CHEMICAL PRODUCT AND PROCESS DESIGN

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ABSTRACT

A template for teaching chemical product and process design was introduced by Seider et al. (2004a) and its relationship to the Stage-Gate product development process was discussed by Seider et al. (2004b). Therein, emphasis is placed on processes involving basic chemical products (commodity and specialty chemicals, biomaterials, polymeric materials). In this paper, the Stage-Gate process is extended to apply for the design of industrial products (e.g., films, fibers, paper, …) and consumer products (e.g., dialysis devices, flat-panel displays, post-it notes, transparencies, drug delivery patches, cosmetics, …). In the *Concept Development* step, emphasis is placed on innovations needed for materials development, process/product development, and manufacturing process development. In the *Feasibility* and *Development* steps, for industrial products, emphasis is placed on constructing the prototype product and process synthesis involving operations for raw materials handling, conversion, primary and secondary forming, and packaging. For configured consumer products, in addition to constructing the prototype product, emphasis shifts toward synthesis of the assembly line involving raw materials handling, conversion, finishing, and packaging.

INTRODUCTION

The design of chemical products begins with the identification and creation of potential opportunities to satisfy societal needs and to generate profit. Thousands of chemical products are manufactured, with companies like Minnesota Mining and Manufacturing (3M) having developed over 50,000 chemical products since being founded in 1904. The scope of chemical products is extremely broad. They can be roughly classified as: (1) basic chemical products, (2) industrial products, and (3) consumer products. As shown in Figure 1a, basic chemical products are manufactured from natural resources.

1. Basic chemical products include commodity and specialty chemicals (e.g., commodity chemicals – ethylene, acetone, vinyl chloride; specialty chemicals - difluoroethylene, ethylene-glycol mono-methyl ether, diethyl ketone), bio-materials (e.g., pharmaceuticals, tissue implants), and polymeric materials (e.g., ethylene copolymers, polyvinylchloride, polystyrene).

2. The manufacture of industrial products begins with the basic chemical products, as shown in Figure 1b. Industrial products include films, fibers (woven and non-woven), and paper.

3. Finally, as shown in Figure 1c, consumer products are manufactured from basic chemical and industrial products. These include integrated circuits, flat-panel displays, dialysis devices, solar desalination devices, drug delivery patches, fuel cells, hand-warmers, Post-it notes, ink-jet cartridges, detachable wall hangers, cosmetics, laundry detergents, pharmaceuticals, transparencies for overhead projectors, and many others.

Many chemical products are manufactured in small quantities and the design of a product focuses on identifying the chemicals or mixture of chemicals that have the desired properties, such as stickiness, porosity, and permeability, to satisfy specific industrial or consumer needs. For these, the challenge is to create a product that has sufficiently high market demand to command an attractive selling price. After the chemical formulation is identified, it is often necessary to design a manufacturing process.

Other chemical products, often referred to as commodity chemicals, are required in large quantities. These are often intermediates in the manufacture of specialty chemicals and industrial and consumer products. These include ethylene, propylene, butadiene, methanol, ethanol, ethylene oxide, ethylene glycol, ammonia, nylon, and caprolactam (for carpets); together with solvents like benzene, toluene, phenol, methyl chloride, trichloroethylene, and tetrahydrofuran; and fuels like gasoline, kerosene, and diesel fuel. These are manufactured in large-scale processes that produce billions of pounds annually in continuous operation. Since they usually involve small, well-defined molecules, the focus of the design is on the process to produce these chemicals from various raw materials.

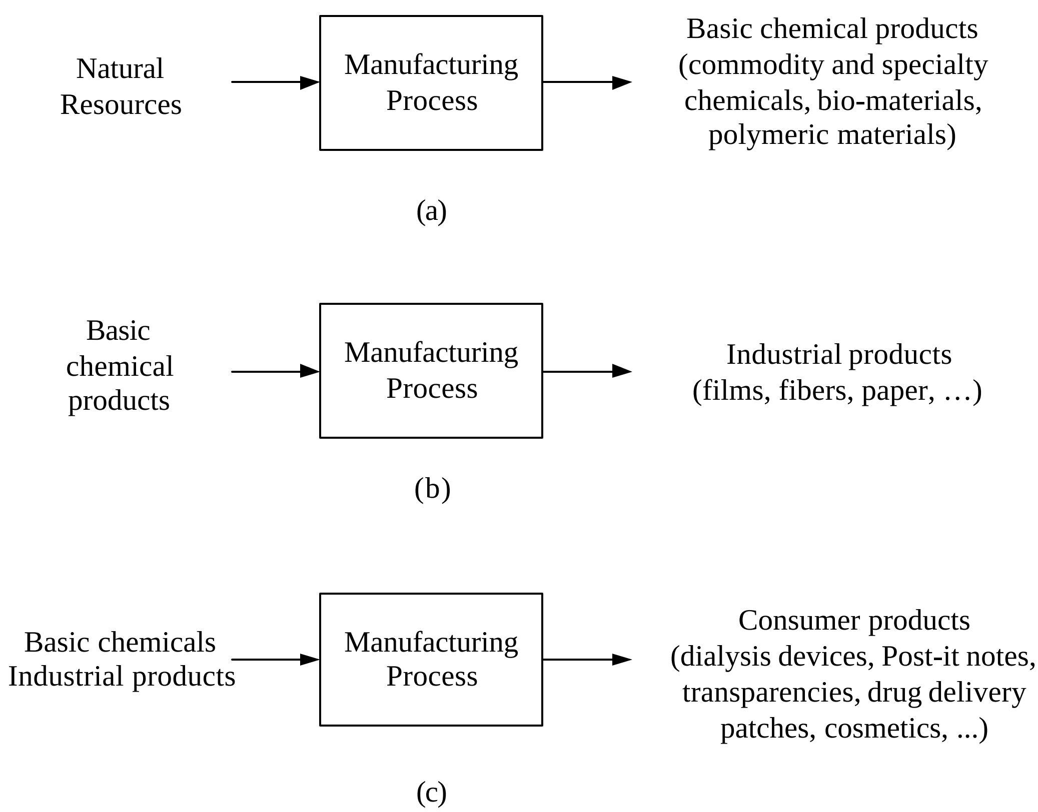


Figure 1. Manufacture of chemical products

Chemical engineers are highly employable principally because of their *process engineering* skills and because they excel in project integration. Consequently, we believe that the chemical engineering curriculum should retain its process-engineering flavor, to retain this edge that our graduates enjoy. However, noting that many chemical engineering graduates, more recently, are finding employment involving materials, semiconductors, and drug manufacturing, all of which are more product-design oriented, a shift in the emphasis of their design courses is justified. To more easily implement this shift, we suggest a combined *product and process design template*, to be discussed later.

Business Decision-Making and Stage-Gate Product Development Process

In an earlier paper (Seider et al., 2004b), a typical sequence of product development involving design engineers, operating engineers, marketing and sales personnel, potential customers, and business decision-makers (BDMs) was presented. Then, steps in the Stage-Gate product development process (Cooper, 2001, 2002) were described, as shown in Figure 2, with a gate following each step in which *Real-Win-Worth (RWW)* evaluation is carried out. Positive results are presented to *BDMs* who provide approval to proceed to the next step. In the *Real* evaluation, the extent of reality is assessed for a potential product. The *Win* evaluation assesses the competitiveness of the product with competitors in the market place (and the ability of the customer's manufacturing facility to accept the product, when applicable). Finally, the *Worth* evaluation assesses the anticipated financial reward of the new product.

