford, Delaware. Nylon stockings went on sale at Wilmington stores in 1939.

In the chronicle above, it is clear that the initial concerns were principally about the product, and the final concerns shifted more and more towards the process. However, much of the decisions made, such as the switch from polyester to polyamide, and the decision to make nylon 66, can be considered to be the best compromise between the optimal product design and the optimal process design. Process research and development continued at DuPont and other places for many decades, resulting in ever-higher quality and efficiency. Nylon is now a commodity, and the fiber division of DuPont has been sold to Koch Engineering, to make room for more innovative new products.

## The case of Chlorofluorocarbons: integrating complexities from molecular to global scales

In 1928, Charles Kettering gave Thomas Midgley an assignment. He said, "Home refrigerators are on the rise, but the refrigerant is sulfur dioxide which is not safe. The press is clamoring for a ban on the 'killer refrigerators'. You assignment is to find a refrigerant that is nonflammable and nontoxic." (Bowden 1994, McGrayne 2001) Midgley did a brilliant analysis and came out with chlorofluorocarbons in three days. He looked at the nonmetals in the periodic table, shown in Figure 2, and observed that flammability decreases from the left to the right, and toxicity decreases from the bottom to the top, thus fluorine is the element that should receive the most attention.

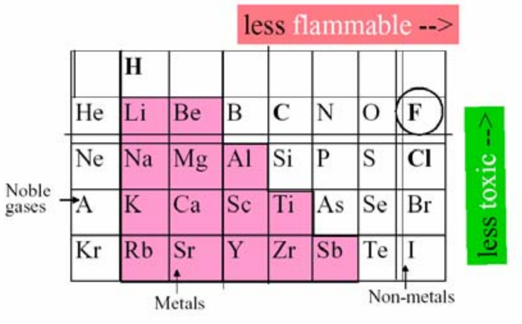

*Figure 2 Midgley's analysis showed that the least flammable and toxic element is fluorine.*

He knew that fluorinated methane has too low a boiling point, and he considered the set of chlorofluorocarbons shown in Figure 3. The top three rows are flammable, and the left border is toxic, which leaves seven compounds to choose from that are neither flammable nor toxic.

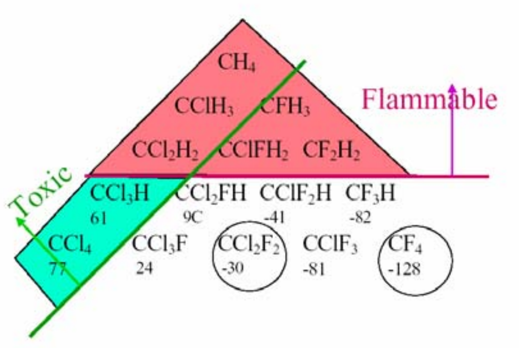

*Figure 3 Midgley showed that CFC with at least one fluorine and at most one hydrogen atom are less flammable and toxic.*

He settled on $CCl_2FH$ as having the appropriate boiling point, and created freon, as a benefit for customers for many years who would have the luxury of home refrigeration without the danger of deadly refrigerator leaks.

The success of freon led to numerous other uses, including air conditioning, blowing aerosols, cleaning computers and fire extinguishing in space capsules. The sales volume rose to 2.5 billion pounds a year in 1988. The extremely stable freon cumulates in the atmosphere to 0.6 parts per billion, and rises to the stratosphere at 20 to 40 kilometers above earth, is broken into chlorine free radicals which consumes the ozone needed to protect earth from deadly ultraviolet radiation. The 1987 Montreal Protocol called for the substitution of CFC with less damaging products, and the current choice is HFC 134a, which is $CF_3$-$CH_2F$ with no chlorine atoms. The story is not ended here for long, as this compound is found to be a greenhouse gas related to global warming. This story demonstrates that the design of a product involves considerations that range from the molecular structure to the global environment.

