Magnetic Resonance: Ongoing and Future Role in Chemical Engineering Research

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Introduction

In 1988, a report by Amundson on behalf of the U.S. National Research Council (Amundson, 1988) identified nuclear magnetic resonance (NMR) spectroscopy as a potentially useful tool for studying catalyst structure and surface chemistry, noting the existence of magnetic resonance imaging (MRI). Fourteen years later, there is a substantial body of evidence to say that magnetic resonance (MR) techniques, far more wide ranging in scope than was originally envisaged, have become integrated into chemical engineering research and are becoming increasingly more popular in this role. This said, the diversity of measurements that can be made and the systems that can be studied are still relatively poorly understood. The opportunities for market penetration are still quite high.

From a chemical engineer's perspective, the most important attributes of MR lie in its ability to record 1-D, 2-D and 3-D images with the resolution as high as 5–10 µm, along with spatially resolved maps of transport characteristics (diffusion, dispersion, and flow vector), chemical composition, and variations in the state of matter being probed—all this information being accessed noninvasively and without the need for a tracer. It is the ability to combine different MR measurements within a single experiment (e.g., combining spectroscopy and transport measurements) that makes it so useful in chemical engineering research. To date, most effort has been focused on transferring the imaging and flow visualization measurements originally developed for medical applications across the nonmedical arena. In itself this is not a trivial exercise, since the MR characteristics of nonmedical systems and their requirements on the detail of implementing the MR experiment are quite different from those of medical subjects.

Ongoing MR Research in Chemical Engineering

MR is established, but is still relatively underused in three distinct areas of application: characterizing fluid flows; visualizing structure-hydrodynamics relationships in process units; and the integrated use of MR with theoretical modeling and numerical simulation studies. The way in which MR is used in each of these applications can be quite different.

Characterizing fluid flows

Until recently, applications of MR to study flow phenomena have almost entirely been restricted to probing the liquid, as opposed to gas, phase—a direct result of the relatively poor signal-to-noise inherent in MR techniques. Nuclear spin densities in the liquid phase are ~10^3 higher than those in the gas, thereby making signal acquisition faster and easier. The potential use of MR in studying fluid flows is huge, because methods can be used to probe molecular displacements over length scales of 10^{-6} m up to the physical dimension of the sample. The time scales over which these displacements can be studied in a single measurement is sample-dependent (and depends on the characteristic relaxation time properties of the system), but can lie in the range of milliseconds to seconds. For those who are brave enough to rise to the challenge of designing new experiments to increase our understanding of spatio-temporal correlations in fluid flows there are exciting opportunities ahead. Advances in this area are limited only by our own scientific insight in designing the appropriate MR experiment to probe specific phenomena.

Most single-phase flow studies have been on transport in a porous media. In this application, so-called pulsed gradient spin echo techniques have been used to measure diffusion and dispersion in a model porous media such as bead packs (Seymour and Callaghan, 1997; Stapf et al., 1998; Manz et al., 1999a). The results of these studies are of immediate relevance to oil recovery technologies, which was the original motivation for much of this work, as well as having applications in the study of transport in fixed-bed reactors and groundwater remediation processes.

Figure 1 illustrates the level of detail that can be obtained in images of the water flow field (any ^{1}H-containing liquid could have been studied) through a packing of spherical glass ballotini. Close inspection of the image in the example sheds much insight. For example, channeling occurs throughout the bed, and within these channels liquid velocities are enhanced by up to an order of magnitude compared to the average liquid velocity in the direction of superficial flow. Furthermore, much of the bed is operating under near stagnant conditions. Therefore, at a practical level, we see directly how the physical shape and size of different packing elements and their method of loading influences the heterogeneity of flow within the bed. In parallel with these direct observations, MR enables us to explore in detail the interrelationships between the 3-D structure of the bed and the transport processes occurring within it (Sederman et al., 1998; Johns et al., 2000).

