

# Systems Integration Design for Chemical and Biological Engineers: Gated Process Development with Digital Interlinks for Bulk Chemicals and Specialty Products Manufacture

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## ABSTRACT

The key systems integration concepts are described with respect to materials and energy flows in successive production units, process automation and supply chain life cycles incorporating also green process and clean technology considerations. The inclusion of environmental impacts monitoring and control as well as incorporation of pollution prevention and emissions abatement technologies to achieve green processing targets require increased levels of co-ordination, communication and functional integration of all the unit operation systems in these three principal domains; namely commercial products (including packaging), waste and emissions life cycles.

Two contrasting industrial case study examples are introduced to demonstrate the application of the concepts developed and discussed above. Each case study example comprises a list of main practical indicators followed by a list of instructions for step wise design application based on the process flow sheets of specific industry applications. These case study examples are introduced also to demonstrate the “open-ended” nature of ideas development and creative solution provision necessitated by complex systems integration design challenges for large scale process applications. It is believed that the case studies built upon the gated process development model will also provide a useful experiential teaching and learning tool for chemical and biological engineers.

**Keywords:** Systems integration design; Environmental impacts monitoring; Experiential teaching and learning

## INTRODUCTION

Holistic integration and optimization of chemical processes and consumer product manufacture require the application of holistic systems modeling in process and product design to evaluate the related environmental, socio ecological and economic impacts. Market research, impact assessment and risk management scenarios are used jointly to establish optimization of the business models for sustainability; combining optimal resource efficiency, and process costs with minimal adverse environmental impacts. These aims are satisfied through the incorporation of supply chain systems that make best use of industrial symbiosis and eco-industrial parks for shared and linked recycle, reuse, and regeneration of utilities, services and materials.

Many of the value added products manufactured in different market sectors rely on gated process development from chemical formulation to microstructural forming and to the manufacture of consumer products with advanced functionality. Product value addition is achieved typically by means of one or more of (i) inclusion of active excipients with targeted and paced chemical/bio-chemical functionality, (ii) incorporation of a dynamic microstructural

transformation in response to a specific environmental stimulus and (iii) maintenance of long shelf life and extended chemical/biological activity to ensure long term benefits with sustained user applications.

These advanced product functionality attributes are introduced typically in a series of gated process development stages that are also accompanied by process scale up and external material and energy flows integration during intermediate microstructural processing and subsequent macro processing stages at increasing levels of product plant throughput.

The paper describes the generic routes for product formulation, processing and manufacture adaptable to many product sectors ranging from foods and pharmaceuticals to healthcare and cosmetics and to a variety of household products which between them make up for some 75% of all consumer product sales. In addition, very similar process and product development routes with a great degree of generic adaptability and versatility are used for applications involving agriculture, transport and urban infrastructure.

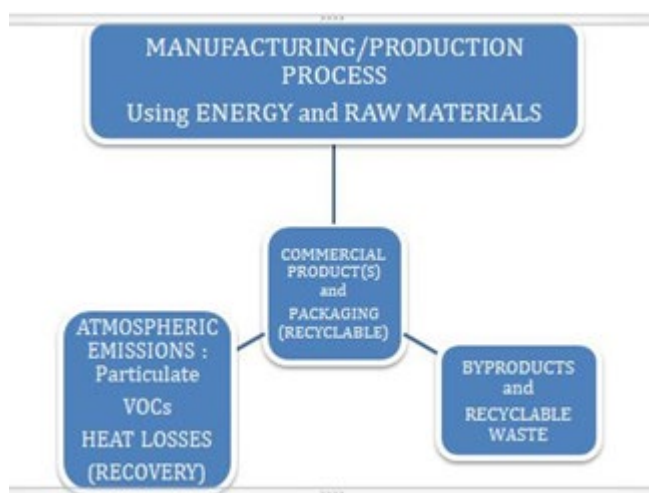
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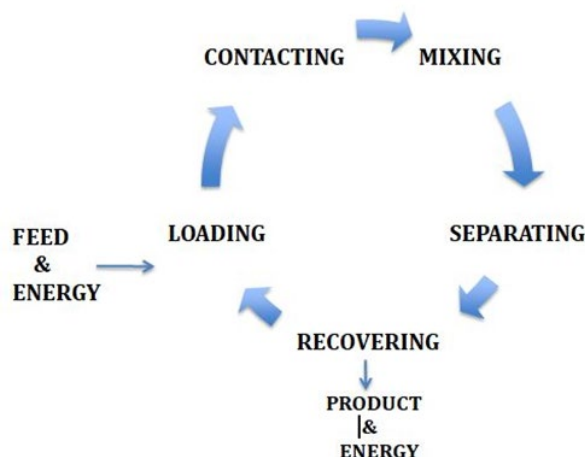
The key systems integration concepts are described with respect to (i) materials and energy flows in successive production units, (ii) process automation and supply chain life cycles incorporating also (iii) green process and clean technology considerations. As seen in Figure 1, the inclusion of environmental impacts monitoring and control as well as incorporation of pollution prevention and emissions abatement technologies to achieve green processing targets require increased levels of co-ordination, communication and functional integration of all the unit operation systems in these three principal domains; namely (i) commercial products (including packaging), (ii) industrial process waste and (iii) industrial emissions life cycles.