Next, the five Stage-Gate steps and the *RWW* evaluation at each step are presented. Notice that the latter becomes more quantitative as the Stage-Gate process proceeds. Also, notice that the steps differ somewhat with the type of chemical product.

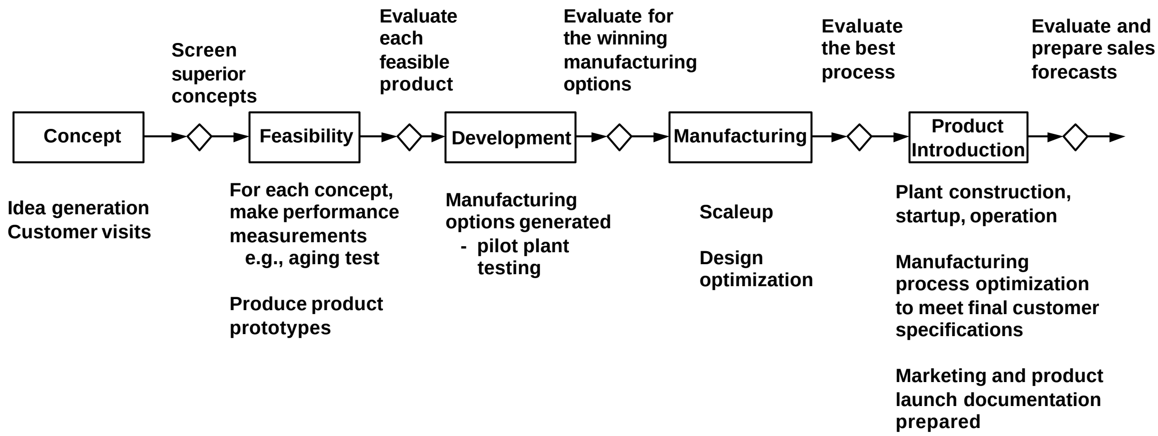


Figure 2. Stage-Gate product development process

Step 1 – Concept Development

This is one of the most creative steps in which ideas are generated, in an unconstrained atmosphere, keeping in mind customer needs. In this step, customer requests are translated into product requirements. Through an iterative process, the requirements are reviewed with the customers and refined as necessary. Product concepts are generated to achieve these requirements. Then, for the best concepts, the *RWW* evaluation is applied. The *Real* analysis evaluates whether the perceived needs for the concept are technically realistic and whether the business opportunity is potentially realistic, given limited information at this stage. Under *Win* analysis, at this point, usually just patent information is available to address potential competition in the marketplace. For *Worth* analysis, only crude estimates of costs and profitability are possible at this stage. Inputs to the *BDMs* consist of the superior concepts, which they screen for acceptability.

Step 2 - Feasibility

In this step, for each accepted concept, a rigorous feasibility study is undertaken. Usually this involves laboratory experimentation, with performance measurements made that correspond to the anticipated product performance. For example, an aging test may be devised to assess the product durability. For basic chemicals, this step begins with preliminary process synthesis. Again, the *RWW* analysis is applied to those products identified as feasible. At this gate, the *Real* analysis confirms that feasibility specifications are met. The *Win* analysis begins to assess the ability of the customer to utilize the feasible product (often in manufacturing facilities). Finally, the *Worth* analysis is refined after feasibility is confirmed. Given more promising inputs, the *BDMs* screen the feasible products.

Step 3 – Development

This step involves generation of the manufacturing options; that is, process synthesis for basic and industrial chemicals, and synthesis of the assembly line for configured consumer products. Often, these options are screened using process simulation and pilot-plant testing. In this case, the most promising processing concepts are evaluated using *RWW* analysis. Under *Real* analysis, the assessment focuses on workability of existing processing techniques. Here, a process that involves a complex separation of solid species might be given a low *Real* evaluation. Under *Win* analysis, the manufacturing process might be compared with others to judge its comparative ease of construction and operation. Under *Worth* analysis, as the manufacturing steps are identified, more meaningful cost estimates may be possible. Once again, the *BDMs* evaluate the most promising results, accepting those that meet higher criteria.

Step 4 – Manufacturing

This step involves the final design. The manufacturing process is scaled-up and optimized when appropriate. Again, the *RWW* analysis becomes more critical. Under *Real* analysis, the assumptions of scale-up must be carefully assessed. Under *Win* analysis, a more carefully conducted comparison of potential operability and controllability with other processes would be assessed. Under *Worth* analysis, the cost estimates should be refined using more detailed methods and databases, enabling a more quantitative assessment. And, consequently, the *BDMs* assessment should be more critical, given that approval leads to the construction of the manufacturing plant.

Step 5 – Product Introduction

This step involves construction of the manufacturing plant, start-up, and operation, with emphasis on quality control. In achieving the product specifications, the process is optimized. Marketing and product launch documents are prepared. In the *RWW* analysis, under the *Real* analysis, the realities of the anticipated channels to the market are evaluated. At this point, the *Win* analysis focuses on the ease of control and operation as compared with other manufacturing alternatives. Finally, the *Worth* analysis involves sales forecasts for the new product. Preferably, these sales forecasts include firm commitments by buyers. This is critical to avoid producing a superior product that does not compete pricewise. When the *BDMs* approve these inputs, operation of the plant proceeds as planned.

In previous discussions of the stage-gate process (Seider et al., 2004a,b), emphasis was on the design of basic chemical products. Beginning in the next section of this paper, the *Concept Development* stage of the Stage-Gate product development process is examined more closely as it applies for the design of the three kinds of chemical products. Then, Figure 1.2b of Seider et al. (2004a) on the steps in product and process design is revisited, it being recognized that it focuses almost entirely on basic chemical products. Finally, an alternate view, which focuses on the Stage-Gate product development process, is extended to apply to the three classes of chemical products.

CONCEPT DEVELOPMENT STAGE

In this section, the *Concept Development* stage is examined for the three kinds of chemical products. Emphasis is placed on the industrial and configured consumer products, of Figure 1, with examples presented to illustrate the implementation of the *Concept Development* stage.