## Teaching Product Engineering at Princeton

I have been teaching a course for several years in Princeton on "Molecular Structure & Property: Product Design", and I am in the process of finishing a manuscript. The course has three major components: history and organization of new product innovations, molecular structure and property relations, and recent cases of product design.

(A). The first four weeks of the semester are concerned with the following topics:

- Historic Product Innovations
- Organization and Phases of Product Development

- Marketing
- Safety, Health and Environment
- Design
- Future Challenges in Product Innovations

We begin by the description of some of the most distinguished new product innovations in history, which also give concrete examples to serve as illustrations of the general principles covered in subsequent chapters. The initial motivation of product innovations can be divided into to the market-pull innovations and the technology-push innovations. Examples of the market-pull innovations include:
vulcanized rubber, Goodyear, 1839; celluloid, Hyatt, 1870; aspirin, Hoffmann, 1898; tetraethyl lead, Midgley, 1921. Examples of the technology-push innovations include:
synthetic mauve, Perkin, 1856; penicillin, Fleming, 1928; teflon, Plunkett, 1930; Post-It, 3M, 1973. William Perkin discovered the synthetic dye mauve in 1856. He was an 18-year-old student of chemistry who had a home laboratory, and he was trying to synthesize quinine for malaria treatment, and found instead a black tar in his tube. He dipped a piece of silk into the tar, and found that it turned to a brilliant purple color, and found that is was also fast; so he started the modern synthetic chemical industry as an accident.

The search methods used in the discovery can also be divided into: (i) Luck, such as in the discovery of mauve by Perkin, the discovery of penicillin by Fleming, and the discovery of teflon by Plunkett. (ii) Sweat, such as in a random search of numerous substance involved in the discovery of Salvarsan for syphilis by Ehrlich, the discovery of carbon fibers for the filament in incandescent bulbs by Thomas Edison, and the discovery of taxol after the screening of 65,000 natural and synthetic compounds. (iii) Planning, such as in the systematic and logical discovery of chlorofluorocarbons by Midgley in three days, based on qualitative associations and trends in the periodic table of elements, and on comparing the physical and chemical properties of the chlorofluorocarbons.

Historians and the press often truncate their stories of innovations at this discovery stage, and neglect the equally exciting stories of the development efforts from an interesting discovery to a valuable product - that would have to be designed to be superior in the marketplace to any existing product, can be manufactured with reasonable raw material and process equipment, and to make a profit to repay the investment in research and new plants. The story of the development of nylon took 10 years from discovery to silk stockings in the stores. Another well-documented story was the introduction of the cancer drug taxol, which was extracted from the bark of slow growing century-old Pacific yew trees, and proven effective against refractive ovarian and breast cancer. But the development took 30 years, as many difficult problems had to be overcome: it takes the high dose of 10 to 20 mg/kg.day to be effective; the yield is very small, as the concentration of taxol in the yew bark is only 40 parts per million, and it takes about six trees to treat one patient; Pacific yews are found only in the Northwest, and it takes a hundred years to grow a tree to 60 feet tall and 30 inches in diameter, and environmentalists were alarmed about the destruction of these old trees (the problem was solved with the development of semi-synthetic taxol that derives from the needles of the common English yew); it has an abysmally low water solubility of 10 ppm by weight, so that its solubility must be greatly increased to inject into the blood stream (the problem was solved by the development of an emulsion with castor oil); the mechanism of action of taxol was not known, so that there was little confidence in its scientific standing (the problem was solved when Susan Horowitz discovered that the mechanism involves cell microtubules, which are used in cell growth and function).