**Figure 1:** Going green in process/production/manufacturing

Figure 1 In plant Energy Recovery, Recycle and Reuse of Materials and Minimizing Atmospheric Emissions and Environmental Pollution Hierarchy of systems integration is completed by describing how an individual plant installation can be placed within an industrial eco-park which makes use of the industrial symbiosis principles [1,2] by association and co-linking of activities for materials and energy supplies and by reciprocal matching of waste recycling and byproduct re-use schemes with other plant installations in close proximity sharing the same eco-space; for further reading See [3,4].

## LIFE CYCLES OF GENERIC ACTIVITIES FOR LARGE SCALE BULK CHEMICALS PRODUCTION



**Figure 2:** Functional life-cycle stages of production

(i) Multiple Feed/Product and Energy Streams are possible as well as further addition/removal of material and energy at each intermediate stage specific to the production system, (ii) Energy (heat) recovery with final product yield also allows power generation

Figure 2 Above shows a functional life cycle schematic of a generic chemical product processing plant. The activities are typically organized to operate primarily in a feed forward mode of material and energy flows through successive unit operation stages that accept input feed streams and produce stage wise output streams. Within each operational unit, generically one primary physicochemical operation is affected at a time such as contacting, mixing, reacting, separating, harvesting and purification of the final product. Additionally, recycle streams of intermediate products and heat recovery is introduced to increase process efficiency and reduce process waste.

The large scale production processes involving high throughput flows of bulk chemicals often comprise continuous plant operations with steady state process control specifications. Such processes are also amenable to high levels of automation of the mechanical equipment operations, automated steady state process control and automatic monitoring of in stream product yield and product specifications including the final product specifications which are looped to provide feed-back control actions on the steady state feed forward process control instrumentation.

Furthermore, in a multiple raw material feed and multiple final product plant operation, the individual plant sections are organized to contain battery of operating units of each type of individual unit operation, functioning in parallel processing mode, with or without stage wise synchronizations involving mechanical shifts with pre-set time lags and/or operational phase frequency changes. The economies of scale of the multiple bulk chemical production process operating in the parallel processing mode drive the overall cost of production of per unit weight or volume per product to quite low values; see for example [5,6] for typical unit sale price quotations at different purity specs.

## DIGITAL PROCESS DEVELOPMENT GATES

To achieve the systems integration mission depicted in Figure 1, it is proposed that the respective life cycles are introduced within a gated process development framework comprising of the following Digital Process Development Gates: (1) Systems modeling for renewable materials and energy flows for large scale production, (2) Microstructural tailoring for advanced product functionality with minimal waste (3) Integration with digital control of the life cycles of multiple product streams in large scale value added manufacture, (4) Digital design for monitoring and control of environmental emissions, and, where possible, in plant abatement of environmental pollution, (5) Digital integration of in and out flows of materials and energy within eco industrial parks to take advantage of industrial symbiosis as described and referenced above.