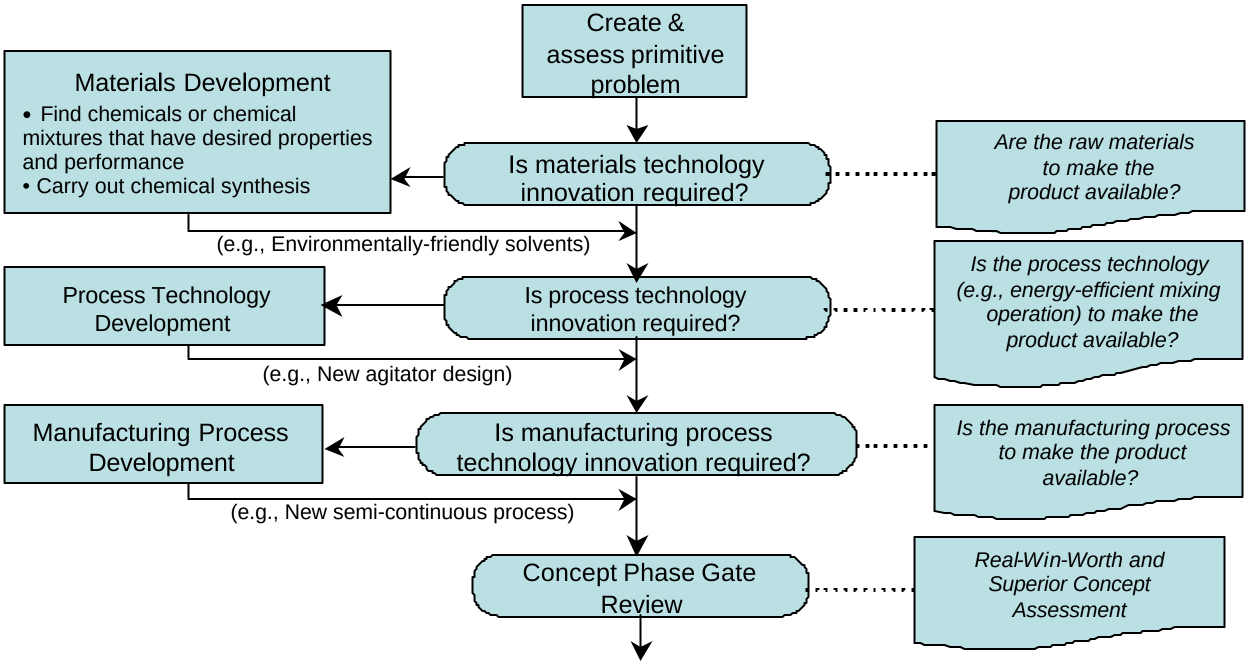
The *Concept Development* stage begins with the creation and assessment of a primitive problem(s) for a potential opportunity. Usually, the opportunity arises from a customer need, often identified by interviewing customers. Given an array of needs, an effort is made to arrive at specifications for the product. In many cases, a development and/or design team engages in a formal session to identify needs and generate ideas for the product. This involves brainstorming to arrive at concepts that are potentially promising in satisfying the needs. However, the ideas or concepts can also come from potential customers, competitors, consultants, etc. Initially, the ideas or concepts should be made without criticism. Having generated the ideas, an attempt is made to select the most promising among them using the principles of thermodynamics, chemical kinetics, heat and mass transfer, etc. In so doing, design teams create and assess *primitive problems* that are most worthy of research and development. These steps are discussed thoroughly in *Chemical Product Design* (Cussler and Moggridge, 2001).

After creating and assessing the primitive problem(s), questions relating to the need for new materials, processing, and manufacturing technologies arise. These are particularly important for the design of industrial and consumer products. To begin, however, consider the design of basic chemical products.

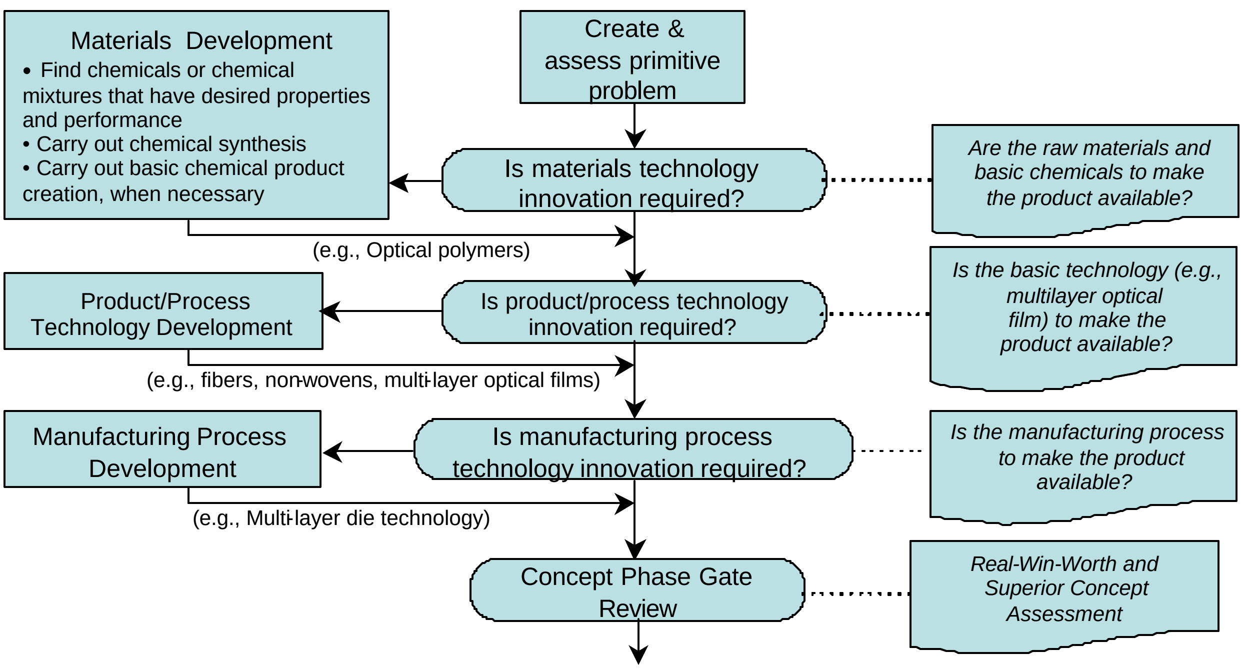
Basic Chemical Products

Figure 3a shows the *Concept Development* stage as it applies to the design of basic chemical products. First, the need for innovation in materials technology is questioned together with the related question of whether raw materials required to make the products are available. When materials need to be developed, this often involves a search for chemicals or chemical mixtures that have the desired properties and performance and/or reaction pathways in chemical synthesis (often referred to as *molecular structure design*). Examples of innovative materials that have been recently created are environmentally friendly solvents, refrigerants, and polymers (Seider et al., 2004a).

Next, the need for innovation in process technologies is questioned; that is, whether the process technology to make the product is available. For example, it may be necessary to develop a new energy-efficient mixing operation to achieve a more uniform molecular-weight distribution in a polymer product.

