WHITE PAPER

Fine and Specialty Chemicals: Global Impact, Advances, and Challenges

The screen or paper on which you are reading this, your chair, the way your drinking water is pre-treated, the pain reliever you reach for to ease that headache – all of these diverse items and processes, plus tens of thousands more, rely on the chemicals industry. The global chemicals industry supports the production of an enormous range of products that are used worldwide. Some chemicals become components of physical products. Others are essential for industrial processes.

Commodity, Fine, and Specialty Chemicals

The chemicals industry is segmented into three major categories: commodity chemicals, fine chemicals, and specialty chemicals. Commodity chemicals are used to produce fine chemicals. Fine chemicals are blended to make specialty chemicals with end-use-specific properties.

The commodity chemicals category can vary among industries. Petroleum and other energy/fuel chemicals are often considered to be organic commodity chemicals. In general, the chemicals industry considers organic commodity chemicals to be those that are mass-produced from petroleum.

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Commodity chemicals are the starting materials for the chemicals industry. They are mass produced in continuous-process chemical plants to meet global demand.

- **Organic commodity chemicals** are petroleum-based (aka, petrochemicals) and are primarily benzene derivatives. A few examples of commodity chemicals include ethylbenzene, xylenes, cumene, cyclohexane, aniline, chlorobenzenes, and phenols.
- **Inorganic commodity chemicals** are based on metals and other minerals. These elements are used to produce acids, bases, oxides, salts, and other inorganic chemicals. Examples of inorganic commodity chemicals are caustic soda and potash, hydrochloric acid, sulfuric acid, iron chloride, and copper oxide.

Fine chemicals are pure, single chemicals produced in customized batches. The production of fine chemicals is a complex, multi-step process that must meet rigorous specifications and produce batches with ultrahigh purity levels. Examples of fine chemicals include active pharmaceutical ingredients (API), peptides and proteins, steroids, alkaloids, and biocides. Fine chemicals are used to produce specialty chemicals that have specific characteristics needed for their target end use. A few examples of industries that rely upon fine chemicals include pharmaceuticals, agrochemicals, electronics, automotive, cosmetics, and construction.

Specialty chemicals are blends of two or more fine chemicals that produce a mixture with a specific function. Specialty chemicals are sometimes referred to as performance chemicals or effect chemicals because the focus is on their action in the end-user's application. A wide variety of products and processes rely on specialty chemicals such as catalysts, corrosion inhibitors, livestock feed additives, photography, paints, inks, coatings, water and waste treatment chemicals, and many others.

History

The modern chemicals industry got its start in the early 1800s when the focus was primarily on explosives and dyes. The organic chemicals industry is considered to have begun in 1856 with British teenager William Perkin. The young chemist was working on developing a process to synthesize quinine, a natural anti-malarial treatment that was in high demand and very expensive. Perkin was experimenting with reacting potassium dichromate with different coal-tar derived salts. After trying aniline salt to no avail, Perkin was using alcohol to clean one of the experimental flasks when a purple solution formed in it. The solution was found to easily and permanently dye fabrics – the first coal-tar aniline dye. Thus began the burgeoning of discovery and production of petroleum-derived organic chemicals.[1,2]

England was the hub of the growing chemicals market for several decades, with Germany taking the lead in the 1880s. France and the United States also had substantial chemicals markets during that era.[1]

The advent of World War I prompted another period of intense innovation and growth in the chemicals industry. Stalled supply lines for much needed medicines and other chemicals spurred such growth in nations around the globe and many new chemicals were discovered and manufactured.[3]

The industry continued to innovate during the 20 years after the end of World War I, including developments in polymers, agrochemicals, and medicines. However, the full commercialization of the new materials lagged until the Second World War. During the 1940s, innovative chemical production and use included synthetic rubber, polymers, light-weight aircraft materials, chemical weapons, and others.[4]

By the 1950s, the pharmaceutical and agrochemical industries were well-established and continued to grow, leading the way in organic chemicals in particular. Distinct fine chemicals and specialty chemicals segments were in place by the late 1970s. The chemicals industry has supported life-changing innovations over the last 40 years, persevering through volatile global economies and raw materials prices.[1,3]

The Chemicals Market

The pharmaceutical industry has been the largest consumer of fine chemicals for several decades. Agrochemicals is another long-time, large-volume consumer. The electronics industry is a growing driver of growth of the fine chemicals industry.