The ability to image the velocity field within a fluid allows MR measurements to provide an *in situ* determination of the rheology of that fluid. In-line monitoring of shear viscosity-shear rate data, ranging from one to over two decades of shear rate from one measurement are now routinely made (Powell et al., 1994; Arola et al., 1997); the effect of shear on the structural evolution of multiphase systems during processing operations can be probed as well (Altobelli et al., 1997). The current state-of-the-art integrates conventional rheological measurements with MR experimentation. Commercially available sample environments can be purchased such that, for example, a cone-and-plate rheology measurement can be performed *in situ* within the MR magnet thereby enabling an image of the velocity field within the sample to be acquired during shear.

This new type of Rheo-NMR measurement has already produced some important insights. For example, Britton and Callaghan (1997) reported visualizations of anomalous behavior such as apparent slip, shear banding, and fracture in systems such as wormlike surfactants during the shear measurement (see Figure 2). Quite apart from the interesting rheology under study, this result demonstrates how MR imaging can give us new insights into the limitations of our day-to-day "macroscopic" materials characterization techniques—in this case the cone-and-plate rheometer.

Does the rheometric characterization provided by the conventional cone-and-plate device offer all the relevant information about the in-use properties of our material? How can this new information be used in optimizing product and process performance? *In situ* Rheo-NMR studies can also be combined with *in situ* MR spectroscopy, which then allows us to characterize molecular rearrangements occurring during shear; such datasets have enormous potential value in testing and validating theoretical models of polymer rheology (Cormier et al., 2001).

What is Magnetic Resonance?

- MR measurements are based on the fact that when a nucleus of nonzero nuclear spin is placed in a magnetic field (typically a superconducting magnetic field of 2–10 T), its nuclear spin energy levels are made nondegenerate. By exposing the system to electromagnetic energy of appropriate frequency (radio-frequency), a resonant absorption occurs between these nuclear spin energy levels. The specific frequency at which this resonance occurs is called the resonance frequency and is proportional to the strength of the magnetic field used in the experiment.
- By exposing the spin system to an additional magnetic field that varies linearly in space, the resonance frequency becomes dependent on spatial position. By applying magnetic field gradients in 1, 2 and 3 dimensions, 1-, 2- and 3-D images are obtained with typically 10–200 µm spatial resolution. 1- and 2-D images can be acquired in any direction through the sample.
- Following the radio-frequency excitation, the return of the spin system to equilibrium is followed as a function of time. The data are Fourier-transformed to give the frequency spectrum or spatial domain image. No model for image reconstruction is required.
- Transport measurements (i.e., diffusion, dispersion, and flow) are also made by imposing gradients in the magnetic field across the sample—no tracer is needed. Displacements from µm scale to the sample size, over time scales of µs to minutes are measured.
- The rate at which a spin system returns to thermal equilibrium following the r.f. excitation is characterized by its nuclear spin relaxation parameters—the spin-lattice relaxation (T_1) and spin-spin relaxation (T_2) time constants. These time constants characterize the physico-chemical environment of the molecules being studied. If a system is characterized by a very rapid T_2 (e.g., many solids), it may not be possible to study it using MR.
- MR is nucleus- and molecule-specific. Any nucleus of nonzero nuclear spin can be studied, but in most chemical engineering applications ^{1}H (referred to as "proton" observation), ^{13}C, ^{23}Na, ^{31}P, ^{19}F, and ^{2}H are of most common interest. Different nuclei have substantially different resonance frequencies, but for a given spin system, say ^{1}H, protons in different H-containing molecules will have measurably different resonance frequencies; hence, the technique also distinguishes between different molecules containing the same elements. In most applications, ^{1}H is the nucleus of choice because of its high natural abundance and high MR sensitivity.
- MR is inherently insensitive compared to other spectroscopic techniques. In other words, spin populations in the excited and nonexcited spin states differ by one part in 10^4-10^5, and, therefore, the nuclear magnetic resonance absorption is weak. This is why gas-phase MR is a relatively specialist field.
- Working at higher magnetic field increases sensitivity and frequency- (and, hence, spatial-) resolution of the Fourier transformed data, but increases the influence of magnetic susceptibility artefacts on the measurement—this can be an important consideration in studying chemical engineering systems.

