# Getting the chemistry right

# MEC: Micro-Engineered Catalyst systems

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**Better reactor performance is currently hindered by the use of conventional, bulk-loaded catalysts in the form of pellets, spheres or extrudates. Micro-Engineered Catalyst (MEC) systems overcome this barrier by significantly improving the contact between the reactants and catalyst, resulting in superior mass and heat transfer. A mechanically strong catalytic web of micro-fibers, thinner than human hair, is engineered and shaped to achieve optimum fluid dynamics. The combination of size and formability significantly enhances catalyst performance – a key factor in overall process economics – providing a major advantage over traditional catalysts and allowing smaller reactors to be built. The system has already been successfully demonstrated on a semi-commercial scale in petrochemical applications, and the first commercial application is anticipated this year.**

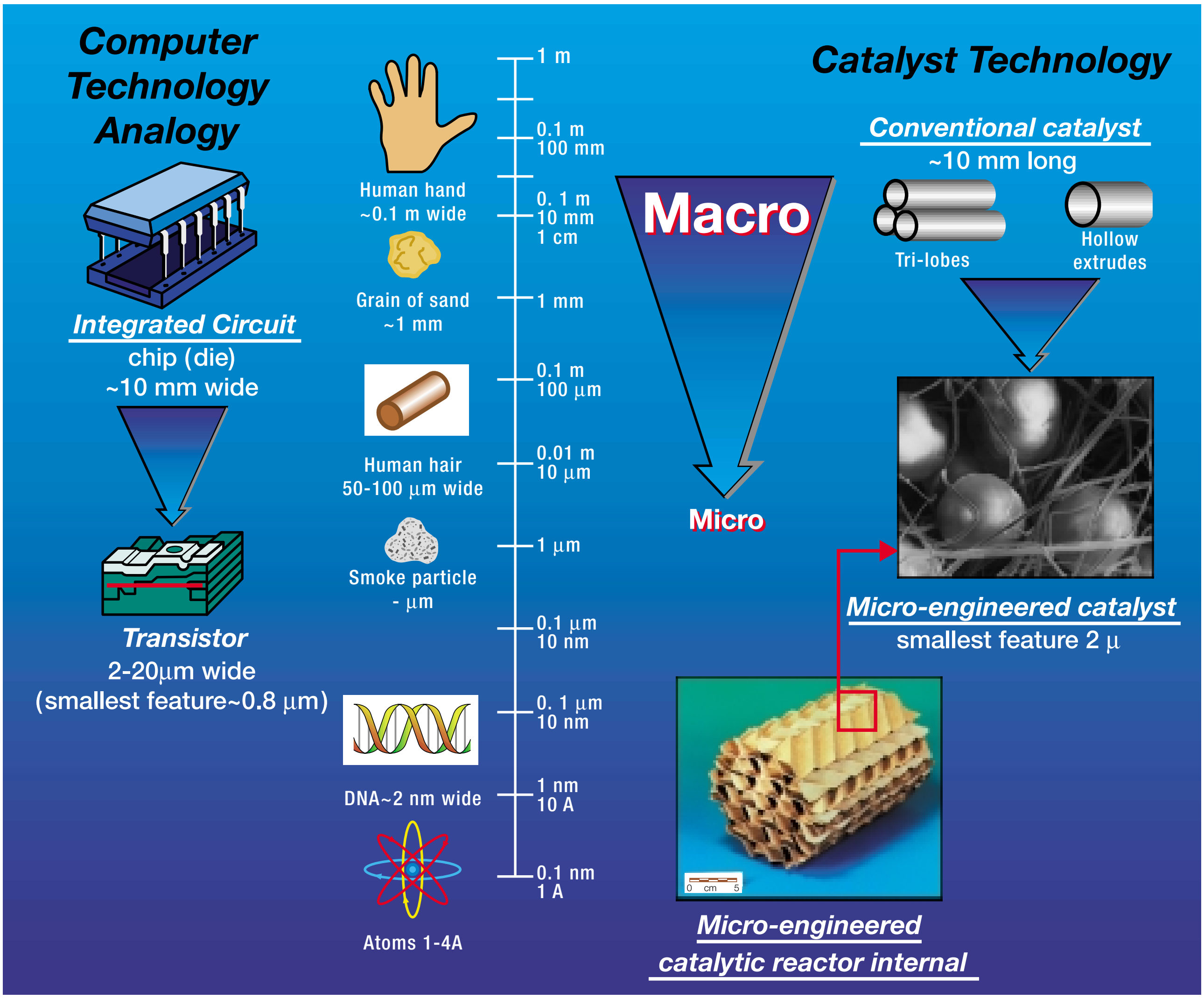
Petrochemicals such as ethylene, propylene and styrene are the raw materials for plastics used in everything from soft drink bottles and contact lenses to engine parts and artificial heart valves. Their use is so widespread today that we hardly give them a second thought. Equally indispensable – and with a much higher profile – are gasoline and diesel oil, which are obtained by refining crude oil. In the process of making all of these products, emissions are generated that must be controlled. To produce them efficiently and at the same time ensure that the environment is properly protected, sophisticated chemical engineering and the ability to control chemical reactions are essential.

