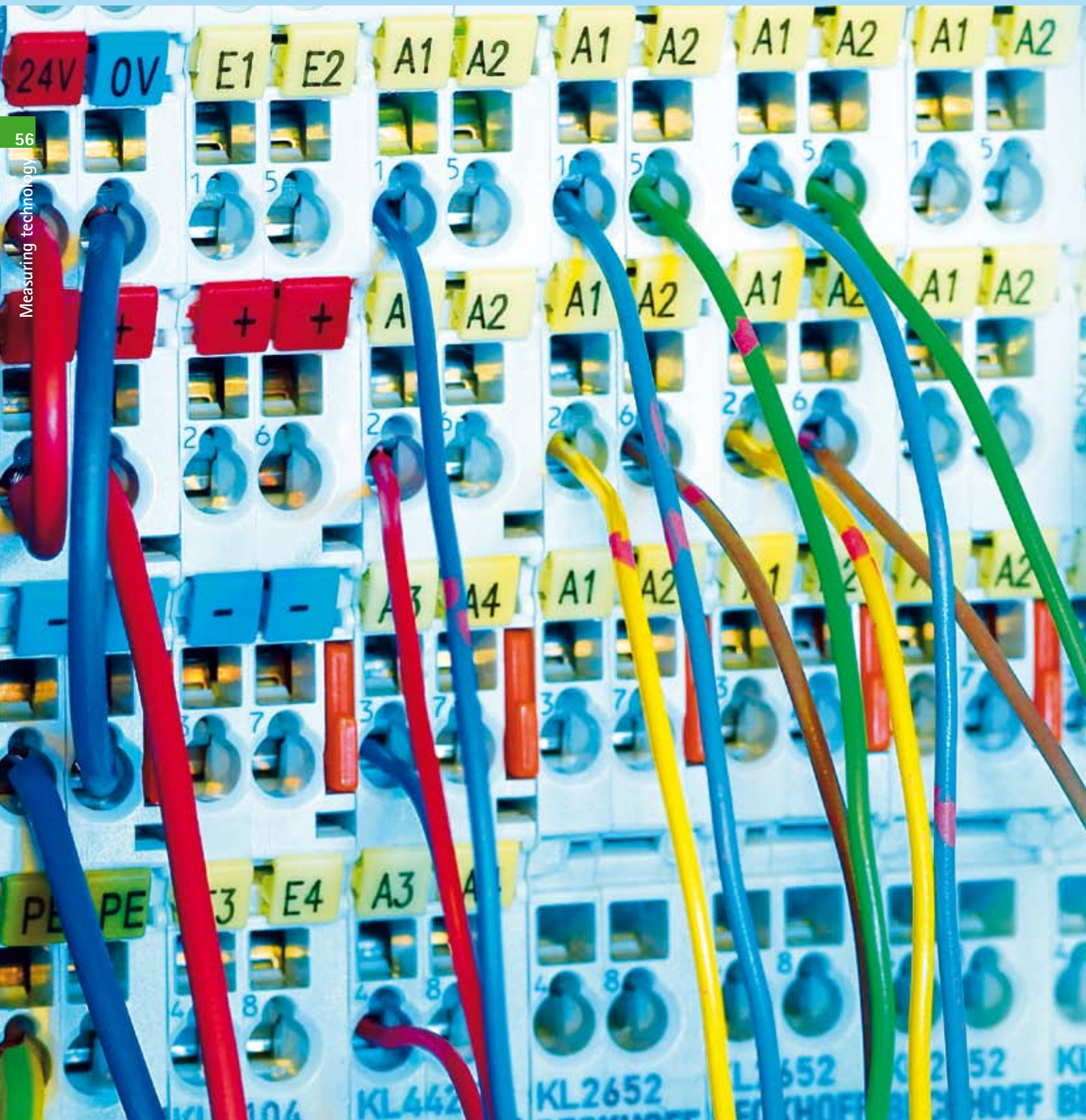


New measuring technologies make chemical reactions visible

“Insider” information



Using infrared rays, telephone cables and lots of mathematics, Bayer researchers have now obtained a new "insider's view" of the goings-on in the chemical industry's steel reaction equipment. They accomplished this feat by making clever changes to tried-and-proven measuring methods and recombining them in unusual ways. The new techniques make it possible to conserve raw materials and energy, which correspondingly reduces the cost of chemical production and is kinder to the environment.