In 2019, the global chemicals industry achieved revenues of 3.94 trillion USD. Global market share is dominated by Asia which has been the case since 2012. China is the largest chemicals producer claiming approximately 36% of global sales in 2018 followed by the European Union (EU) at 17% and the United States (US) at 14%.[5,6]

Commodity Chemicals	Fine Chemicals	Specialty Chemicals
Single basic chemicals	Single complex chemicals of ultrahigh purity	Mixtures of fine chemicals
High volume production Low cost	Low volume production (<1,000 tons/year) High cost (>$10/kg)	Quantities and costs based on end-use industry
Mass produced in continuous-process plants, using standardized reactions, to meet global demand	Produced in customized batches	Blended in customized batches
Use is based on their versatility as raw materials	Use is based on specific molecular characteristics	Use is based on specific functionality

Fine chemicals make up the largest portion of the global chemicals market. Global fine chemical revenues were 155.55 billion USD in 2018 and are expected to grow to 219.49 billion USD by 2024. Europe and North America lead the way in fine chemicals production. In 2018, fine chemicals revenues were 46.31 billion USD in Europe and 36.17 billion USD in North America. The Asia-Pacific region is growing in fine chemical production, especially China and India.[7]

The pharmaceutical industry has been the largest user of fine chemicals for many years. Fine chemical purchases by the pharmaceutical industry were 78.2 billion USD in 2016 and are projected to increase to 153.7 billion USD by 2025. The continuous growth is considered to be driven primarily by the aging global population as well as an increasing demand for preventive healthcare innovations.[8]

The global specialty chemicals market generated 630 billion USD in 2019. It is projected to grow at a rate of 3.7% between 2020 and 2027. This market growth is being driven by increasing demand for high-performance and function-specific chemicals across the end-use industries such as oil and gas, pulp and paper, and personal care and cosmetics. These chemicals are referred to as specialties because they are produced in lesser volumes and cater to only a few applications unlike the rest of the fine and commodity chemicals.[9]

Through July of 2020, the top five specialty chemical segments globally were polymers, electronics/electrical, industrial and institutional cleaners, surfactants, and flavors and fragrances. Combined, these segments comprised approximately 38% of the specialty chemical market. China was the largest consumer of specialty chemicals, followed closely by North America. Together, they use nearly 50% of global specialty chemicals.[10]

The COVID-19 pandemic of 2020 has impacted the chemicals industry in various ways. For example, during second quarter 2020, BASF experienced much lower demand from the auto industry for materials, surface technologies, and basic and performance chemicals. At the same time, the company's nutrition and care business earnings grew and agrochemical earnings were steady. The result of these contrasting activity levels was an overall sales decrease of 12% compared to second quarter 2019. Other chemical company's report similar slowdowns in the automotive sector with concurrent stability in others.[11]

Activity within the chemicals industry has also been affected by the Covid-19 pandemic. During the first half of 2020, the volume of acquisitions/sales/mergers among chemicals companies decreased significantly from 2019 levels. The only large deal announced was INEOS's acquisition of BP's Global Aromatics and Acetyls business.[12]

Challenges

Reliable production and use of chemicals is only possible when the industry's technical needs and challenges are successfully met. Some needs and challenges are common to all chemical sectors, others are segment-specific or end-use specific.

From raw materials to end product, chemical manufacturing uses a series of integrated steps that include QA/QC checks throughout the process. The first step in every chemical manufacturing workflow is analysis of raw materials for composition and purity before they enter the production process. As the production workflow proceeds, monitoring is conducted at strategic checkpoints to ensure the process maintains high efficiency, yield, and throughput.

Fine Chemicals

Fine chemicals have stringent customer requirements, many of which are based on end-use industry or regulatory standards. For example:

- The pharmaceutical industry is required by law to adhere to good manufacturing practices (GMP) throughout the production process, including the composition, concentration, purity, and stability of active pharmaceutical ingredients (API), inactive components, and packaging materials.
- The agrochemicals industry is required by law to adhere to strict standards for active pesticide ingredients, including composition, concentration, purity, and stability.
- The electronics industry is guided by SEMI Standards that define the ultra-high purity levels needed for chemicals used in the electronics and semiconductor industry.

Thus, in fine chemicals manufacturing, intermediate chemicals must be closely monitored for adherence to customer and regulatory specifications. Key characteristics that are typically monitored for all fine chemicals include:

- Molecular structure
- Potential contaminants
- Chemical properties

Process QA/QC

Production QA/QC Considerations		
Raw Materials QA/QC	**In-Process Monitoring**	**Final Product QA/QC**
• Composition • Concentration • Purity	• Molecular structure (fine) • Presence of contaminants • Phys/chem properties • Efficiency • Yield • Throughput	• Composition • Molecular structure (fine) • Concentration • Purity • Stability • Phys/chem properties • Functionality (specialty)

Intermediates are also monitored for batch-specific requirements. The final batch of each fine chemical production run undergoes the same analyses conducted on process intermediates, plus determination of its final composition and concentration, purity, synthesis residues content, and batch-specific requirements.