## The essential ingredient

Catalysis – the enhancement of a chemical reaction between two or more compounds through interaction with a catalyst – lies at the heart of most chemical processes. Approximately 90% of all chemical products require at least one catalytic step in their manufacture. Generally, the key to overall process economics and environmental control is the reaction step combining reactor and catalyst performance.

Catalysts are usually produced as millimeter-sized pellets, spheres or extrudates with active catalytic agents dispersed in the interior of the particle. In a conventional catalytic process, reactants flow through a reactor containing the bulk-loaded catalyst. The arrangement, shape and size of the catalyst govern flow dynamics and pressure drop. In a conventional packed bed, the flow pattern is random, making fluid dynamics and heat-management difficult to predict and control. The use of active catalytic agents can also be inefficient since, in many cases, only those agents close to the exterior surface of the particles are available to the reaction. Catalyst effectiveness is therefore well below the theoretical maximum, and much of the potential activity of the catalytic agents is unused. This results in higher raw material and operating costs as well as increased production of less valuable byproducts and waste.

Now, a multi-national team of ABB chemical engineers working with top university scientists has invented a system that improves reactor and catalyst management by applying and effectively utilizing catalyst particles on a much smaller scale than is currently applied in industry.



1 ‘From macro to micro’: how ABB catalysis technology has progressed

**A catalytic web of fibers thinner than human hair**

The Micro-Engineered Catalyst (MEC) systems technology is able to overcome current reactor performance barriers by utilizing the catalyst on an extremely small particle level. The MEC system is composed of a mechanically strong catalytic web of micro-fibers – thinner than a human hair – in which microscopically small catalyst particles are entrapped. The size of these catalyst particles is about a 1000 times smaller than that currently in use in industry. There is a clear analogy between this size reduction and developments in computer technology; transistors were originally about a thousand times larger than they are today. Currently, an integrated circuit of the same size contains many, much smaller transistors 1.

The new material with the included catalyst can be formed into a variety of catalytic shapes and structured packings, especially tailored to their application. In effect, the name ‘Micro-Engineered Catalyst’ is coined to emphasize the two key attributes:

- Micron-sized catalyst particles result in unmatched efficiency of expensive catalyst components.
- The material can be formed to achieve the optimum geometry for a given reactor.

By significantly improving contact between reactants and the catalyst, excellent mass transfer, superior heat transfer and optimal pressure drop are achieved in the catalytic reactor. The catalyst system is tailored and designed to make more products efficiently using much less catalytic material. As catalyst technology and reaction and process engineering can now be integrated in a very effective way, the reaction system is able to reach performance levels previously considered unattainable on a commercial scale. The resulting enhanced catalyst performance enables smaller reactors to be built, which reduces the capital cost of the reaction system, and therefore the cost of operating the plant. This will allow ABB customers to operate more competitively and reduce their impact on the environment.

