

Creating Successful Custom Catalyst Manufacturing Partnerships

Almost every chemical compound used in significant quantities requires a catalyst at some point in the manufacturing process. Often, these catalysts are the key to the economical production of a chemical, so the development of catalysts with high activity and selectivity towards the desired product are critical to many companies' success. To this end, many chemical/petrochemical companies have significant research groups dedicated to the development of catalysts that will provide a unique advantage in a highly competitive market. Once the Intellectual Property (IP) has been established through the patent process, the scale-up and commercial production of these unique catalysts becomes the keystone in supporting the overall technology package. In order to do this, a company may have in-house facilities that can be used but, increasingly, the high capital cost of such facilities make it more economical to partner with a specialized catalyst producer, such as BASF, to manufacture what becomes a "Custom Catalyst".

BASF has over 50 years of experience in custom catalyst manufacturing, 36 manufacturing locations around the world, and a pool of over 650 catalyst research scientists. Such knowledge, skill, and competence are necessary to convert a customer's research and development (R&D) effort into a commercial catalyst which can be produced consistently and economically. This allows the customer to install a competitive technology which may be used internally or licensed to

others. Over many years, BASF has developed an understanding of its customers' needs, particularly with respect to the sensitive nature of the IP involved with Custom Catalysts, which has allowed BASF to cultivate many long-term partnerships. Through these collaborations, BASF has developed and commercialized custom technology for chemical catalysts, polyolefin (polymer) catalysts, refining catalysts, and adsorbents. Examples of BASF partnerships in the public domain are:

- Sasol — Fischer Tropsch catalysts
- CBI Lummus — Olefin Conversion Technology
- Oxy Vinyls LP — Fluid Bed Oxychlorination catalysts



Why Choose BASF Custom Manufacturing?

Catalyst manufacturing is capital intensive and often requires very specialized equipment that is only useful for processing catalyst materials. Typically, a catalyst manufacturing facility is multipurpose, allowing the fixed cost of these investments to be spread over a number of products, thus reducing the cost for any individual product. At BASF, we understand the fundamentals and complexities of catalyst manufacturing. With our global network of production plants, research units, and site communities, our capabilities are unparalleled for meeting the specific catalyst needs of our customers. BASF puts all the pieces together with its understanding of international standards and sustainable development. We do this by:

- Optimizing costs by avoiding capital expenditures and reducing manufacturing charges
- Delivering high quality products within an accelerated commercialization time frame
- Synchronizing our customers' core competencies with BASF's catalyst expertise

While it is not unusual to manufacture a custom catalyst at a single BASF location, BASF has the unique advantage of having several manufacturing locations with equivalent unit operations that can be cross qualified to provide flexibility in its custom catalyst production. With multiple facilities around the world, a back-up location can eliminate potential downtime and keep projects on track when schedule conflicts occur. Additionally, by manufacturing within a common tariff zone, e.g., the European Union, import tariffs, which can be as high as 6.5%, may be avoided.

The key element in any custom catalyst project that BASF recognizes as essential is confidentiality. BASF recognizes that confidentiality is crucial to ensure our customer's catalyst or process profitability is maximized. Thus, we have established a compartmentalized system that guarantees that a customer's IP is held within a very limited group within BASF. The protocol includes legal agreements for IP protection and information dissemination limitations on a "Need-to-Know" basis. Our internal computer network includes an electronic

database with restricted access. BASF also takes the time to select skilled personnel for each project. In the laboratory, the R&D teams are carefully selected to avoid conflicts of interest. The R&D project leader guides the plant process engineer to prevent any cross contamination. Access to the progress reports is limited to a restricted list of personnel.

Finding the Right Developmental Scenario to Meet Specific Needs

BASF understands that different customers have different needs; thus, we support a spectrum of development arrangements for custom catalyst formulation and manufacturing, four of which are illustrated in Table 1.

	Customer Contribution	Technology Flow	BASF Contribution
A	Fully commercialized manufacturing process (toll manufacturing)	→	Manufacturing (quality, reproducibility, price)
B1	Fully developed formulation (bench scale)	→	Black box scale-up and manufacturing
B2	Fully developed formulation (bench scale)	→ ←	Scale-up and manufacturing
C	Partially developed formulation (bench scale)	→ ←	Formulation assistance, scale-up and manufacturing
D	Joint development	→ ←	Simultaneous development of catalyst & process

Table 1: Development arrangements for custom catalyst formulation and manufacturing

A: Fully Commercialized Manufacturing Process (Toll Manufacturing)

In a pure **toll manufacturing model**, the customer designs and scales up the catalyst to the point where it has been proven commercially and the product specifications are clearly defined. The information is delivered to BASF where a qualification trial is performed using BASF's unit operations, and then product is produced to an agreed specification.