Specialty Chemicals

The growing diversity of specialty chemical blends requires even more sophisticated quality control protocols. Advanced analytical instrumentation is needed to:

- Determine the complex composition of specialty chemical blend
- Confirm each blend's purity level
- Verify that it meets the functionality specifications required for its intended end use

Upon final product analysis of each fine or specialty chemical batch, a detailed compositional certification should be generated and provided to the customer with the shipment. An integrated analytical platform can auto-generate and record the required documentation following completion of each final batch analysis.

Regulatory Compliance

Chemicals manufacturers need to maintain compliance with all applicable regulatory requirements in their countries of operation and their locales. A few nearly universal compliance requirements are considered here.

Permitting

A facility that uses materials that are classified as hazardous will need to be permitted to obtain, store, and use those materials. The permit stipulates the types and amounts of materials the facility can obtain, store, and otherwise use in their operations. It also defines the monitoring, record-keeping, and reporting requirements to maintain the permit.

Air permitting is required for chemicals manufacturing operations. The requirements of the permit will depend on the content of the air emissions and the location of the facility. Air permits stipulate the monitoring, record-keeping, and reporting requirements to maintain the permit.

On-site Materials Management

The chemicals manufacturing facility must have a materials management plan for all chemicals present at the facility, both hazardous and non-hazardous. The plan must address how the materials will be loaded and unloaded, stored and moved within the facility, and spill prevention and containment measures. The plan will include maintenance and monitoring schedules, spill response plans, reporting procedures, and record-keeping procedures.

A stormwater pollution prevention plan may be required, depending on the extent of outside storage or operations at the facility. The plan includes sampling and analysis procedures for stormwater discharges, remedial action plans, and record-keeping and reporting procedures.

Off-site Materials Transport

The transport of produced chemicals to customer and other downstream facilities must comply with federal, state, and local transportation regulations. Considerations for transport planning and compliance include vehicle and container requirements, proper placarding and other labeling, and appropriate routing for specific classes and/or volumes of chemicals. The transport operator must also have proper training and certification in emergency response procedures.

Waste Management

Process wastewater and other process wastes are generated by manufacturing facilities of all types. The contents of these and other waste streams produced by a chemical production facility depends on the materials and processes used at the facility.

Process wastewater discharge to an off-site treatment facility requires a permit from the facility and periodic sampling and analysis. The treatment facility will set the parameters for testing, waste volume and content limitations, and reporting. Some chemicals manufacturing facilities use on-site wastewater treatment operations. The treated water may then be discharged to a local system or as a point-source discharge to a nearby water body. Permits are required for both options and will require sampling and analysis, volume and content limitations, reporting, and other locale-specific requirements.

Other process wastes may include off-specification or contaminated materials. Characterization, storage, and transport of the wastes must comply with national, state, and local requirements. A special permit may be required if any wastes are classified as hazardous or otherwise specially regulated. The waste disposal or treatment facility will require analytical data on the content of each unique waste stream to ensure their acceptance of the waste complies with the terms of their operating permit.

Employee Health and Safety

The materials used and produced at chemicals manufacturing facilities must be closely controlled to prevent employee exposure. Potential routes of exposure include inhalation of volatile and semivolatile organic compounds and airborne particulates, dermal absorption of chemicals, and incidental ingestion of chemicals and particulates.

Production QA/QC Considerations		
Permitting	**Material Handling and Storage**	**Waste Management**
• Hazardous materials • Air • Location-dependent permits	• Materials management and transport • Spill prevention and response • Storm water pollution prevention	• Hazardous waste • Process wastewater • Other process-related wastes

A comprehensive exposure prevention and monitoring program is essential to protect employee health and comply with regulatory standards. Some of the components of an effective health and safety program include:

- Personal protective equipment (PPE) requirements
- Target parameters to be monitored
- Sampling and analysis schedule and SOPs
- Analytical sensitivity requirements
- Remedial action alternatives
- Regulatory reporting requirements, schedule, and means
- Record-keeping practices
- Other regulatory-specific requirements

A well-designed, consistently implemented employee health and safety program not only protects employees, it also helps the company avoid costly regulatory penalties and liability lawsuits.