### MEC systems – engineered for optimum performance

MEC systems could be considered as a unit operation which, within the reaction zone, can be engineered for optimum catalytic performance to improve:

- Mass transfer
- Heat transfer
- Catalyst density
- Pressure drop

2 shows two current MEC technology concepts. In both, a highly porous metal sheet is used as a rigid carrier for very small, micron-sized, catalyst particles.

### Application of paper technology

The original concept, 'encapsulated micro-catalyst particles', was based on paper-making techniques in which metal micro-fibers and catalyst particles are added to cellulose pulp to form a composite paper. The cellulose is then burned out and the metal fibers are sintered to produce a rigid metal sheet. This concept was scaled to semi-commercial size in cooperation with Auburn University and the Swedish Corporate laboratories.

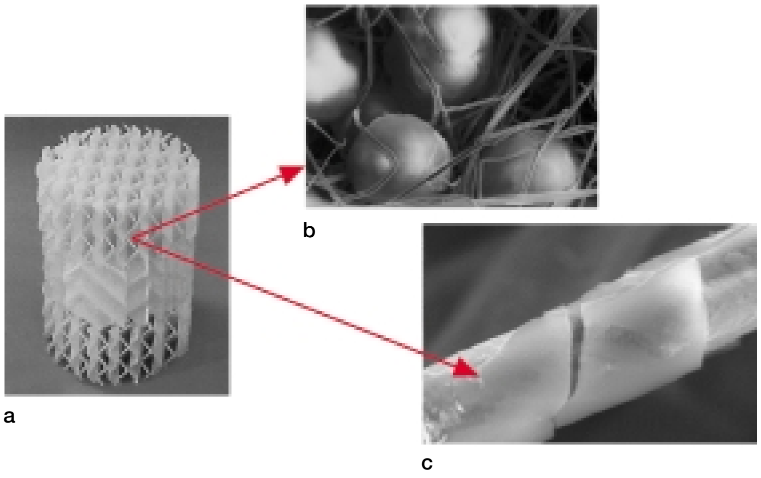
### From laboratory to demonstration

The laboratory tests comprised the production of hand-size micro-fibrous sheets to study forming and wet laying of the mix of cellulose and metal fibers. Good quality sheets were produced with simple mixing equipment.

The first semi-commercial size tests were performed at the Swedish Paper Producers Education Center in Markaryd during 1997. The tests produced about 500 meters of micro-fibrous paper sheet of various types. 3 shows two stages in the production process.

Even though the original test was relatively successful and proved that the principles of paper-making could be applied to produce MEC, several problem-areas in the process were identified. These included the mixing of the metallic and cellulose micro-fibers and the sequence of the various steps. Further research, development and optimization in the Swedish Corporate Research Center and at Auburn University led to a variety of solutions and inventions, which were tested in 1998 in a second semi-commercial test run.

Several patent applications have been filed on the various production concepts. Although this route appears to be very attractive, there are some technological barriers that must be overcome prior to commercial implementation.



2 Micro-Engineered Catalyst system concepts

a *MEC internal, made from highly porous metal fiber sheets*

b *Encapsulated micro-catalyst particles*

c *Coated micro-catalyst*

3 During semi-commercial size tests in Sweden, some 500 meters of micro-fibrous paper of various types were produced. Two stages in the production process are shown.

## New coating technology

The current approach is based on catalyst being coated on the micro-fibers. The MEC support material is made from a generally metallic, micro-fibrous sheet. Coating of this carrier has been demonstrated on a laboratory scale based on core in-house developments in Bloomfield and at the Corporate Research laboratories in Heidelberg. By focusing efforts on this route, we were able to accelerate the MEC development program and have been able to develop a commercially viable product.