BASF offers two options for customers who bring a complete bench scale formulation for scale-up and manufacturing:

B: Fully Developed Formulation (Bench Scale)

Option 1: In cases where a customer does not want to be "contaminated" with the knowledge of BASF's operations, we offer what we call "black-box" scale-up based exclusively on the customer's formulation.

Option 2: Joint scale-up with a two-way flow of technology between BASF and the customer.

C: Partially Developed Formulation (Bench Scale)

In many cases, a customer has **partially developed** the catalyst formulation, but there are still options that can be explored prior to finalizing the design, some of which can impact the commercial production economics. This provides an opportunity to tailor the design to suit available manufacturing operations or raw materials. With this set-up, BASF also provides formulation assistance along with scale-up and manufacturing.

D: Joint Development

Finally, the **joint development** option requires the most extensive R&D input from BASF. We work closely with the customer on the simultaneous development of the catalyst and manufacturing process.

This option requires the highest resource commitment, but also tends to offer the greatest opportunity for optimizing both the custom catalyst and the production process.

BASF has successful partnerships with each of these models, so no single model is "better"; it all depends on the specific project circumstances.

The 5-Phase Approach to Custom Catalyst Development

With our long history of successful catalyst manufacturing, BASF understands that an outstanding custom catalyst requires a well-established partnership. For all of the previously described developmental scenarios, BASF utilizes a detailed methodology that relies on the creation and maintenance of an open dialogue with the customers as outlined in these 5 phases. The level of detail to which we will go will be greater when applied to a Joint Development Scenario (D) than a pure Tolling Scenario (A).

The steps are:

Phase 1: Initial Meeting – Goal Identification

Phase 2: Planning and Specification

Phase 3: Development in the Laboratory

Phase 4: Pilot Plant Scale-Up

Phase 5: Commercial Demonstration

Note, the next step is Product Launch.

Phase 1: Initial Meeting – Goal Identification

This typically begins with the initial contact by a BASF Account Manager. A preliminary meeting is arranged to ascertain if there is a fit between customer needs and BASF capabilities. An in-depth view of BASF is provided to determine how the requirements can best be met. This includes a detailed presentation of our custom catalyst capabilities and may involve tours of the plant and/or labs. This preliminary discussion also includes the various joint development scenarios along with possible options for cost sharing. At this stage in the relationship, it is normal to have executed a one-way or two-way secrecy agreement to protect any technical disclosures made by the customer and/or BASF.

Phase 2: Planning and Specifications

After a preliminary agreement is reached, an R&D team and project leader are selected. The selection of the group members is done to minimize any conflict of interest with other BASF in-house or custom development projects. Detailed planning for the projects includes:

- Set of objectives
- Creation of a timeline
- Determination of project milestones
- Resource requirements
- Projection of manufacturing costs

Next, BASF performs literature and patent searches related to the initial catalyst design. Business approval from both BASF and the customer must be obtained before the project can proceed further. If necessary, a cross functional team is formed to assist in the authorization. Once approval is received, the official joint development agreement is signed. The customer and R&D team then meet to confirm the planning details, assign specific responsibilities, and complete the technical disclosure.

Phase 3: Development in the Laboratory

After receiving the customer's sample(s), BASF performs a detailed analysis. When the evaluation is complete, the material is replicated on the bench-scale level in the lab. The customer inspects the reproduction, as the next phase cannot start without the approval of the lab sample. While the customer is reviewing, the R&D team works on different research methods, including alternative process steps that are based on Sustainable Energy Development (SED). In compliance with Environmental Health and Safety (EH&S) guidelines, the necessary Material Safety Data Sheets (MSDS's) are started. If necessary, Pre-Manufacture Notices (PMNs) and Consolidated Federal Air Rules (CARs) are filed with the Environmental Protection Agency (EPA). At this point, BASF discloses the technical project specifications to the plant engineers involved in the manufacturing process.

Phase 4: Pilot Plant Scale-Up

In preparation of moving the R&D lab to full production, BASF creates a pilot plant scale-up procedure that simulates manufacturing. This step allows us to identify and optimize

any rate-controlling steps for the proposed process. The scale-up tells us the effect of scale on the quality of the final product. The samples are characterized based on their ability to withstand production on a large scale while maintaining the initial attributes. All Quality Control (QC) tests are reviewed with key plant personnel. Based on any process modifications, new estimates for costs and yields are determined, and MSDS's and other necessary documentation, such as REACH registration are completed. From the pilot scale results, the final methodology for the manufacturing run is generated. No plans are activated until the customer has evaluated and approved the final sample from the pilot lab.