Minimizing Environmental Impacts

Chemicals manufacturers must consider the environmental impacts of their operations. In addition to meeting permitting and other regulatory requirements, attention to a facility's environmental impacts can help control costs and increase operational sustainability.

A few practical steps that can move a facility toward these goals are:

- Improving process controls to reduce waste generation and air emissions. This can also increase production efficiency and control costs.
- Using R&D efforts to minimize use of potentially toxic materials in the production process. This can reduce costs for waste disposal and the need for special permits or restrictive permit conditions.
- Using R&D efforts to increase the recyclability of intermediate and final products. This can improve operational sustainability and contribute to advancement of the circular economy.

Trends

There are numerous trends developing in the chemicals industry. The following are a few of the more commonly noted trends.

Biobased Materials

Biobased materials are products that are made from biomass (living matter) or by processes that use biomass. Biotechnology research and development has been underway for some time and continues to grow in scope and success. Even in times of low petroleum prices, biobased chemicals innovation is being driven by consumer demand for more sustainable materials and product manufacturer demand for higher-performing chemicals.

Biobased commodity chemicals are being produced from carbohydrate biomass, creating a new basis for a sustainable chemicals industry. The use of biomass feedstocks for the chemicals industry can help reduce greenhouse gas emissions while also circumventing the fluctuations in cost and availability of fossil fuel-based feedstocks.

Innovative biotechnology companies are developing biobased chemicals that can be used to produce more sustainable materials. Examples of the wide range of biobased products being produced today include:

- Bioplastic packaging
- Biodegradable diapers
- Biobased films for touch screen displays
- Biobased coatings and adhesives
- Microbe produced enzymes used in industrial processes
- Agricultural biochemicals
- Biopharmaceuticals

As the innovation continues, the chemicals industry will likely see improved sustainability in their operations that can lead to higher efficiency and costs savings.

Pharmaceuticals

The COVID-19 pandemic has had tremendous impacts on the plans, priorities, and performance of nearly every industry, including pharmaceuticals. Most pharma companies have shifted the focus of some of their R&D efforts to developing effective drugs to prevent and treat COVID-19.

In the midst of the pandemic, previously existing trends continue to demand the attention of the pharmaceuticals industry. The growing global geriatric population and rates of chronic disease continue to be primary drivers of innovation in pharmaceutical development. In response to both COVID-19 and longer term medical conditions, the chemicals industry is continuously challenged to meet the emerging needs and applications with new fine chemical APIs and specialty chemical blends.

Pharmaceutical company leaders report that strengthening their R&D efforts and successes is a top priority for their companies now and in the foreseeable future. They expect their efforts to include prevention, early detection, and non-pharmacological interventions in addition to new drug therapeutics. The fine chemicals industry will need to continue providing highly-specific, innovative solutions for APIs, preventative treatments, and diagnostics.[13]

The biosimilar drugs industry continues to expand as consumers and health care payers demand lower-cost therapeutics. The total number of biosimilars under development or in the market has grown 208% since 2013. Biosimilars are very much like, but not exact duplicates of, brand-name drugs because they don't contain identical ingredients. Thus, to be approved for market, biosimilars must be tested and shown to provide the same therapeutic and clinical results as the brand-name drug. The chemicals industry will continue to be relied upon to provide innovative fine chemicals to enable continued growth in biosimilar development, efficacy, and availability.[14]

Chemicals Recycling

The terms chemical recycling, advanced recycling, and transformational technologies are used interchangeably.

Chemical recycling of plastics entails the breakdown of used plastics into one or more of their original building blocks that are then used as feedstocks for the synthesis of other chemicals. The term chemical recycling differentiates the technology from traditional mechanical recycling of plastics. Mechanical recycling is effective for newer and purer plastics, such as water bottles. More complex plastics—such as multi-layer plastics, heavily contaminated plastics, or unsorted plastic waste—are not amenable to mechanical recycling, which is where chemical recycling comes into play.

Advanced recycling uses solvents or heat to break down the plastics for reuse. This greatly reduces the amount of plastic waste requiring disposal via landfilling or burning and, combined with mechanical recycling successes, decreases use of non-renewable resources such as petroleum.

The chemicals manufacturing industry is gradually increasing their use of recycled raw materials. Some companies are even integrating plastics recycling operations into their production facilities. Such efforts will strengthen the industry and advance development of the circular economy.

The three primary advanced recycling methods are:

- Purification uses a solvent to dissolve the plastic so that additives can be removed, resulting in a purified polymer resin.
- Depolymerization breaks the plastic's molecular bonds to release its monomer building blocks so they can be used for other chemical synthesis.
- Conversion breaks the plastic's molecular bonds and recombines the molecules to form hydrocarbons and chemical feedstocks similar to organic commodity chemicals.