### Current state of coating technology

In modern powder coating of solid bodies, a variety of low-cost coating procedures are employed, the most common of which are spray-coating, dip-coating and wash-coating. These coating technologies have the following common limitations:

- They are used for coating simple structures.
- Coating homogeneity and the process itself are intrinsically controlled by surface tension and wetting properties.
- There is no effective direct control of the coating properties.

### Need for new technology

Because of these constraints, the known coating technologies were found to be inadequate for uniformly coating each single micro-fiber. Coating the complex three-dimensional micro-fibrous structure required a new, significantly more versatile coating technology. In addition, a modern process control parameter was desired, eg an electrical parameter for controlling the coating thickness. Moreover, the process had to be as cost-effective as dip-coating or wash-coating.

### Electrophoretic coating

Electrophoretic coating was investigated to determine its ability to meet the defined quality targets. This technique, used by ABB Flexible Automation for coating car bodies, is known as cataphoretic- or paint-coating and is based on colloidal particles, such as micro-catalyst powder particles dispersed in a fluid medium, being mobile in an electric field. In principle, two electrodes of opposite electrical charge cause colloidal particles to migrate to one of the electrodes. After release of their charge to this electrode, they will attach to the surface of the electrode. This process can be roughly compared to electroplating. However, MEC features two completely new processes: coating of the 3-dimensional fibrous network and controllable coating of each fiber within the network.

The combination of applicable process know-how and colloidal chemistry expertise at the Corporate Research Center in Heidelberg smoothed the development of this coating technology. With the team cooperating closely on all levels, a material with an optimized structure for electrophoretic coating was developed, ie with defined void volume, void morphology and fiber diameter, while catalyst powder and colloidal suspension know-how was also generated. The new coating technology can be considered as a breakthrough for the following reasons:

- It can coat complex structures.
- There is current and voltage control of the coating process.
- A combination of current, voltage and time determine coating thickness.
- The process is easily adapted to modern process controls.

The product of the coating process development, shown in 4, clearly demonstrates that each fiber in the three-dimensional structure is coated. Several patent applications covering the technology have been filed.