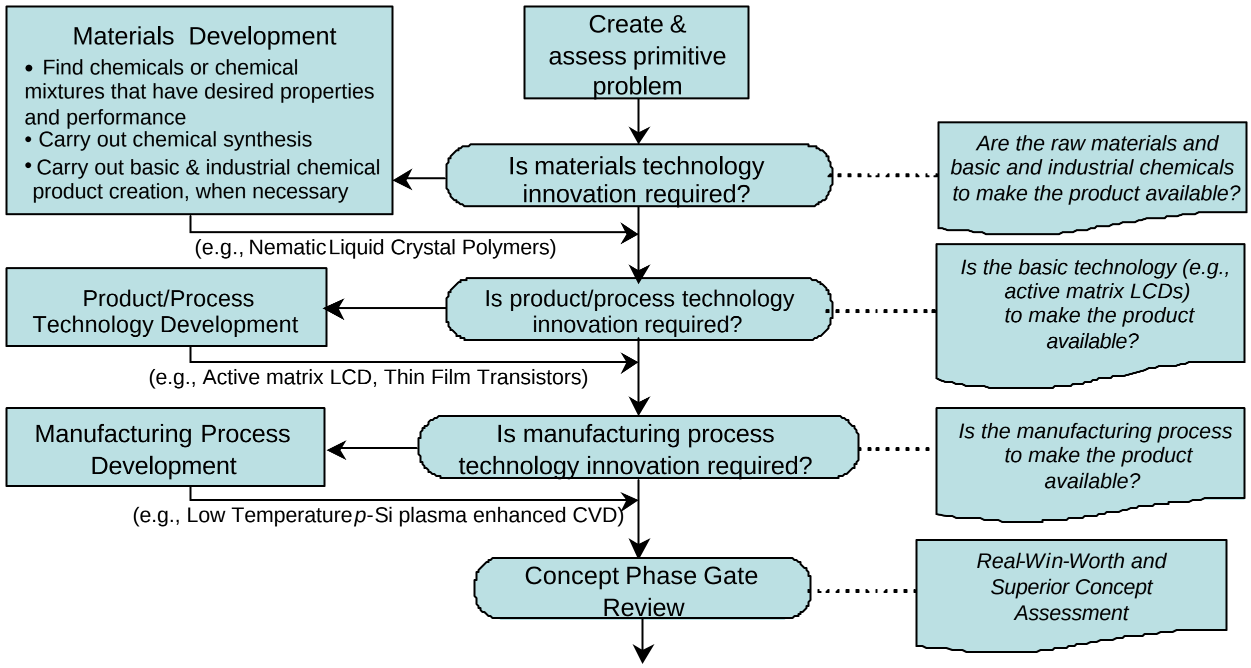


a. Basic chemical products



b. Industrial products

Figure 3. Concept development stage



c. Consumer products

Figure 3. Concept development stage (cont'd.)

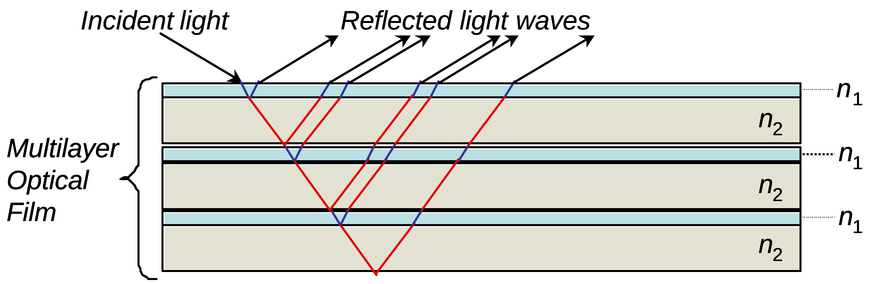
Finally, the need for innovation in manufacturing process technologies is questioned. As an example, when intermediate quantities of a specialty chemical are required, throughputs may be too small to justify continuous processing and too large to justify batch processing. In this case, it may be desirable to design semi-continuous manufacturing operations.

Industrial Products

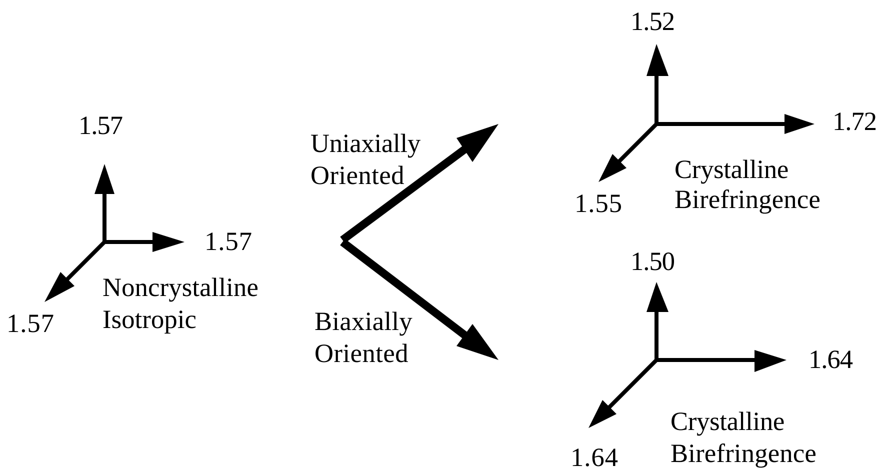
For industrial products, such as films and fibers (woven and un-woven), the concept development stage is extended as shown in Figure 3b. Here, when considering innovation in materials technology, it is necessary to question whether the raw materials and basic chemical products to make the product are available. Under materials development, in addition to searches for chemicals and chemical mixtures having the desired properties and performance, and reaction paths for chemical synthesis, it may also be necessary to carry out these searches for basic chemical products. Under product/process technology development, often new methods are needed; for example, methods for creating multilayer films. And, finally, under manufacturing process development, an example of something new would be multilayer dies for producing multilayer films.

To clarify the concept development stage for industrial products, consider the design of multilayer polymer mirrors (Weber et al., 2000). This industrial product combines thin polymer films, each having a different refractive index, to achieve prescribed properties of transmission, refraction, and reflection of light in specific wave lengths, as shown schematically in Figure 4a, where n_1 and n_2 are the refractive indices of the two films involved. These properties vary with the thickness and refractive index of the individual films. When creating multilayer stacks of polymer films, the first step in concept development involves finding the proper combination of layers to achieve the desired properties. Multilayer polymer mirrors are used in many consumer products such as: (1) coatings to tint automobile windows, allowing visible light to pass through, while reflecting infrared light waves, (2) protective coatings for rare paintings, permitting visible light to pass through, while reflecting ultraviolet light, and (3) mirrors for the backing of flat-panel displays and screens of laptop computers, thereby increasing their brightness.

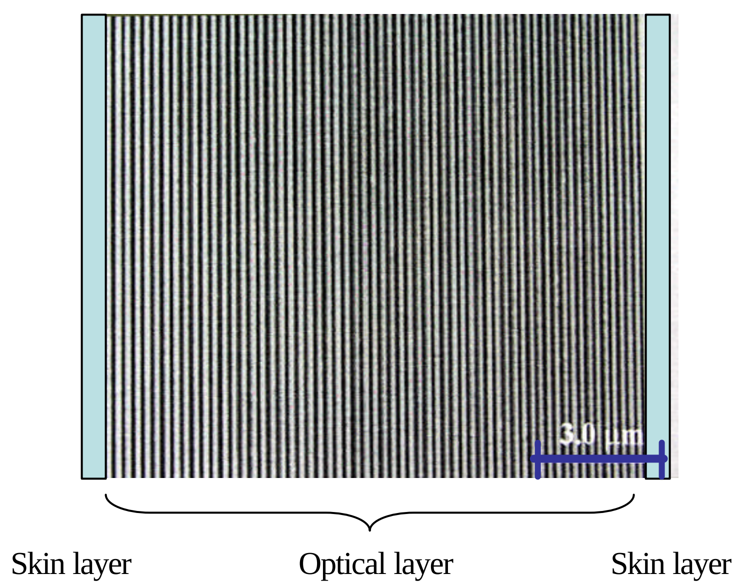
Typical materials selections are noncrystalline organic molecules, such as polyethylene-terephthalate (PET), polyethylenenaphthalate (PEN), or polymethyl-methacrylate (PMMA). These can be re-oriented uniaxially and/or biaxially (i.e., stretched) to produce optical birefringent polymers with non-isotropic refractive indices, as shown in Figure 4b (where the axes are annotated with refractive indices). When these films are constructed in alternating layers with thicknesses in the range of 10 nm to 1 mm, they can maintain or increase light reflectivity with increasing incident angle. This is a significant advantage as compared with conventional isotropic films that are characterized by a Brewster angle (angle of incidence at which no light is reflected from the mirror surface.) For non-isotropic polymer films, the Brewster angle is eliminated and the intensity of reflected light is increased over a broad range of incidence angles.