## INDUSTRIAL CASE STUDY

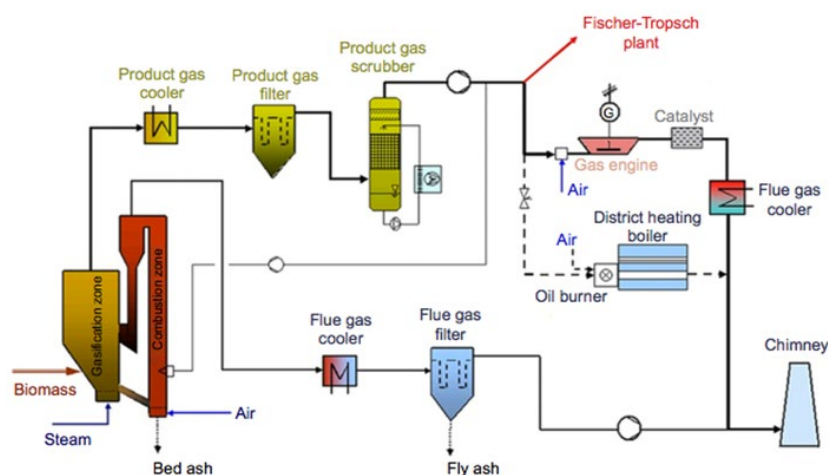
### Large scale production with gated parallel processing

Farm and forest residue is gasified in a fast internal circulating fluidized bed under high temperature and pressure to produce syngas with low NO<sub>x</sub> (<3%vol) and high H<sub>2</sub> (35%-45% vol) content that can be either used;

- (i) In a gas engine to produce heat and electricity or
- (ii) As feed gas to a Fischer-Tropsch Synthesis plant to produce biofuels (e.g. bio-methane, bio-diesel and dimethyl-ether (DME) [7].

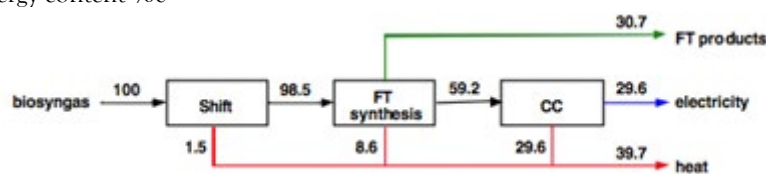
### Recommended reading

Chapter 12: Fischer Tropsch Synthesis to Biofuels (BtL Process), IN: Triantafyllidis, K.S., Lappas, A.A., Stocker, M., (Eds), The Role of Catalysis for the Sustainable Production of Bio-Fuels and Bio-Chemicals, 397-443, Elsevier Science, ISBN: 978-0-444-56330-9 [7].



(i) The flue gas is cooled, cleaned of ash and released into the atmosphere by a chimney as above. (ii) Bed ash and fly ash could be sold to construction materials manufacturing sector whilst (iii) CO and CO<sub>2</sub> emissions from chimney are monitored. (iv) Dry hot gas and wet cooled gas cleaning [7] are used with the Fischer-Tropsch synthesis to biofuels (Figure 3).

1. Using the schematic process flow sheet above, identify the process units above which can be linked to the individual digital process development gates (1-5).
2. Using the box diagram flow sheet below, identify the chemical reaction steps and conversions in the tri-generation stages of Water Gas Shift, Fischer-Tropsch (FT) Synthesis and Combined Cycle (CC) Power Generation units (numbers on flow streams correspond to the split of total energy content %)



3. Identify the steps that could be taken to modify the split of energy content between FT products, CC electricity and heat output streams i) in favour of more FT products, or ii) more power and heat; and indicate which option will result in reduced GHG emissions and/or greater overall energy efficiency and less waste.

**Figure 3:** Combined Heat and power (CHP) plant using Fischer-Tropsch synthesis to generate biofuels

## PROCESSING OF SPECIALTY PRODUCTS WITH VERTICAL INTEGRATION FOR VALUE ADDED MANUFACTURING

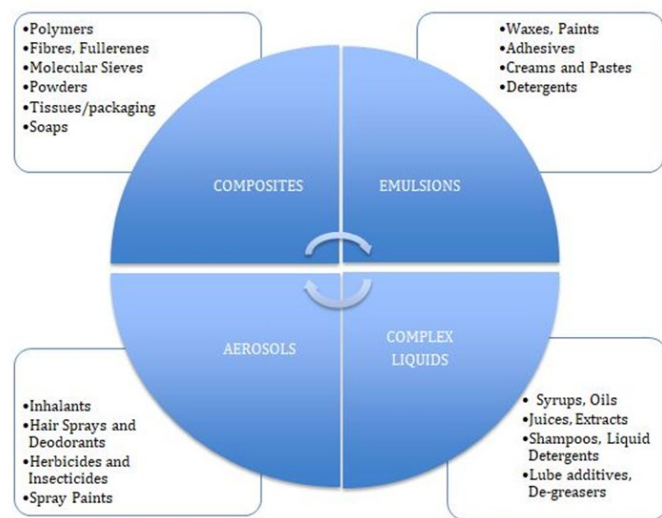
In contrast to the large scale processing of bulk chemicals, the specialty components produced with microstructural processing are often embedded, mixed and blended, encapsulated with other materials when produced at large scale; see for example [5,8] for more product details. Quite clearly, the systems for process unit operations are inherently not only parallel but also vertically integrated to provide the complex “value added” functionality that comes with the specialty applications.

