KnowGenix *sustainable strategies*

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Transformations in chemical manufacturing

Since 2000 chemical manufacturing technologies have gone through rapid shifts in the way they have been developed and deployed. These transformations have largely been driven by developments ranging from climate change and sustainability mandates; rationalisation of business models and structures; shifts in product portfolio strategies; emergence of new manufacturing models; emergence of stringent regulations, energy efficiency models and complex supply chains; polarisation of global markets and migration of manufacturing, to name a few.

During this period, enhancing performance, reliability and safety have been the three pillars of the chemical industry. This involved meeting critical goal posts for the industry; some of which are;

- Higher product selectivity and yield by minimizing side reactions
- Tailored high quality materials through precisely controlled process conditions
- Accelerated development and optimization of new chemical processes
- Opening novel process windows: for processes which are not feasible hitherto
- Increasing productivity through higher reaction rates
- Improved process control

Chemical industry cutting across diverse sectors has been focused on identifying new strategies across the entire business chains The mandates to adopt policies which balance social, economic and environmental dimensions set forth by sustainable development protocols have a high impact on strategic decision making in chemical manufacturing. New digital technologies are ushering in a new era of sustainable and elegant manufacturing driven by data analytics and mining tools.

Differentiated products and services, customer engagement models, and real time analysis of market dynamics have become crucial as the industry strives to create sustainable value. Besides, innovation in plant engineering, material efficiency, resource optimisation, supply chain and facility management are gaining attention. With innovations happening more in the interphases of various disciplines the industry is geared today to develop newer operating models and identify newer skills development models to train its workforce handle the complexities of new technologies.

Game changers in the chemical industry

Chemical engineers work in diverse sectors far removed from traditional domains of the 90s. From petrochemical, refining and downstream segments they are now working in fields like like sustainable management, business, law, and a host of other disciples. The decade witnessed several game changing developments that redefined industrial growth.

Healthcare, energy, agriculture and other key economic sectors went through major transformations and drove far reaching innovations within the chemical industry. In the fine and specialty chemical industry there was an increasing focus on developing technologies that ensured full control of product properties than yields. These were complemented by rapid development of sustainable processes. New technologies, feedstocks, tools and the consumer have now emerged as the key game changers within the industry (1).

Technologies: Fuel-cell technologies, energy storage technologies; Carbon dioxide capture and valorisation technologies; molecular engineering, nano technologies; micromachining technologies; genetic engineering and gene shuffling technologies etc.
Practices/ enablers: Process intensification, process integration, advanced catalytic technologies, bio-transformations, waste valorisation, product engineering etc.
Manufacturing models: Distributed production, flexible manufacturing, shared manufacturing etc.
Tools: Advanced algorithms, scale spanning models, computational tools.
Sustainable models: carbon management, eco efficiency tools, newer feedstocks sources

The most profound shift in the chemical and allied industry came from the emergence of biology as a key chemical engineering science and the validation that synthetic biology is in fact based on chemistry. It did provide a tool to develop an improved understanding of modelling of cellular processes, and systems biology. In recent years the move towards addressing the needs of sustainability, healthcare, water, natural resources, functional products for ageing and disabled and related social dimensions have led to a shift in the way chemical industry focused its growth platforms.

Advanced materials for medical devices, customised drugs, protein products and innovative therapies using biomarkers have opened up new opportunities. Functional colorants for diverse applications made far reaching changes in several fields. Industrial biotechnology and nanotechnologies ushered in far reaching developments. Future regulatory domains will demand more attention for molecular engineering and molecular probes. Molecular engineering to develop new materials and new molecules and molecular probes that track and control the path of each molecule are on the anvil. Development of solid state chemicals for APIs and computational tools for smart manufacturing plants are being explored with fervour. In addition molecular transformations, multi-scale analysis and systems analysis and synthesis have attracted significant research dollars (1).

Emergence of new production concepts: Flexible manufacturing models

With ever increasing focus on sustainability in chemical manufacturing diverse options were explored by the industry in its efforts to rationalise manufacturing infrastructure and ensure safer, resource efficient, sustainable and flexible output. Rising demands for customised products and services pose immense challenges in manufacturing facilities. Since a decade chemical and pharmaceutical industry have been exploring newer approaches to further production efficiency. One of the primary approaches involved shifting from batch to continuous-flow and modularized production to ensure competitive, sustainable and faster to market products.

Competitive and high quality process intensification has been identified as a key challenge for the future industrial competitiveness of the chemical and related process industries. This is due to fast changing markets, shorter product life cycles, diversification of highly specialised products and shortage of raw materials and production capacities. Competitive manufacturing in the future will have to leverage the promise of intensified processes and new production concepts, to enable process efficiency, improve sustainability and speed up market launch.

There is an urgent need for flexibility in production to make it adaptable to product diversity and short product life-cycles as well as a need to improve eco-efficiency by using renewable decentralised feed-stocks. In traditional batch processing complex chemistries and chemical engineering practices synergise to produce high value products. This involved multi step processes and high investments. The continuous-flow and modularized process model is emerging as an competitive alternative to batch process to ensure simultaneous energy and resource efficiency- both critical components of sustainable manufacturing systems.