Marketing is one of the least understood subjects in engineering, as it involves the inverse paradigm of inductive logic. Engineering students are used to learning immortal principles handed down by Olympian scientists such as Newton and his law of motion, Maxwell and his equation of electro-magnetism, and Carnot and the Second Law of Thermodynamics, and derive results from these theories to solve practical problems. Marketing is the exact opposite, of trying to extract guiding information from thousands if not millions of voices, from people in the street who are incoherent and inconsistent. The customers are always right, but how do we find out what they are not articulate enough to say? Product innovation must begin by first finding out what are the real needs of the marketplace, how the product can enhanced the lives of the customers, how much do they want to buy and at what prices. The innovators must also study the products already in the marketplace, what are their volumes and prices, what are their strong points, and what are the weak points that offer an opportunity for improvement. The course discusses a range of products from the most simple to the most complex: bottled drinking water, fuel for Tomahawk missiles, ink for inkjet printers, zeolite adsorbents to separate normal from iso-paraffins, and controlled drug release devices.

Historically, Green Engineering began with attempts to clean up the plant effluents as an add-on activity to well-established products and processes. This stopgap method has limited effectiveness. Gradually, the work broadened to the cleanup of spills, went upstream to re-design the processes, and more recently to re-design the products to minimize on the use of potentially hazardous and irreplaceable substances. The designers of a product need to take all of these into consideration. A design project is assigned at this point, giving adequate time for the students to read the literature and to consult experts, culminating in an oral presentation and a written report in the third part of the course.

(B). The next 7 weeks are devoted to the study of molecular structure and property relations, which is the intellectual toolbox of product innovations.

- Search methods
- Literature and database
- Quantitative predictions from theory
- Quantitative correlations
- Qualitative associations and trends
- Strategies of Random Search
- Research frontiers of structure property relations

The forward search can be thought of as establishing a function $y = f(x_1, x_2, ...a_m)$. Here y is the property in question, which can be:

- Structural - bond lengths and angles, conformation, symmetry
- Physical - density, boiling and melting points

- Chemical - reactivity, kinetics
- Thermal - heat and free energy of formation, entropy
- Biological - toxicity, pharmaceutical activity
- Economic - price, volume of sale

The parameters $x_1$ to $x_m$ are either structural parameters or other properties that are more readily available. The quickest way to search for a property y may be to look them up in a database, a handbook, a research journal, or the more modern electronic methods of a CD or a web address. The molecular structure of the substance, and a few physical-chemical properties can be computed from first principles, or more often from semi-empirical methods involving empirical parameters and force fields, such as the heat capacity of a bi-atomic molecule. This involves the use of software such as Gaussian, HyperChem and Atomic Microscope. Many more properties can be estimated by correlations with molecular structure, or with other more commonly available properties, such as the boiling points of normal paraffin with the number of carbons, and by the group contribution methods, such as the boiling points of numerous organic compounds with heteroatoms. This involves using statistical software, which can be a spreadsheet as Excel, and group contribution method software such as Cranium. Qualitative associations and trends are relied upon when the more quantitative and data-intensive methods are not available, such as the case of Midgley's use of the periodic table to single out fluorine as the most promising element for a nonflammable and nontoxic compound.

The reverse search can be formulated as the reverse function $x = g(y_1, y_2,...y_n)$, where x represents the main quest for the product engineers for a suitable product, and $y_1$ to $y_n$ are a set of properties that are desired. With a traditional handbook of properties, this reverse search is very laborious and time consuming. Some electronic databases are now equipped with a reverse search capability, so that one can ask for "all compounds that boil between 0 and 1 C, and have a density less than 1". The availability of reverse search capabilities is still in its infancy, and one usually has to fall back on combining the forward search with interpolation to simulate a reverse search. For instance when three points $\{x_a, x_b, x_c\}$ in the X-space has been forward mapped to three points in the Y-space $\{y_a, y_b, y_c\}$, which forms a convex space containing the desired point y*, one can attempt a linear representation of y* by the three y points and project that the desired structure x* has the same linear combination by the three x points. When these methods have been exhausted, the next resort may rely on qualitative associations and trends, as well as unproven rumors and folklores. The last resort would be the random search, which was used successfully by Ehrlich in a search for an arsenic-based cure of syphilis, by Edison for a filament for the incandescent lamp, and by the National Cancer Institute for a cure of cancer that resulted in taxol. Combinatorial chemistry is a much-discussed new method that has not yet made any major discoveries.