Phase 5: Commercial Demonstration

Before full-scale production, the customer evaluates samples from the plant's trial batches. Based on data obtained from the other phases, a reassessment of the yields, throughput, and manufacturing costs is performed. Next, specifications are modified based on manufacturing capabilities. A small production run is conducted to gather at least 40 data points. Afterwards, the specifications are finalized and full production begins.

The catalyst launch is based upon the customer's commercial request for the product. If necessary, BASF orders and installs any additional capital equipment to facilitate the manufacturing process.

BASF understands that the development of a custom catalyst is a careful and deliberate process, which customers often have to run in a Process Demonstration Unit (PDU) to develop the data required for either internal investment or for process licensing. From formulation to initial production for a PDU, it can typically take two to three years after which a commercial plant may take another two to three years until it is commissioned. In some cases, this progression has taken as long as 10 years. BASF is willing to take a long term view of such developments when the economics of the business case support a level of return that meets BASF's goals.

Catalyst Performance Testing

As the project plan is defined, the performance testing aspects need to be clearly understood. Most often performance testing is done by you, the customer. However, it can sometimes be beneficial for both BASF and the customer to have performance testing capabilities. This can often improve the speed to market and support the development of a better optimized catalyst.

BASF has wide experience in designing and building such test units in-house with all the associated on-line analysis techniques and data acquisition systems.

BASF Value-Added Manufacturing Process

Why do companies around the globe turn to BASF for catalyst development and production? BASF has a wide array of potential processing routes but, more importantly, a deep understanding of how each step of a manufacturing process impacts both product properties and production costs. So, from precipitation through reduction, we can define an optimum process that not only meets our customers' business objectives, but also adds value at each step.



Figure 1: Typical Process Flows

BASF Chemical and Process Engineering Expertise

BASF is unique amongst catalyst companies in that we have a group of over 200 scientists, dedicated experts in their fields focused on all aspects of manufacturing processes. This group, with the support of a staff of technicians using equipment scaled to mimic BASF's operations, can run rigorous tests on the unit operations needed to make a catalyst. We can draw on these experts to provide support in choosing the right equipment for a specific catalyst we are producing. In addition to recommending the correct equipment for, say, filtration, they can advise on the choice of materials of construction which can be critical for optimizing the longevity and maintenance needs of equipment.

Since this group is independent of any specific supplier, their recommendations are based on price/performance criteria and the synergy of such a group of experts allows them to consider the integration of different unit operations that can lead to lower overall production costs.

Precipitation

For many catalysts, the final product properties are set by the material made during the precipitation process. Key factors such as particle size, the ratio of active components, and the distribution of promoters are impacted by process flow rates, temperature, pH, agitator speed, and residence time. These are a few of the control parameters that BASF has the knowledge and experience to manipulate to achieve the desired properties. In our worldwide facilities, we offer a wide range of precipitation systems along with scalable pilot plant equipment. Our plants can perform batch, continuous, sequential, and simultaneous precipitation.

Zeolite Crystallization

The synthesis of specialty zeolites typically requires high pressure and complex organic templates to develop the correct morphology. BASF is uniquely positioned, as it is a manufacturer of a number of the template molecules used in

zeolite synthesis. As a consequence of the use of organic templates, the ability to treat the off-gas generated during the process is necessary to meet environmental regulations. BASF has state-of-the-art technology to handle this off-gas treatment at its manufacturing locations.

Filtration & Separation

The goal of any filtration/separation/washing system is to maximize the retention of the desired product, while minimizing the generation of effluent, which has to be treated in a wastewater treatment plant. Experience in choosing the correct filter media for a particular material plus online pH and conductivity monitoring allows BASF to identify the optimum equipment and cycle times for each product. All BASF filtration systems have reverse osmosis and/or deionized water available to achieve the highest possible purity levels during the removal of unwanted ions.

Drying

Although BASF has the capability to prepare catalytic materials in organic liquids, the majority of products that require drying are concerned with the removal of water. The rate of water removal can impact the location of active metals or promoters. An understanding of the impact of drying rate which, in turn, is related to residence time and drying temperature, is key to designing the optimum drying route. From conventional belt and tray drying techniques, to spin-flash or spray drying equipment, and other variations, BASF is capable of drying most materials from fine powders to large formed catalysts.

Calcination

Calcination is applied to catalysts in two main ways:

1. It is used to fix the particular structure desired for the support materials prior to addition of the catalytically active metal.
2. Active metals are typically added to the support as a compound in solution e.g. nitrate, which is dried to remove excess moisture and decomposed by calcination, which fixes the active metal at specific locations within the support structure.

By understanding the effect of calcination temperature, atmosphere, and residence time on catalyst and catalyst support properties, BASF can optimize catalyst properties while reducing energy and material costs. At BASF, we have a wide range of calciners that can be used to produce catalysts with the right quality parameters, that also meet the capacity requirements of our customers.