Checks: sophisticated measuring techniques can be used to monitor chemical processes inside reactors (left). The temperature provides Dr. Martin Gerlach (above right) with important information about how the reaction is proceeding.

Dr. Martin Gerlach's office is broiling in the heat of the sun. The chemist at Bayer Technology Services is not fazed by the sauna-like temperature in the room, however. He is more interested in temperatures such as those in the huge reaction vessels and distillation equipment used in the chemical industry. "Each synthesis process consumes or generates a characteristic amount of heat. As a result, the temperatures on site supply valuable information about the course of the reaction," explains Gerlach.

His team has now developed a new type of thermometer which can take measurements at various points of the reactor simultaneously. Until now, this was only possible to a limited extent since conventional resistance thermometers and thermal elements ascertain temperatures via electrical effects and require individual wiring. If measurements have to be made at several points in the reactor with such thermometers, the strand of cables needed soon becomes as thick as a man's arm and may itself impair the sensitive process of chemical synthesis even in the large vessels used in the industry.

In contrast, the temperature sensor in the new Bayer thermometer is especially delicate. It unites umpteen measurement points in a glass fiber cable just half of a millimeter thick and, if needed, up to six meters long. The new sensor is furthermore entirely free of electric currents and voltage. This is an additional advantage, as it makes the

sensor insensitive to electromagnetic radiation and suitable for safe use even in explosive mixtures.

The heart of the new technology is actually a mass-produced article: "We use glass fibers from the communication technology sector," reports Dr. Wolfgang Borchers of Bayer Technology Services, who played a key role in the development of the thermometer. Glass fiber cables conduct light as well as invisible radiation, such as the longer wave infrared rays, from one end to the other. In order to make the fibers suitable as thermometers and not just for relaying telephone calls, they are spot treated with UV light by the Advanced Optics Solutions (AOS) company in keeping with instructions from Bayer researchers. This creates sections with special optical properties, known as Fiber Bragg Gratings.

One fiber measures at numerous sites simultaneously

When the researchers send infrared rays through the glass fibers, part of the transmitted light reflects on each grating, just as it would on a window pane, while the other wavelengths can proceed unhindered. As the temperature grows warmer or colder, the mesh of the grating changes in size as the atoms squeeze closer together or move further apart. This alters the wavelengths of the reflected rays, which then serve as a gauge for the distance between atoms in the manipulated



Measuring temperature with light

This thread-like glass fiber (in front) can be used to measure temperatures at several sites simultaneously. To this end, Fiber Bragg Gratings (shown on the rear right in the illustration) are created at the measurement points. Every section of such a grating reflects only very certain wavelengths (red). The light from other wavelengths can pass through unhindered and thus be reflected by another Fiber Bragg Grating (blue and yellow). If the glass fiber cable becomes warmer or colder, this changes the wavelength of the reflected light (e.g. from red to dark red). Bayer researchers use infrared thermal radiation invisible to the human eye instead of visible light in the glass fiber thermometer.

sections of fiber. The reflected wavelengths are measured with an infrared spectrometer that is now a standard component of many production facilities. These spectrometers are usually used to measure levels of substance concentrations, thereby also providing information about the progress of chemical reactions. "Upgrading the devices with the temperature-sensitive glass fibers is very easy," underscores Borchers. The new thermometer has long since proven its worth in pilot systems and has been demonstrating its talent for supplying "insider information" in two industrial production plants since late summer 2006.

A minireactor optimizes production

Exploring chemical processes is also a favorite hobby of Dr. Ricarda Leiberich from Bayer Technology Service. The chemist and her team have developed a teapot-sized measuring cell in which miniature versions of industrial syntheses processes are conducted. Using