For the academicians and researchers, molecular structure-property relations is a fertile field for research advances: theoretical understanding of structure-property relations, measurements and compilations of more comprehensive databases, synthesis of new materials and measurements of their properties, and predictive methods for more properties of more substances.

(C). The last 3 weeks are devoted to presentations and discussions of contemporary cases of product development. It is very useful to have guest lecturers from industry to describe and to analyze recent cases of new product development, which adds reality to basic principles. We have had guest lectures on the development of the synthetic lubricant Mobil-1, which is a poly alpha olefin, on the missile fuel for increasing the maximum range of Tomahawk, and on the cancer drug taxol. Then we have the oral presentations of the student design projects, which has included: hair removing cream based on a cancer drug, impact resistant polymer faceplate for cellular phones, foot warmer powered by shoe insert that generates electricity upon compression, and disposable contact sun glasses.

## The Case of Sistine Chapel Ceiling: Integrating Complexity in Design

Chemical engineers hav been and should continue to derive new ideas and concepts on the successful design and optimization of complex artifact by other disciplines. Michelangelo and Leonardo da Vinci were both successful engineers, skilled in the design and execution of large and complex military and civilian works. Let us look at Michelangelo’s ceiling for the Sistine Chapel. (Seymour 1972, deVecchio 1992, Partridge 1996) The design can be divided into four different scales:

(A) The structure of the overall ceiling has an impressive scale of 131 feet long by 42 feet wide, and is 65 feet above the floor, shown in Figure 4. It is divided into: nine central rectangular panels, which tells stories from the Old Testament, such as *God Creating the Sun and the Moon*, and the *Fall and Expulsion from Eden*; four corner spandrels contain stories, such as *David and Goliath*; twelve inverted triangles contain seven prophets and five sibyls; twelve triangular lunettes and two coves for the ancestors of Christ.

*Figure 4 Ceiling of the Sistine Chapel*

(B) The structure of the central panel of the *Creation of Adam* has a scale of 18 feet by 8 feet, shown in Figure 5. The energetic and dynamic God on the right is wrapped in a cloak, extending a finger of his right arm to animate a finger of the left arm of the totally inert Adam, sprawling on the left; the left arm of God is wrapped protectively around the not yet created Eve, who stares at Adam her future mate.

*Figure 5 The Creation of Adam*

(C) The structure of the figure of the *Delphic Sibyl* has a scale of 9 feet by 5 feet, shown in Figure 6. This most lovely woman in the entire ceiling is seated, but with restless energy endowed by the sinuous twists in her body, or *contraposto* - her eyes are looking to the left, her arms are pointed to the right, her hips are twisted to the left, and her knees are turned to the right.

*Figure 6 The Delphic Sibyl*

(D) The structure of the single head of God in the *Creation of Sun and Moon* has a scale of 3 feet by 2 feet, shown in Figure 7. It shows a majestic God, charged with authority and purpose, with flowing gray hair, moustache and long forked beard, and stern eyes surveying his creation. He is advancing with his right arm pointed towards the sun, and his left arm pointed towards the moon. Once again, notice the consistent symbolism of the dominant and energizing right side, and the passive and receiving left side.