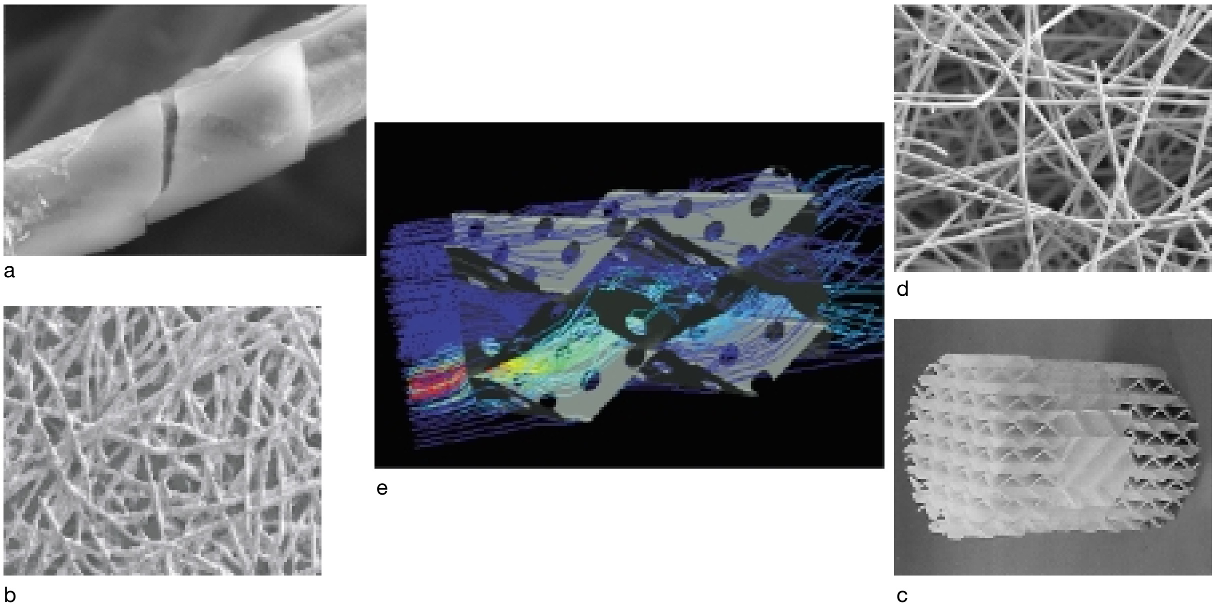
## Novel catalytic packing designs

Through close collaboration of the various project partners, and making special use of the knowledge base at the Corporate Research Centers in Switzerland and Sweden, novel catalytic structures with optimized fluid dynamic performance and catalyst utilization were designed. ABB utilized its strengths in the design of burners and turbines extensively by employing Computational Fluid Dynamics (CFD) in concert with detailed aerodynamic measurements to support the design of the new structures.

### Development of knowledge base

A solid foundation was laid by executing a detailed review of flow characteristics and design criteria for non-catalytic structured packings. The existing literature confirms that surface characteristics, as well as deliberate coalescence and break-up of droplets and bubbles, promote, respec-tively, heat and mass transfer in packings. From geometric analysis, it was deduced that a favorable packing geometry should spread the flow in a three-dimensional manner and should not have predomina-ting characteristics in certain directions.

Based on this, the project team developed a first theoretical basis of mixing and its description by CFD modeling, where mixing efficiency is defined as a measure of the degree of mixing. In addition, it developed an algorithm to solve the single and two-phase fluid flows within a fiber network using commercial CFD codes.



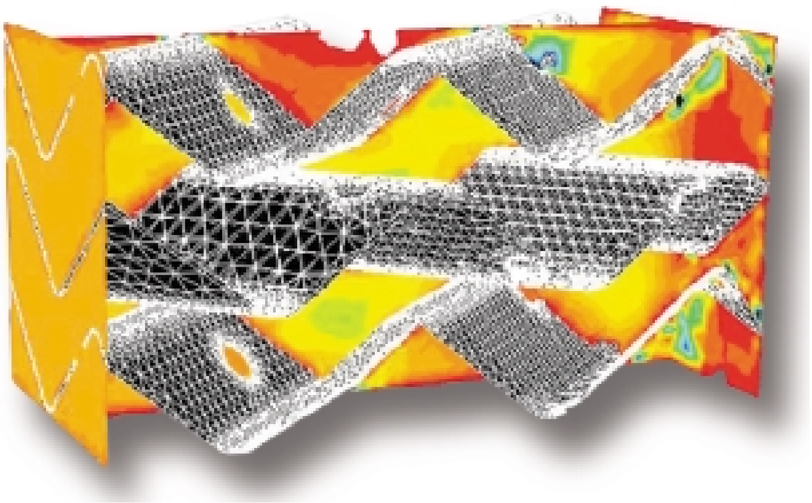
**4** MEC compilation

a *Magnification of coated fiber*
b *Coated micro-fibrous web*
c *MEC packing*
d *Uncoated micro-fibrous web*
e *CFD simulation of flow through MEC structure*