a. Product concept



b. Nonisotropic birefringence



c. Gradient multilayer polymer film

Figure 4. Multilayer polymer mirrors

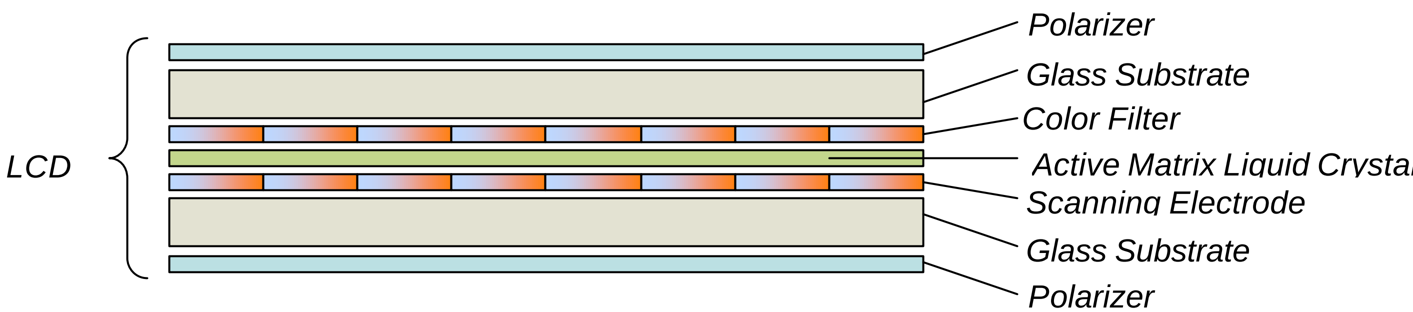
To produce multilayer polymer films, as illustrated in Figure 4c, it is often necessary to develop new processing units for precision extrusion, co-extrusion, and orientation (i.e., stretching). For co-extrusion, two techniques are commonly used: multiple manifolds with merger of effluents downstream of the extruder, and feed-block designs with effluent streams from the feed block sent to a single cavity extruder.

Finally, the new manufacturing process concepts often involve the design of new dies for continuous operation of precision extrusion, co-extrusion, and orientation.

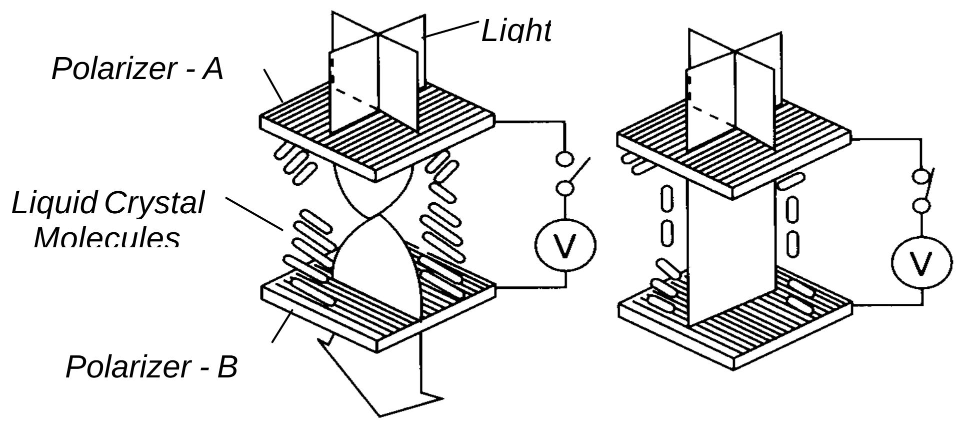
Consumer Products

For consumer products, such as hemodialysis devices, solar desalination units, flat panel displays, transparencies, hand warmers, and many others, the concept development stage is extended as shown in Figure 3c. Here, when considering innovation in materials technology, it is necessary to question whether the raw materials and basic and industrial chemical products to make the product are available. Under materials development, in addition to searches for chemicals and chemical mixtures having the desired properties and performance, and reaction paths for chemical synthesis, it may also be necessary to carry out these searches for basic chemical and industrial products. Under product/process technology development, new methods, for example, may be needed for creating active matrix LCDs. And, finally, under manufacturing process development, often innovations are needed in sequencing an efficient assembly line, for example the implementation of a clean room.

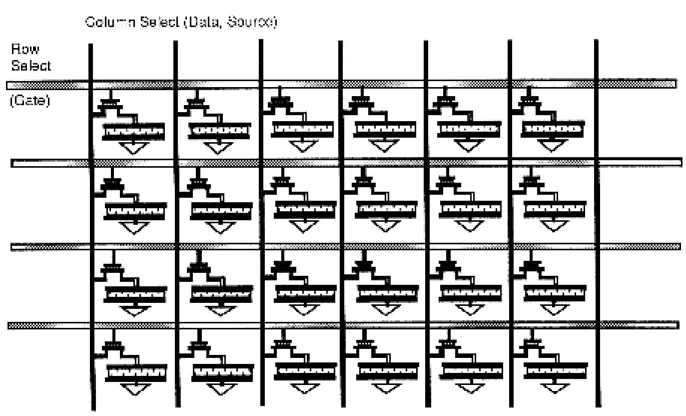
As an example of the concept development stage for consumer products, consider the design of flat-panel displays (Koike and Okamoto, 1999). These are rapidly replacing bulky cathode ray tubes to provide compact computer monitors and light-weight laptop displays. One product concept is shown in Figure 5a in which a sheet of liquid crystals arranged in an active matrix is bounded by a scanning electrode on one side and a color filter on the other. This sandwich sits within thin glass sheets, which are surrounded by polarizer layers. This multilayer structure is commonly referred to as the liquid crystal display (LCD). It often sits on a multilayer polymer mirror, which reflects a large fraction of light from a broad range of incidence angles, as discussed in the previous section on industrial products.



a. Product concept



b. Polarization of pixels



c. Active matrix LCD

Figure 5. Flat panel display

Under materials development, the key innovation involves finding organic molecules, that is, basic chemicals (e.g., 4-methoxy benzylidene-4'-butylaniline (MBBA) and its derivatives in Coates (2000)**),** known as liquid crystals, which can be re-oriented by applying an electric field. As shown in Figure 5b, because these materials are optically active, their natural twisted structure can be used to turn the polarization of light by, for example, 90 degrees. The two polarizers, A and B, transmit light in orthogonal planes. Light that exits polarizer A is naturally twisted 90°, and consequently, it can pass through polarizer B, producing a bright pixel associated with a specific cell. However, when an electric field is applied, the helical structure of light moving between A and B is unwound. As a result, light doesn't transfer through polarizer B, resulting in a dark pixel.