Nanotechnologies

The development of an ever-expanding number of nanotechnologies is introducing some exciting advances to the chemicals industry, including use of nanoparticles as catalysts and in drug delivery.

Catalysts

The chemicals industry relies on catalysts to increase reaction times throughout the production workflow. Nanotechnology developers strive to produce catalysts that are highly selective and active while having low energy requirements and long lifespans. These performance characteristics are achieved by carefully considering key chemical and physical characteristics during particle development, such as:

- Size, shape, and spatial distribution
- Surface composition and electrical structure
- Thermal and chemical stability

Nanocarbon particles are being used as catalysts in the fine chemicals industry. Nano-sized carbon particles have advantages over traditional carbon materials thanks to new insights into nanocarbon curvature, confinement, heteroatom doping, and improved electron transfer. Other types of nanocatalysts being developed for industrial use include those based on metals and oxides.[15,16]

Carbon-based Nanocatalysts	Metal-based Nanocatalysts
• Graphite • Graphene • Carbon nanotubes (CNT) • 3D porous nanocarbons	• Platinum group metals • Titanium, Cobalt, Silver, Iron, Aluminum, Nickel, others • Metal oxides

Drug Delivery

Nanoparticles are being used as drug delivery systems for many pharmaceutical therapies. Lipids, metals, polymers, and carbon are commonly used materials for drug delivery nanoparticles at this time.

Nanoparticle systems provide numerous advantages over traditional delivery methods such as tablets and capsules, advantages such as:

- More specific targeting
- Lower cytotoxicity
- Enhanced bio-distribution and metabolism
- Sustained and controlled release
- Delivery of poorly soluble drugs

Challenges in drug therapies that continue to be addressed via nanoparticle delivery systems include overcoming drug resistance in target cells, moving drugs across the blood-brain barrier, and precisely characterizing molecular targets.[16,17,18]

Industry 4.0

Industry 4.0 is considered the fourth industrial revolution, and for good reason. Industry 4.0 is the integration of a facility's physical manufacturing operations with an advanced digital technology platform, creating a seamlessly integrated system across processes. The physical-digital interconnection empowers communication throughout the system with continuous, real-time data gathering.

The platform's advanced analytics scrutinize the data and produce insights and automated control actions that are invaluable for operations and business parameters such as:

- Workflow optimization and QA/QC
- Energy efficiency
- Supply chain management
- Preventive maintenance
- Safety management

The chemicals industry is gradually adopting Industry 4.0. One initial way it has begun using its integrated system is for research and development of new or improved products. The advanced analytics platform can use historical data and materials parameters to conduct product simulations, reduce R&D failures, and enhance the effectiveness of laboratory testing.

Summary

The chemicals industry has experienced incredible growth and innovation over the past 150 years. It will undoubtedly continue to evolve as new technologies, end-uses, and materials are developed within the diverse industries that rely upon chemicals. Advanced analytical capabilities and platforms will be an important part of the success of the chemicals industry and the businesses it supports.

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Addendum

Analytical Resources for Fine and Specialty Chemical Manufacturers			
Material characterization	**Organics**	**Inorganics**	**Air-specific parameters**
Infrared spectroscopy systems: • Spectrum™ FT-IR spectrometers • Spectrum™ 3 FT-IR spectrometer • Spotlight® 200i FTIR microscope systems	Chromatography systems: • LC 300 UHPLC and LC 300 HPLC System • Clarus® 590 and 690 GC • Clarus® SQ 8 GC/MS with TurboMatrix TD • QSight® Triple Quad LC/MS/MS • Flexar FX-20 HPLC/UHPLC	ICP instruments • Avio® Max ICP-OES series • NexION® ICP-MS series • PinAAcle™ flame/graphite furnace AA spectrometers • FIAS/FIMS® mercury analysis series • Titan MPS™ sample preparation system	Clarus® 590/690 GC with TurboMatrix TD for ozone precursor analysis
LAMBDA™ UV-Vis and UV-Vis-NIR spectroscopy systems	LAMBDA™ UV-Vis spectroscopy systems	LAMBDA™ UV-Vis spectroscopy systems	Spotlight® FT-IR series for analysis of $PM_{2.5}$ and other particulates
FL 6500 & FL 8500 fluorescence spectroscopy systems			Spectrum™ 3 FT-IR spectrometer series for hazardous air pollutant analysis
Thermal analysis systems: • DSC • TGA • STA • TMA • DMA			

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