During the thermal treatment process, our hold times can range from minutes to days. Calciners are equipped with effluent gas treatment capabilities ranging from NOx abatement to organic off-gas incineration.

Forming

In fixed bed catalytic applications, the size and shape of the catalyst particles are important variables that impact pressure drop, activity, selectivity, and cycle length. The forming technology can impact manufacturing costs, so selecting the right manufacturing technique is a crucial part of the development process.

It is vital to understand how different binders can affect important parameters such as strength, density, porosity, etc.

The most common forming techniques are:

Extrusion

Although the process is like making pasta, the components are rather more abrasive and require a great deal of skill and knowledge. Shapes from basic cylinders to complex star shapes can be made with a capability to extrude to less than 1mm diameter.

Tabletting

Although similar to the process of making vitamin pills, again the abrasive nature of the materials requires a high degree of technical knowledge of the ability for the machinery to withstand wear so that consistent tablets of the same size and strength are produced. Solid tablets are generally very strong and require the least costly tooling while shaped and hollow core tablets provide more geometric surface area but require more expensive tooling.

Spheres

Commonly used for support materials, there are various techniques which can be used to form lower or higher density spheres.

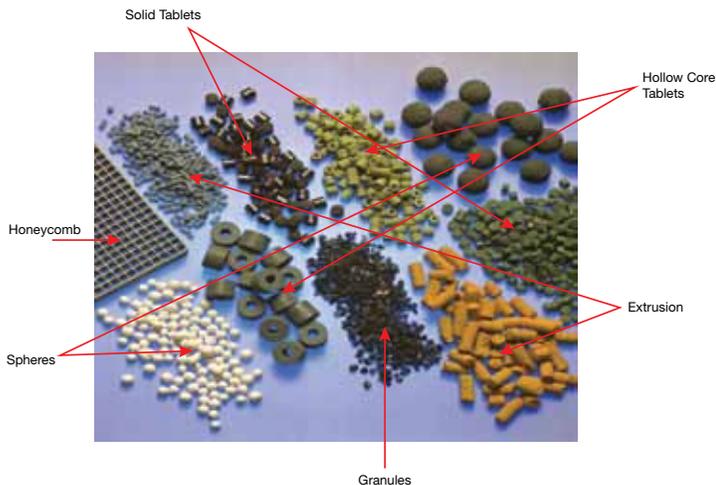


Figure 2: Examples of Formed Catalysts

Impregnation

Improved control of the impregnation process can create a more homogeneous distribution of the active component(s). BASF has expertise in surface coating, sub-surface coating, and uniform impregnating of various precious metals and base metals onto different supports, including ion exchange capability for precious metals loading.

Reduction

If the custom catalyst requires pre-reduction, BASF can reduce the catalyst in up to 100% hydrogen, followed by surface passivation with O_2 or CO_2 . The common designation for these catalysts is Reduced and Stabilized (R&S). BASF also has capabilities to package reduced catalysts under protective liquids compatible with our customer's application, or take reduced powders, surface coat them with wax, and form wax pastilles.

Custom Manufacturing Around the World

Custom catalyst development is a stringent process that involves collaboration between scientists, engineers, and plant personnel. At BASF, we have strategically-positioned manufacturing sites to better meet our customers' needs. The site selected for production is based on the technology available and specifications from the customer. We can now provide custom catalysts to our global clientele regardless of location.

- Elyria, OH (USA) — Chemical Catalysts
- Erie, PA (USA) — Chemical Catalysts
- Seneca, SC (USA) — Chemical Catalysts and Precious Metal Catalysts
- Ludwigshafen (Germany) — Chemical Catalysts and Precious Metals
- Rome (Italy) — Precious Metal Catalysts
- De Meern (The Netherlands) — Chemical Catalysts

At BASF - The Chemical Company, we combine a comprehensive and proven portfolio of custom catalyst manufacturing services with an infrastructure of chemists and researchers who have the knowledge and skills to turn a catalyst into commercial reality. From manufacturing to development, BASF has the foundation to support even the most challenging design and processing requirements. Using our assets and resources, we have the ability for rapid scale-up and mass production in a cost-efficient manner. Our worldwide manufacturing facilities are equipped with the necessary machinery for every step of the production process. BASF has the business model, technical expertise, and commitment to customer satisfaction that translates into custom catalyst success.

About Us

BASF's Catalysts division is the world's leading supplier of environmental and process catalysts. The group offers exceptional expertise in the development of technologies that protect the air we breathe, produce the fuels that power our world and ensure efficient production of a wide variety of chemicals, plastics and other products, including advanced battery materials. By leveraging our industry-leading R&D platforms, passion for innovation and deep knowledge of precious and base metals, BASF's Catalysts division develops unique, proprietary solutions that drive customer success.

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