Moreover, these have minor ecological footprint, smaller equipment, lowered process cycle times besides maximising costs, quality and safety. It also is based upon new human-machine interaction approaches and digital technologies based on Internet of Things. Continuous-flow production is fully integrated and offers a facile option for those reactions that could not be made in batch mode (2).

Advances in flexible and modularised plant concepts

In speciality chemicals manufacturing modularized plant systems operating in a continuous mode permits faster response to increasing or decreasing market demands. The primary objective behind the use of modular plant systems is to use standard modules for continuous manufacturing processes; wherein different modules and components are integrated. They are also multi-scalable to accelerate modelling and process design. The dual process of synergising these components into modules along with associated integrated information modelling from the process design to the initial operation, are key to reduce throughput times and at the same time optimize energy efficiency of the process.

Integrated and multi-scalable reaction, separation, and other hardware modules form the basis of these modules and components to transfer laboratory reactions directly into commercial mass production. This approach eliminates pilot projects and supports the concurrent development of hardware modules for recurring process steps. These modules have to be integrated into a planning tool that supports the entire design process from early process development in the laboratory up to the 3-D plant model. Such modularisation enables increased efficiency and reduced time to markets. This leads to competitive production by enabling optimal balance between investments and operating costs.

Innovative flexible production projects

Combining **P**rocess **I**ntensification-driven Manufacture of Microstructured **R**eactors and Process Design regarding to **I**ndustrial **D**imensions and **E**nvironment (CoPIRIDE) and Flexible, fast, future (The F³ Factory) are two of the projects that have developed innovative technologies to support the shift towards greater versatility and smaller environmental footprints. They have led to novel technologies, processes and manufacturing concepts that find use in the design and operation of innovative chemical plants.

CoPIRIDE

CoPIRIDE is an EU-project that focuses on developing new technologies, processes and manufacturing concepts for the designing future chemical plants(3). One of the demonstration projects involved a chemical factory embedded in a special flexible and moveable container. This needed two different facilities, each equipped for a different process step. Another demonstration addressed the need for lower production ranges. This required a modular multi-purpose 'mini-plant', the construction of which was led by a consortium partner from the small and medium-sized enterprise (SME) sector. A separate demonstration plant was set up to allow researchers to explore the feasibility of producing biodiesel from waste oils in supercritical conditions. The demonstration targeted cost efficiency, greater competitiveness and improved sustainability compared to other starting materials and processing conditions.

The F³ Factory project

F³ Factory is a €30 million collaborative research programme that seeks to strengthen the European chemical industry's global technological leadership through faster, more flexible production methods. The F³ Factory consortium is made up of 25 leading companies and research institutions from nine EU Member states. They are collaborating on new technologies for process intensification and innovative new production concepts. Some of the key applications targeted within the F³ Factory project include solvent-free polymers, innovative surfactants, compounds for the healthcare industry and materials from renewable resources. Process intensification is a key challenge for the future industrial competitiveness of the chemical and related process industries in view of short product life times, high diversification and shortage of resources (4).

The F³ Factory consortium laid emphasis on the competitiveness of the chemical industry through novel manufacturing models and in specific modular continuous processes for low to medium scale production rates. The novel technology is suited to produce a range of diversified products, or to react fast to fluctuating raw materials supply or product demands. The operation of such a plant is more economical and more sustainable than the operation of continuous processes at world scale or (ii) the operation of batch processes at low to medium scale.

The new technologies and innovative production concepts developed by the interdisciplinary consortium are characterised by a *plug–and–produce* philosophy based on three main functional elements (5).

- A generic backbone facility constituting an interface
- A standardised process equipment containers (PEC) and process equipment assemblies (PEA) for high–quality chemicals production
- A holistic process design methodology, applying process intensification concepts and innovative decision tools.

The F^3 Factory project focused on reconciling the seemingly conflicting requirements of flexibility and resource efficiency in a novel way. It led to the development of a standardised, modular type of plant which was designed for easy deployment for any chemical manufacturing. Typically it represented a *plug-and-play* container-based production facility which involved design of design of software to facilitate and streamline the process design. The consortium partners expect a reduced time-to-market by up to 50%, lowered operating expenses and capital expenses by as much as 20% and 40%, respectively.

The F^3 Factory project combines the efficiency, consistency and scalability of a world scale plant with the versatility of batch plants in terms of the speed of introduction of a new synthetic process at low capital cost (up to -40%) in a data lean environment. It accelerates process and product development and delivers a substantial reduction in footprint of the production systems with respect to energy consumption (up to -30%), waste generation, raw material usage as well as increased yields (up to 20%) and plant volumes as a result of process intensification (up to the factor of 500) (5).