Many of the value added products manufactured in different market sectors rely on gated process development from chemical formulation to microstructural forming and to the manufacture of consumer products with advanced functionality. Product value addition is achieved typically by means of one or more of (i) inclusion of active excipients with targeted and paced chemical/bio-chemical functionality, (ii) incorporation of a dynamic microstructural transformation in response to a specific environmental stimulus and (iii) maintenance of long shelf-life and extended chemical/biological activity to ensure long term benefits with sustained user applications.

These advanced product functionality attributes are introduced

typically in a series of gated process development stages that are also accompanied by process scale up and external material and energy flows integration during intermediate microstructural processing and subsequent macro-processing stages at increasing levels of product plant throughput.

Figure 4 depicts the typical product life cycles resulting in microstructural changes to intermediate products to achieve advanced functionality. The gated integration steps taken in successive stages of specialty chemicals production, harmful emissions and material and energy waste are contained within the integrated process flow sheet linking chemical synthesis precursor formulation product manufacturing; refer also to Figure 4. This interlinked process design approach allows for the necessary steps of (i) environmental containment and (ii) energy efficiency considerations to be integrated throughout all plant operations; [9,10] for the design and operation of an integrated continuous vacuum processing and indexed manufacturing system that provides for vacuum filtration, cake washing, pressing and drying of high solids slurries. The design also can integrate steaming, counter current washing as well as allowing for the mother liquor and the wash filtrates to be recovered individually and re-circulated/recovered/reused for a more efficient and versatile plant operation utilising multiple parallel product formulation routes.



**Figure 4:** Life-Cycle Stages of Microstructural Products

(i) The unit operations cycle involves selective and successive additions of solid and mixing of liquid components followed by selective thinning and aeration of liquids and pulverization and deposition of solids, (ii) selections of commercial consumer products accessible at each life cycle stage are also shown.

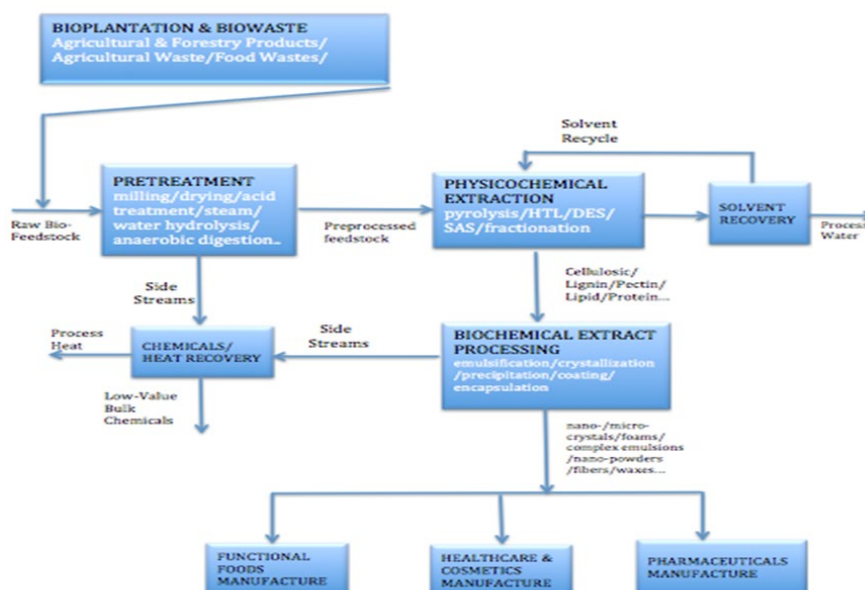
## INDUSTRIAL CASE STUDY

### Value added manufacturing from bio-feedstock

- Vertically Integrated Physicochemical Processing
- Specialty Bio-Chemicals Production
- Value Added Consumer Products Manufacture
- Recovered Process Water/Process Heat/Low value bulk chemicals can be regenerated/re-used either (i)“in process” or (ii) in other process applications.