Innovative product/process technology centers about the active matrix LCD and thin-film transistor technologies. The active matrix LCD permits each LC cell to be addressed, with each cell corresponding to one monochrome pixel. In its simplest form, the active matrix LCD contains one thin-film transistor for each cell, as shown in Figure 5c. A row of pixels is selected by applying a voltage to the selected line connecting the thin film transistor (TFT) gates for that row of pixels. When a row of pixels is selected, the voltage is adjusted according to the data line. The TFT active matrix can be considered as an array of ideal switches that turn on and off a row of pixels.

Commonly, either amorphous-Si (a-Si) or polycrystalline-Si (p-Si) is used for the TFTs. To manufacture the TFT cells, a clean room is required [within Class 100 ($\leq$ 100 particles larger than 0.5μm/ft^3 air) to 10,000 ($\leq$ 10,000 particles larger than 0.5μm/ft^3 air)]. An innovative manufacturing process would include: (1) plasma enhanced chemical vapor deposition, (2) sputtering, (3) lithography, (4) wet processing and cleaning, (5) dry etching, and (6) TFT cell fabrication and assembly.

TEMPLATE FOR PRODUCT AND PROCESS DESIGN

In the preceding section, the *Concept Development* stage of the Stage-Gate product development process was extended to address the design of industrial and consumer products. In this section, the design template in Figure 1.2b of Seider et al. (2004a), shown here as Figure 6a, is mapped to the Stage-Gate product development process and extended to address the design of industrial and consumer products.

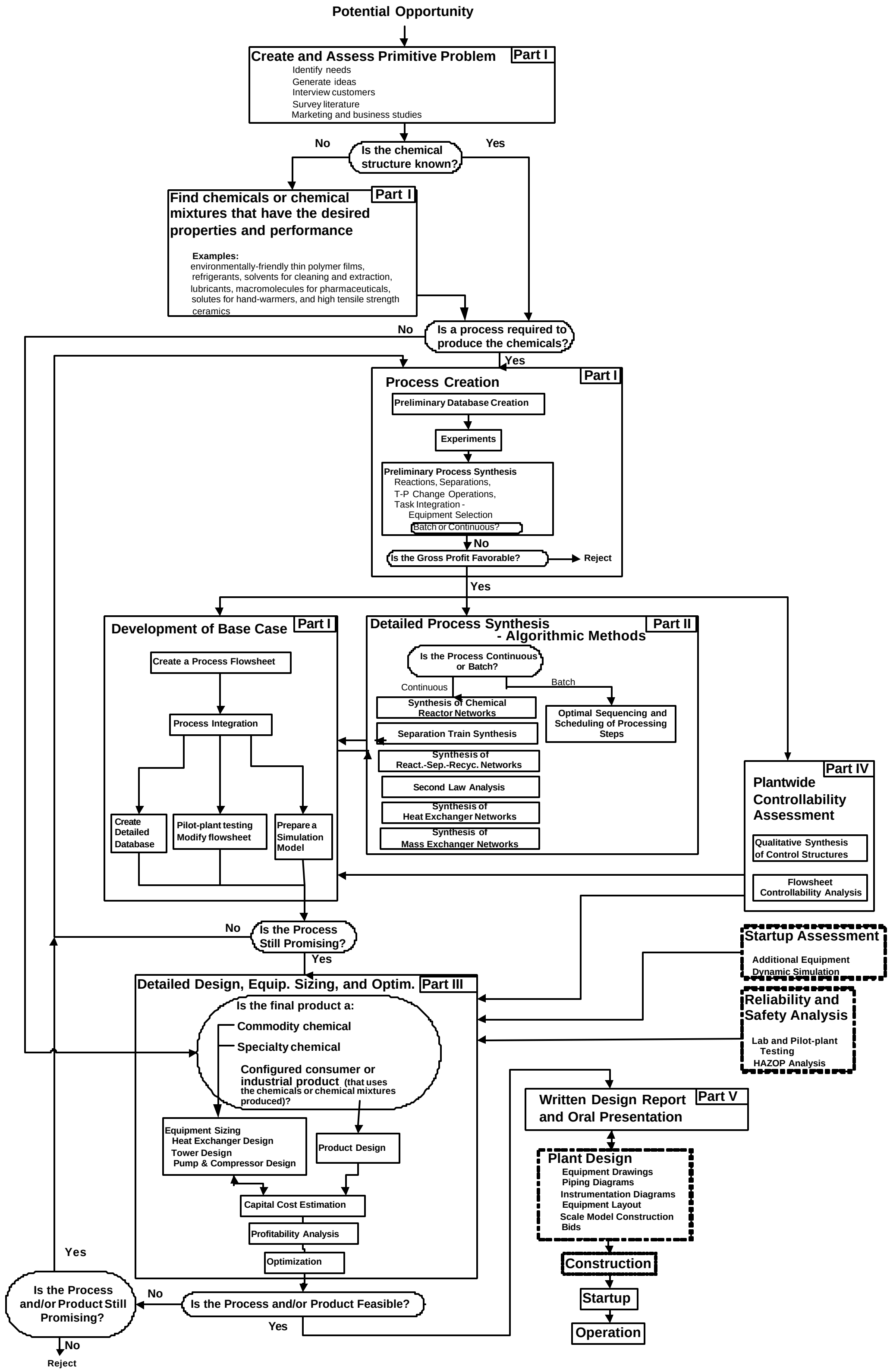
Basic Chemical Products

The template in Figure 6a focuses on the technical steps in generating design alternatives and preparing a product/process design, as applied to basic chemical products and processes. These steps are also carried out in the Stage-Gate product development process and it helps to understand the relationship of this template to the Stage-Gate product development process. Beginning with a potential design opportunity, the template shows the step, *Create and Assess the Primitive Problem*, which involves identifying needs, generating ideas, interviewing customers, setting specifications, surveying the literature (especially patents), and carrying out marketing and business studies. Then, if necessary, a step is carried out to *Find Chemicals or Chemical Mixtures that Have the Desired Properties and Performance.* These two steps correspond to the *Concept Development* step in the Stage-Gate process, as shown in Figure 3a.

When a process is necessary to manufacture the chemicals, the *Process Creation* and *Development of Base Case* steps in the template correspond closely to the *Feasibility* and *Development* steps in the Stage-Gate process. Note that pilot-plant testing and preparation of a simulation model are included under *Development of Base Case.* Note also that the methods of *Detailed Process Synthesis* and *Plantwide Controllability Assessment* also correspond to the *Development* step.