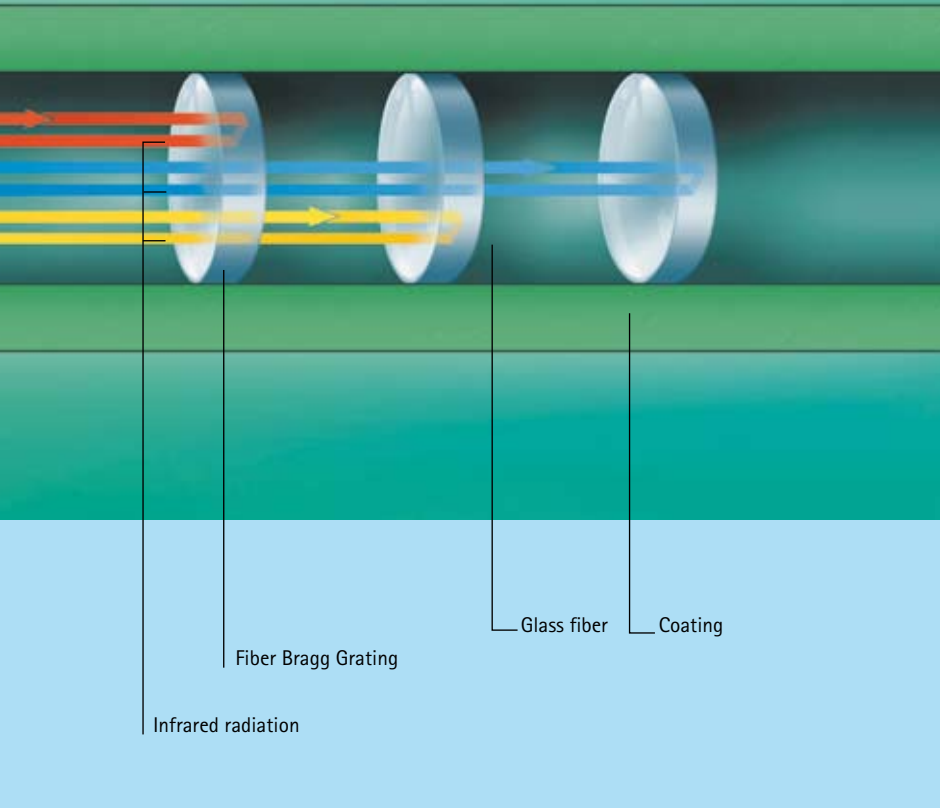
the new measuring technology, she can uncover secrets about reactions that take place faster than the blink of an eye. These reactions play a key role in the production of numerous plastics, for instance. The results of the measurements indicate which reactor designs and operating conditions are optimum for syntheses, prevent fast reactions from slowing down and keep the formation of undesirable byproducts to a minimum. Thanks to the findings from Leiberich's laboratory, Bayer has saved millions of euros in the operation of existing systems and in the construction of new ones – reason enough to honor the team of researchers with the Otto Bayer Medal in the spring of 2006.

It was long considered impossible to observe molecular unions, which take place within milliseconds. Problems began with the mixing of the starting substances, reports Leiberich: "If you mix substances more slowly than they react with one another, you have no opportunity to measure anything useful." The researchers at Bayer

therefore developed a jet which mixes all of the substances together within microseconds. Because analysis techniques have become considerably faster over the course of the past few years, scientists can now obtain a very detailed picture of the reaction process.

Focus on chemistry with video microscopy

In order to do so, they illuminate the reaction solutions several times per second with infrared rays of varying wavelengths which are absorbed by the starting substances, products and undesirable byproducts. The changes in the wavelength spectrum indicate which amounts of what substances are still involved in the reaction at which time points. The scientists use a reflection infrared spectrometer that provides reliable measurements even in cloudy mixtures for this purpose. In another run, the researchers film the process through a microscope. Filming is used because the starting substances are frequently in different phases, e.g.



Sensitive measuring technology: using this tiny glass fiber, Dr. Wolfgang Borchers (above) can monitor the temperature inside production facilities and therefore follow what is going on. Dr. Ricarda Leiberich (center) and Peter Lobert (below) analyze the courses of reactions in their specially constructed measurement unit using infrared light, video microscopy and a great deal of mathematics.

in liquids that don't mix but form droplets which drift around each other like oil in cooking water.

After the insider information comes the mathematics

In such cases, chemical reactions take place primarily on the surface of the droplets. The smaller the droplets, the larger the surface and the faster the reaction. In the filmed recording, the researchers can then watch how the

droplets gradually merge into one large puddle, thus slowing synthesis.

Additional work is needed to convert the multitude of information from laboratory trials into concrete advice for process engineers: "We develop complex mathematical models used to project the conditions in industrial reactors," explains Leiberich. The success of these calculations has long since ceased to be a secret, and the next plant to benefit from them is already under construction.



www.micromemanalytical.com/ATR_Ken/ATR.htm

Another application for ATR infrared spectroscopy is the analysis of water filters, as explained by the California analysis laboratory for the Orange County Water District.