### Recommended reading

Cadman, J.E., Zhou, S., Chen, Y., Qing, L. 2013, On the Design of Multifunctional and Microstructural Materials, Journal of Materials Science, 48(1), 51-66, Springer Publ., DOI: 10.1007/s10853-012-6643-4.



1. For each tier of the vertical integration, identify the process stages from the block diagram that correspond to the successive Digital Process Development Gates.
2. Identify the microstructural transitions depicted in Figure 4 above that correspond to the (i) physicochemical extraction, (ii) biochemical extract processing and to (iii) consumer product manufacture; investigate further one branded product application in one of the consumer products sectors.
3. Comment on the significance of byproduct recovery, heat and solvent recovery steps leading to process water and bulk chemicals production and suggest possible process units for cost effective solvent recovery and bulk chemicals and process heat recovery from side streams.

**Figure 5:** Gated Process Development for Microstructural Processing of Specialty Products

## GATED DIGITAL INTERLINKS BETWEEN PILOT DEMONSTRATION COMMERCIAL PLANTS REFERENCES

The intermediate product processing would normally be carried out in pilot plant units with a scale up factor of 10-100 in the gated Pilot Plant Stage (PPS) seen in Figure 5. In contrast to the chemical and bio-chemical active excipient formulation, the pilot plant scale is used to produce intermediates that accommodate (i) a structured distribution of the active components inside macromolecular chains, and/or (ii) by adsorption and deposition on solid substrate (e.g. cellulosic, sol-gel matrices, nanoparticles) supported scaffolds or (iii) aggregation and agglomeration using hydrophobic binders [8].

Figure 4 demonstrates a selection of physicochemical process steps used to generate the intermediate products with advanced functionality going into hybrid final product manufacturing plant designated as demonstration plant stage (DPS) in Figure 5.

Advanced functionality provided in the microstructural processing life cycles shown in Figure 4 can be gated for the final stage of scale up leading to commercialization of multiple product streams at a further 100-1000 fold production scale as seen in Figure 5. Figure 4 also provides examples of consumer products accessible at different intermediate product microstructures with increasing and decreasing levels of solid and liquid phases. Such consumer products are produced at commercial large scale industrial plants incorporating multiple product brands with a variety of specialties offered for consumer choice.

## DISCUSSION

### Interactive teaching and learning using digital gated process development

Digital gated process development framework described and exercised with the two contrasting case studies above allows for an experiential learning process through considerations of different configurations of (i) materials and energy flows, (ii) material splits for intermediate microstructural processing steps, (iii) solvent, waste heat, process water and bulk chemicals recovery steps and (iv) split between different final products and power production in hybrid energy process plants (HEPP) [11]. This approach is based on the principles of metacognitive learning that recognises the development of the active use of self-awareness, self-regulation of the individual's cognition, and the continual self-evaluation of their progress [12]. Recognize two types of metacognition: Reflection ("thinking about what we already know"), and self-regulation ("managing how we go about further learning"). This requires the self-centred learning approach by the student of transferrable skills (i) to make connections with what is already known and (ii) to re-evaluate progress when confronted with new concepts, constraints and development gates. To help the student to acquire these interactive learning skills in a cooperative learning environment, a number of metacognitive (self-awareness

support) activities are implemented in practice; for more details [13].

## CONCLUSION

An entirely generic framework for gated process development is presented connecting pilot plant, demonstration plant and commercial plant activities. Furthermore, the gated process development stages also include consideration of energy and material life cycles and environmental impacts directly in tandem with the development from pilot scale to large scale production. Use of interactive digital platforms enabling gated process development could and should also be used to facilitate interactive teaching and learning of the dynamic systems development and integration. Two industrial case study examples are considered for value added manufacturing of bulk chemicals and specialty products respectively by mapping the systems integration activities required for digital gated process development steps onto the individual process flow sheets. The most significant benefit of the approach lies in the ability to develop sustainable and environmentally friendly plant installations that can also take advantage of the dynamic local industrial eco system through effective symbiosis of energy and material supply chains by adaptable reconfigurations of the process flow diagrams as demonstrated in the two industrial case studies for interactive teaching and learning.

## ACKNOWLEDGEMENTS

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