The unique aspect of this modular and container-based platform is that it can use any type of feedstock in contrast to conventional bulk processing which is tailored to a specific feedstock. The stakeholders also explored and integrated opportunities for process intensification into this technology. The F^3 Factory plant was designed either in a dedicated manner or as a multipurpose facility, without any changes to the design concept.

Four levels of standardised modular elements were involved in the process. These are:

Novel process intensified reactor technologies and downstream unit operations capable of fulfilling the requirements of a F³ Factory. (*PI optimised reactor technology: jet-loop reactor; PI optimised separation technology: organophilic nanofiltration membrane*)

Process Equipment Assembly (PEA) as the smallest modular element associated with one or several unit operations (*a jet loop reactor with integrated membrane separation module*)

Process Equipment Containers (PEC) which constitute a superstructure holding PEAs in position and providing the services required for operating the PEAs. (*logistics functions, process control elements, etc*.)

Backbone Plants providing general services to the PEC(s). A F³ Factory plant can have one or more backbone plants.

Case studies using The F³ factory technologies (5)

Demonstration of a new 'transformation methodology' for increasing throughput of early phase pharmaceutical materials (Leadership: AstraZeneca)
It involved the development of a proof of principle concept for the flexible, continuous production of pharmaceutical development materials for toxicological and clinical studies. A new generic transformation methodology for the formation of pharmaceutical intermediates was developed and validated.

Development and validation of modular, continuous production concept on medium scale plant level (20-30 kilo-tonnes/p.a.) for decentralised production based on renewable resources (Leadership: Arkema)
The key aim of this project was to demonstrate the technical and economic viability for the production of high volume intermediate chemicals in a modular, medium-scale plant. The target was the production process of acrylic acid and its derivatives from biomass-based glycerol.

Process intensification and solvent-free production of high viscous polymers (Leadership BASF/Bayer)
The primary objective was to demonstrate a concept for multi-product, small-to-medium scale production of high viscous polymers in a solvent-free manufacturing process. This involved development of a new flexible reactor

technology which can be demonstrated within a modular, continuous production unit.

Transfer of a multi-step synthetic batch process for pharma intermediates to a fully continuous manufacturing process (Leadership: Bayer)

The focus was to develop a modular, flexible continuous production of active pharmaceutical intermediates. The shift of a multi-step synthetic batch process for pharmaceutical intermediates to a fully continuous manufacturing process in a modular, flexible infrastructure - including downstream processing was investigated and demonstrated.

Demonstration and economic evaluation of new modular production technologies for highly exothermic reactions (Leadership: EVONIK)

This project involved the demonstration of the flexible, continuous production of intermediate chemicals. A generic methodology for modularised production plants of medium scale was developed, validated and exemplified on two different technologies: structured catalyst packing and jet-loop reactor with integrated “cold” membrane separation.

Evaluation and demonstration of step-change process intensification in the production of anionic surfactants for local markets (Leadership: PGB)

This study involved validating a new intensified reaction technology for surfactants production. In addition it aimed at a step-change process intensification in the production of anionic surfactants. It concentrated on two key reaction stages (S02 oxidation and sulphonation) using novel reaction technology and modeling of the economic viability of the concepts.

Demonstration of the F^3 Factory concept to enable transition from batch to continuous multi-product plant for different polymers (Leadership: Rhodia/BASF)

This project was aimed at developing a flexible, modular production of water soluble speciality polymers. It was planned to design and build a continuous, multi-product pilot plant to demonstrate the technical and economic viability of the F^3 Factory concept for the production of solution polymers. It included investigation of two model polymer systems: acrylic acid-based copolymer and homo-polymerization of acrylic acid and copolymerisation of acrylic acid with second monomer with extremely different copolymerisation parameters.

Future road map for innovative production platforms: an imperative

Of late there have been reports of flexible plants being implemented with capacity and location flexibility. Most of these plants have been in segments like fine and specialities and pharmaceuticals. At present public-private initiatives in flexible production are EUROPIC, Britest (UK), FISCH (Belgium), Provide (TNO in the Netherlands) and INVITE (BTS in Germany). In addition diverse private collaborations and platforms exist.

Primary drivers for flexible plants are shortened time to market; fast response to market demands; enabling quick market entry and reducing CAPEX risks. Chemical production can be flexible in multiple ways; in capacity, product type, innovation, location and feedstock. At present advances in tools and systems have enabled the implementation of flexible plants as the modular design offers the needed flexibility to increase or decrease capacity. This is aided by key enablers such as process intensification and continuous processing, novel manufacturing technologies like 3D printing, to name a few. At present the concept is being applied to R&D and pilot setting.

The chemical industry and in particular the fine and speciality chemicals industry is opting for decentralised, flexible production capacity and in this effort an ideal flexible plant should meet key norms; competitive production of high value and small volume chemicals; and product, innovation, feedstock and location flexibility. In practice it is possible to have only a couple of flexibility and there is no plant operating with all the needed flexibility (6). For the chemical industry stakeholders developing collaborative business and technology roadmap for innovative production platforms will be key to ensure sustainable, competitive and low footprint chemical plants.

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