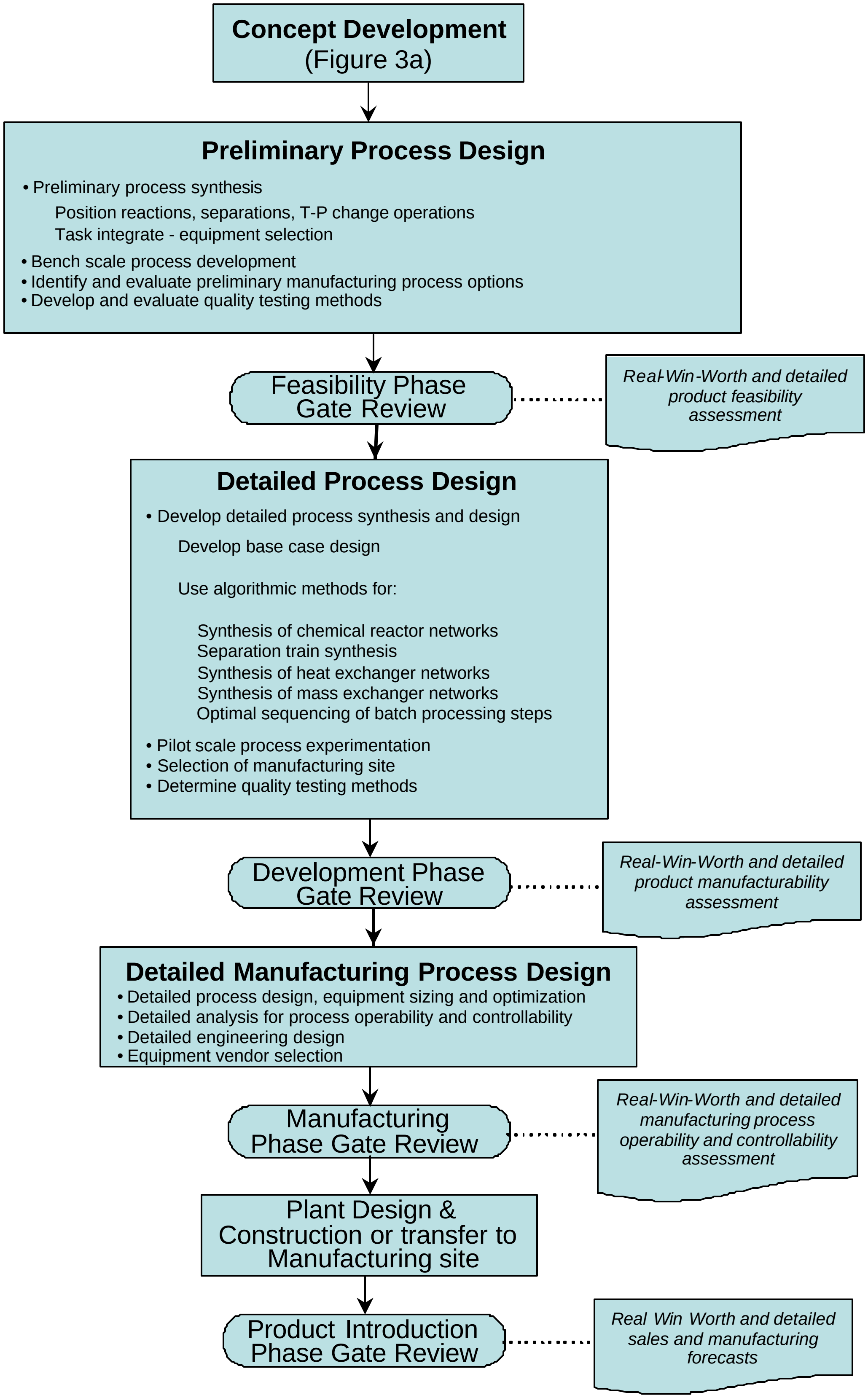
Finally, the *Detailed Design, Equipment Sizing, and Optimization* step in the template corresponds, in part, to the *Manufacturing* step in the Stage-Gate process.

An alternate view, which focuses on the Stage Gate process, is provided by Figure 6b. This template will be altered for the design of industrial products and consumer products, in the sections that follow.



(a) Seider et al. (2004a)

Figure 6. Template for steps in basic chemical product and process design



(b) Stage Gate development process

Figure 6. Steps in basic chemical product and process design (Cont'd.)

Industrial Products

Figure 7, when compared to Figure 6b, shows significant differences when industrial products, rather than processes, are designed. After the *Concept Development* step (see Figure 3b), preliminary product design occurs in the *Feasibility* step of the Stage-Gate process. Initially, a product prototype is constructed, usually in a laboratory. Then, the preliminary options for a manufacturing process are identified and evaluated at a bench or pilot scale. Methods for performance testing are developed and evaluated. Finally, the prototype product undergoes a preliminary evaluation by selected customers.

In the *Development* stage, detailed product design is carried out. This begins with the coordinated synthesis of the product and the manufacturing process. Alternate operations are considered for raw-materials handling (including feeding, pumping, web handling, drying, etc.), conversion (including extrusion, blending, and compounding), primary forming (including die/profile extrusion, pultrusion, and molding), secondary forming (including scaling, stamping, thermal/light treatment, etc.), and packaging. As these operations are selected, the design team begins to consider the ease of scale-up from the bench or pilot scale to the full-scale manufacturing process.

The *Manufacturing* stage involves the detailed design of the manufacturing process. This begins with the detailed design of the process units, including equipment sizing, cost estimation, and optimization. Detailed analysis for process operability and controllability is carried out next. Then, detailed engineering design and selection of the equipment vendors is undertaken.

Consumer Products

Figure 8 shows additional differences when designing consumer products. After the *Concept Development* step (see Figure 3c), in the *Feasibility* step, for consumer products, prototypes are constructed for both the product and the parts needed to assemble the product. Then, the preliminary options for a process design are identified and evaluated at a bench or pilot scale, as well as the preliminary options for the parts assembly process. As for industrial products, methods for performance testing are developed and evaluated, and the prototype product undergoes a preliminary evaluation by selected customers.

In the *Development* stage, both the operations for process design and the options for parts and parts assembly methods are considered. Alternate operations are considered for raw materials handling (including web/fiber handling, belt conveying, etc.), conversion (parts making including cutting and molding), finishing, and packaging. The other steps parallel those for industrial products in Figure 7. Likewise, the *Manufacturing* stage parallels that for industrial products.

CONCLUSIONS

Product design is a multi-disciplinary activity, especially in the design of industrial and consumer products. These products, as compared with basic chemical products, involve unit operations that are less commonly studied by chemical engineers, often involving solids handling and shaping, and chemical and physical vapor deposition. These have been enumerated in the templates containing the steps for the Stage Gate product development process.