*Figure 7 God in the Creation of Sun and Moon*

Michelangelo designed the entire ceiling and executed the painting over a period of four years. The process encountered many technical problems that needed innovative solutions. Fresco was the technique used, which starts with a plaster made of lime, sand and water. Each of the first two rough coats of plaster were applied and then allowed to set. In the meantime, the artist made a full-scale cartoon of the image the he intended to paint, transferred the outlines of the design onto the wall from a tracing made of the cartoon. The final smooth coat of plaster was then trowelled onto as much of the wall as can be painted in one session. The boundaries of this area were confined carefully along contour lines, so that the edges or joints of each successive section of fresh plastering were imperceptible. The tracing was then held against the fresh plaster and lined up carefully with the adjacent sections of painted wall, and its pertinent contours and interior lines were traced onto the fresh plaster. As the wall dried and set, the colors were imbibed into the surface and bound with the lime and sand particles. This gave the color great permanence and resistance to aging, since they were an integral part of the wall surface, rather than a superimposed layer of paint on it. The painter must work fast while the plaster was wet, but cannot correct mistakes by over-painting.

To paint on the ceiling, a scaffold must be built so that the painter could lie on his back to apply the plaster, to attach a cartoon or sketch to the ceiling, to score the plaster through the sketch, and to apply the paint with the brush. There was plenty of opportunity for the plaster and the paint to drip into the painter's eyes. Michelangelo designed the scaffold out of flat wood with brackets built from the wall, near the top of the windows. He also built zigzag ladders from the floor to the platform. The area covered was 131 x 42 = 5502 square feet. It has been estimated that Michelangelo painting on the average of 6 square feet per day, roughly the size of the head of God! The coordination of almost a thousand pieces of 6 square feet pieces must have been enormous task to ensure that the outlines and colors have continuity and harmony. No wonder fresco wall painting went out of existence after Raphael, and was not revived till the 1920s by Diego Rivera.

The world of chemical engineering design was traditionally concerned with processing equipments in meter scale, and with systems such as refineries and chemical plants in hundreds of meters. The degree of complexity has been greatly expanded by recent events from the nanometer scale of molecular design to the 10,000-kilometer scale of global environment of phenomena, such as the ozone hole and global warming. Figure 8 shows six scales, from molecular to colloidal, from particles to equipment, and from plant to global environment. This span of 16 orders of magnitude is becoming the drawing board of chemical engineers.

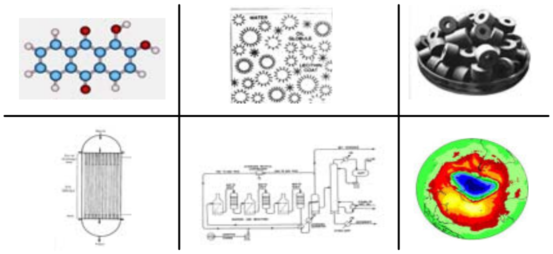

*Figure 8 Six scales of chemical engineering: molecule, colloid, particle, reactor, plant, and global.*

## Conclusion

In the world of today, the prosperity of the chemical engineers depends on the creation of a stream of new products that are often sold in small quantities and with short product life cycles. In service to these needs, chemical engineering research and education should be focused on these new demands. We need to teach product engineering as a complement to the teaching of process engineering, and to integrate these two topics. We need to emphasize the subject of molecular structure-property relations as the principal tool of product engineering. We also need to integrate these designs involving a complex set of scales from the nanometer of molecules to the ten thousand kilometers of global environment.

## References

Bowden, M. E., 1994 "Chemical Achievers", Chemical Heritage Foundation, Philadelphia.

Hermes, M. 1996 "Enough for One Lifetime: Wallace Carothers", American Chemical Society, Washington DC

de Vecchio, Pierluigi. 1992 "The Sistine Chapel: a glorious restoration". Harry N. Abrams, New York.

Hounshell, David A. and John Kenly Smith, 1988 "Science and Corporate Strategy: DuPont R&D 1902-1980", Cambridge University Press, UK

McGrayne, Sharon B. 2001 "Prometheans in the Lab: Chemistry and the Making of the Modern World." McGraw-Hill, New York

Partridge, Loren W. 1996 "Michelangelo: the Sistine Chapel ceiling, Rome" Braziller, New York

Seymour, Charles, 1972 "Michelangelo, the Sistine Chapel ceiling", Norton, New York