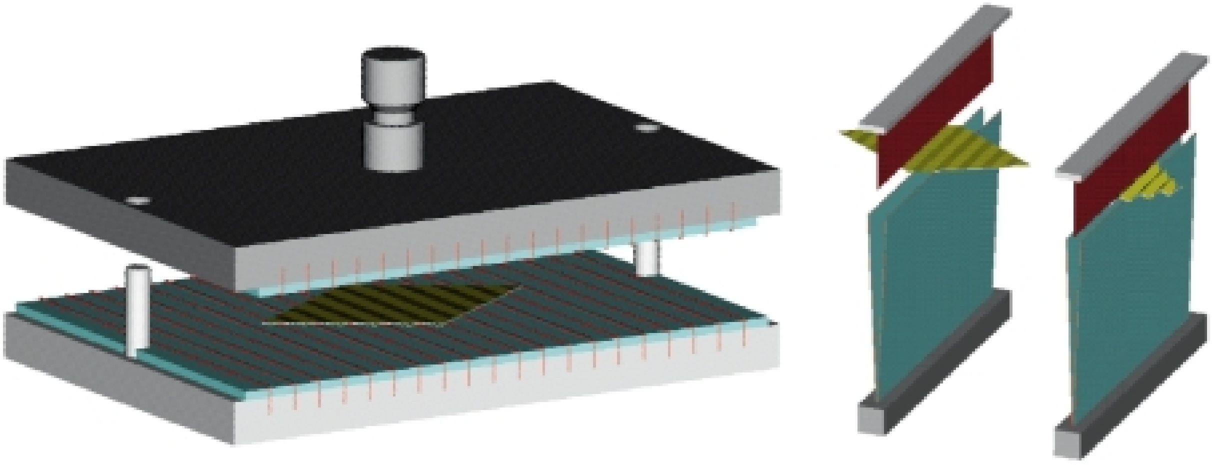
## Experimental approach

In the initial developmental program, the Corporate Research team in Baden, Switzerland, developed a series of experimental techniques to benchmark existing commercial packings in single and two-phase environments. Among these techniques were flow visualization, Laser Doppler Velocity Profiling, pressure drop measurements, quantification of two-phase liquid/gas distribution and mass transfer (gas desorption from liquid). This work identified the requirements for high-performance, structured packings in various reactive environments. The project team had to design novel structures to optimize both fluid distribution and catalyst utilization. Effective use of the large surface area of the porous fiber substrate – one of the key advantages of MEC – added additional constraints to the design.

Using CFD, the teams at the Corporate Research Centers in Switzerland and Sweden optimized the amount of flow into the internal fiber network while simultaneously minimizing total pressure drop across the packing. Using unstructured grids for quick mesh generation, the Swiss team rapidly modeled commercially available structured packings in single-phase flow using unstructured CFD grids, and compared the results with experimental investigations. Visualizations of the



**5** CFD simulation of the novel MEC structure showing velocity contours for velocity components perpendicular to two surfaces



6 Special tools have been developed that take into account the the unique properties of the MEC paper. The tool on the left is for creasing, that on the right for bending.

results of CFD calculations are presented in 4 and 5 . The CFD results agreed closely with experimental results.

### New packing designs

Using the knowledge accumulated from CFD and experimental modeling, both groups developed various novel designs. The Swiss team tested and optimized these, also using CFD, and eliminated the less efficient designs. Evaluation of the critical design criteria enabled the group to continually optimize the designs.

Using structured CFD grids, the Swedish team performed two-phase flow simulations in order to understand the phenomena of gas-liquid flow in structured packing. It was found that liquid tended to collect in certain areas rather than spread evenly. Another discovery was that mixing could be enhanced via properly shaped and sized holes, which needed to be distinctively placed in the packing. Various designs were created on the basis of the CFD calculations. The Swiss team subsequently used experimental methods to optimize gas-liquid distribution using actual models of the developed structures. Two generic, novel structured packing families designed in this fashion are covered in two patent applications. The established design procedures are now used for the optimization of structures for various spin-off applications that can exploit the advantages of MEC.

### Description of flow in an MEC structure

Finally, the team developed and verified a model for calculation of flow through porous media which allows simulations of flow through the fiber-based material. This model can be used to assess whether the catalyst in the three-dimensional structure should be distributed at or near the surfaces of the porous medium or uniformly inside the material. The fibrous support medium can then be tuned for optimum reaction performance.