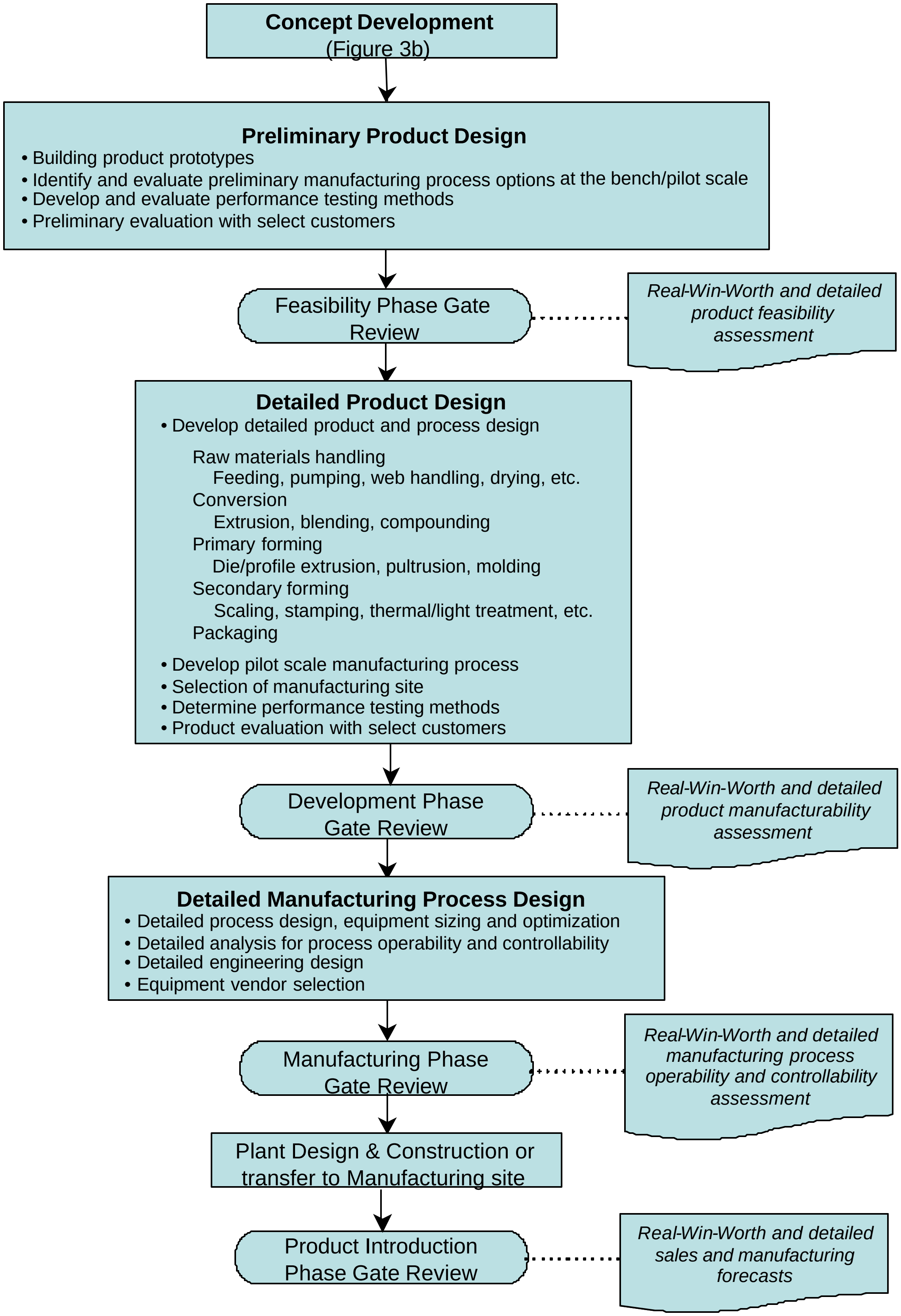


Figure 7. Steps in industrial product and process design

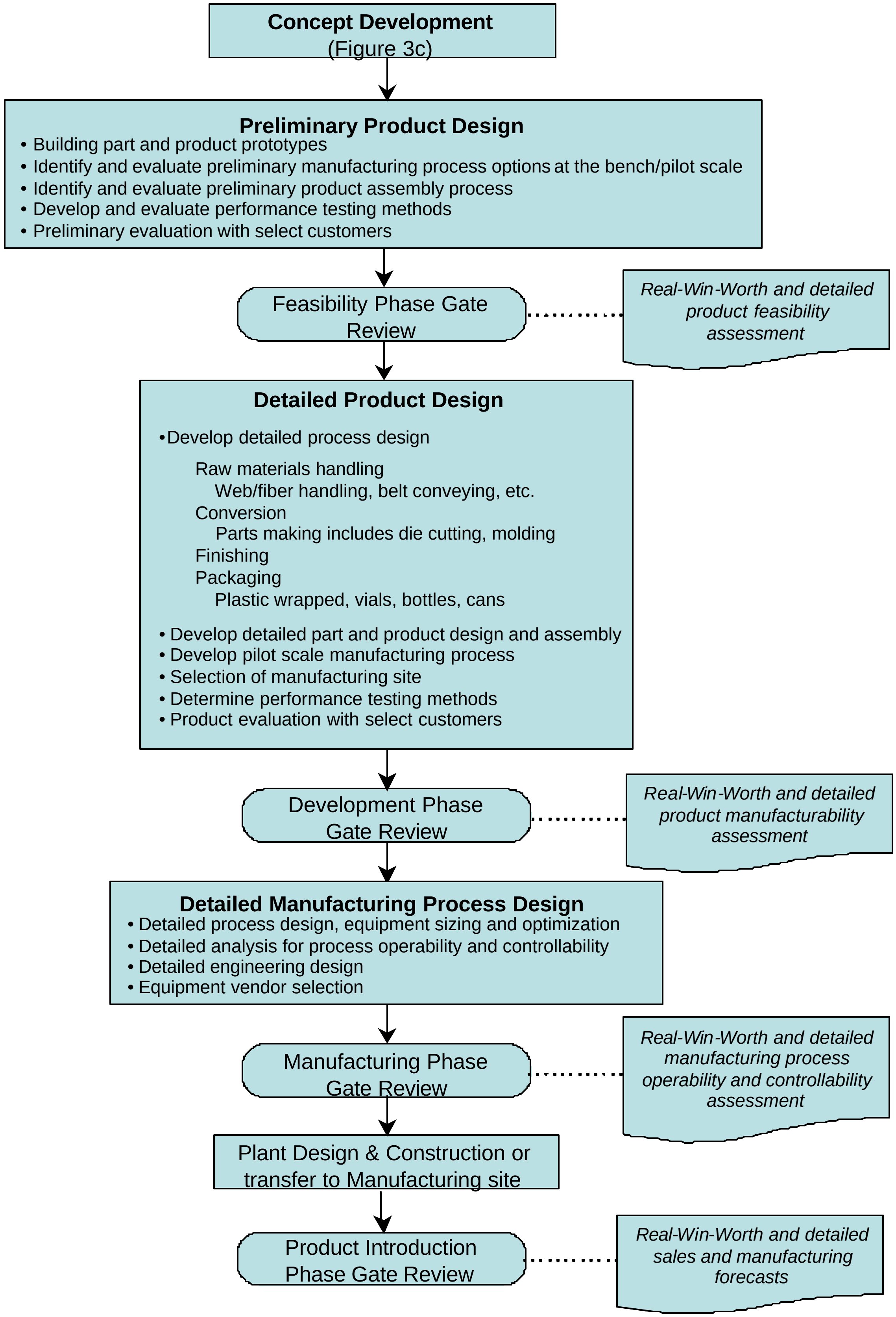


Figure 8. Steps in consumer product design

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