### Structure manufacturing scale-up

Once the most promising mechanical design had been identified through small-scale pilot testing, scale-up to industrial size using automated production was addressed. At the Corporate Research Center in Switzerland special tools were designed, constructed and tested for the production of catalytic packing elements that took into account the unique properties of the MEC paper. These tools were used for the manufacture of a six meter MEC packing for a large-scale pilot test in Pasadena, Texas, which took place during the autumn of 1998. Designs of some of the developed devices are shown in 6 . The uniquely designed tools are the subjects of a separate patent application.

### Road to commercialization

At the development stage, MEC systems showed significant advantages in a broad range of applications, both traditional and non-traditional. Various MEC designs were tested, both in-house and at customers' facilities, in a variety of application areas. Significant progress was achieved in the applications listed in the *Table* opposite. Based on these test results, several application experts expressed interest in joint development. Bringing the concept to market, however, presents many challenges and associated risks. Commercialization efforts are currently being focused on DeNOx and hydrogenation.

### Hydrogenation

The use of MEC as a hydrogenation catalyst system is viewed as a relatively easy target for initial commercialization and market penetration, given ABB's experience and stature in this area. ABB is also a premier licensor of ethylene technology and several selective hydrogenation processes exist within this process. Use of a superior hydrogenation system will only serve to ensure that status. Proof of concept and demonstration in hydrogenation was first achieved in 1998, and further demonstration in several additional hydrogenation applications has since been achieved. Specific target hydrogenation applications are currently being evaluated. In these applications, the use of MEC has been shown to enhance selectivity (minimization of undesired by-products) and catalyst efficiency, thereby improving product quality and reducing reactor volume and capital investment.

### $NO_x$ abatement

DeNOx is chosen as a focus application because we believe that MEC can provide a cost-effective solution to a current technology need. In particular, MEC has proven potential in a narrow area with a significant market potential, namely $NO_x$ abatement for gas turbine applications. At this point no cost-effective, or possibly even technically sound, solution is known for this application which meets the ultra-low $NO_x$ emissions ($<$2.5 ppm) as defined by the newest US emission regulations. Economic and technical evaluations for DeNOx for specific power plant applications have been completed, and indicate that the use of an MEC will have the following major advantages:

- The ability to meet new $NO_x$ emission regulations
- Reduced tail-end system pressure drop (substantial annual operating cost savings)
- Reduced ammonia slip for SCR-DeNOx
- Reduced reactor volume and capital investment

MEC is being exploited as the vehicle for process licensing based businesses with partners. However, if certain markets cannot be penetrated on this basis or if the application is in an area where ABB has no licensing interest, then general sales of MEC catalyst will be pursued if justifiable profits can be generated. The targeted catalyst market exceeds US$5 billion annually. Including technology license fees, each one percent captured represents US$75 million in annual revenues.

## Key to Success

### A multi-disciplinary, multi-national project team

**Micro-Engineered Catalyst (MEC) systems technology improves reactor and catalyst management by applying catalyst particles on a much smaller scale than is usual in industry. With corporate High Impact/High Risk funding, an R&D team headed by ABB Lummus Global has succeeded in developing and demonstrating the novel technology in only two years. The nucleus and key to success of the project has been a multi-disciplinary team composed of engineers and chemists from ABB Lummus Global's Technology Division in Bloomfield, New Jersey, the major ABB Corporate Research Centers in Switzerland, Germany and Sweden, and various universities, particularly Auburn University in Alabama.**

**Table: Demonstrated MEC application areas**

| *Application* | *Achievement* | *Date* |
|---|---|---|
| Hydrogenation | Pilot demonstration | 9/98 |
| | Commercial slipstream demo | 8/99 |
| SCR-DeNox | Proof of principle (small pilot unit) | 4/99 |
| Synthesis gas | Proof of principle (small pilot unit) | 12/98 |
| Ethylene oxide | Proof of concept (bench-scale) | 3/99 |
| Phthalic anhydride | Proof of principle (small pilot unit) | 9/99 |

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