Visualization of the internal structure of solids by conventional means is limited by opacity. MR provides one of the few means to visualize solids' flows. The flow of solids is limited to the study of materials that give a detectable MR signal under the relevant experimental conditions and usually restricts studies to particles that have a ^{1}H-containing liquid-like (i.e., relatively long T_2 relaxation time) core. Typical systems are, therefore, oil-filled plastic beads or seeds, which will have a naturally high oil content. Early studies focused on imaging the particle distribution at rest within the container, following perturbations to the system. Such studies have been able to probe convection phenomena within granular systems resulting from vibrations of granular beds (Ehrichs et al., 1995) and to follow the evolution of segregation in rotating granular flow (Hill et al., 1997). Imaging measurements have also been reported while motion is occurring. For example, MRI has been used to visualize the formation of high-shear bands within vibrating granular beds (Caprihan et al., 1997), to obtain spatial distributions of collisional correlation times during 3-D granular flow in a horizontal rotating cylinder (Seymour et al., 2000), and to quantify the time-averaged density variations and the random motion of granular particles in the presence of gas flow in a model gas-fluidized bed reactor (Savelsberg et al., 2002). Increasingly, we are seeing a transfer of the MR techniques used to measure random and nonrandom transport processes in fluids to granular systems, along with the concomitant development of the appropriate formalisms to interpret the data obtained from these new measurements.

Process applications

Many industrial and academic research laboratories now have MR integrated fully into their research programs and use MR spectroscopy, diffusion, dispersion, and flow velocity measurements directly in problem-solving applications. The two most well established areas of process application, both using MR on a day-to-day basis, are food engineering, and the characterization of hydrocarbon bearing sedimentary rocks in well-logging applications. Food materials are excellent systems for MR inspection because of the similarity in their MR characteristics (e.g., relaxation times, low magnetic susceptibility variation) to those of medical subjects. Recent developments include the use of model food systems to demonstrate MR's temperature mapping capabilities (Nott et al., 1999) and a quantitative evaluation of mixing in food-processing operations (Lee et al., 2001). Small spectrometers dedicated to quality control applications in food production are already in use.

What Can You Measure?

- Flow velocities ranging from ionic drift velocities 10^{-3} mm·s^{-1} to pipe flows of ~10^{2} cm·s^{-1}.
- Molecular diffusion coefficients >10^{-14} m^{2}·s^{-1}. The probability distribution of molecular displacements for a given "observation" time is often reported, which is called the MR propagator.
- All measurements can be made in optically opaque samples and with multiple phases and components present.
- Phase separation—and state of mixing in general—can be followed by exploiting intrinsic differences in relaxation time, resonance frequency, and molecular self-diffusion coefficients among the individual components of the mixture.
- The state of phase of a system (e.g., the spatial evolution of a crystallization process) can be mapped by exploiting relaxation time variations among the same chemical species in the gas, liquid, gel, or solid phase.
- Temperature can be mapped by measuring the variation of relaxation times, molecular self-diffusion coefficient, and resonance frequency of a specific species within the sample.
- Droplet sizes in multiphase systems are obtained from measurements of molecular diffusion over varying time scales. The kinetics of denaturation processes, protein folding and aggregation processes can also be followed using measurements of molecular self diffusion.
- Molecular interactions in mixtures can be quantified by monitoring the difference in the value of the resonance frequency of a nuclear spin in the mixture compared to that found in the pure compound.
- Chemical speciation can be spatially resolved by combining spectroscopy and imaging methods within the same experiment.
- 2-D image acquisition times are typically a few seconds to minutes. However, the so-called ultrafast MR techniques allow data acquisition times for 2-D images, diffusion and propagator measurements to be as short as 10–50 ms, enabling imaging of transient phenomena.
- MR is limited to the study of nonmagnetic systems. MR cannot be used to study systems containing significant amounts of paramagnetic species. Whether or not a sample containing some paramagnetics can be studied can be decided only by preliminary investigation. Even if signal acquisition is possible, extreme care should be taken in extracting quantitative information from such data.
- Current commercial magnet systems limit the maximum diameter of samples to be studied to 2.5–~30 cm, depending on the strength of the magnetic field. For specific applications, study of samples outside the magnet ("inside-out") experiments are possible.

In contrast to food systems, well-logging applications are extremely demanding of MR methods—most rocks will contain significant amounts of paramagnetic impurities and exhibit strong spatial variations in magnetic susceptibility. However, the need to obtain a quantitative characterization of the fluids contained within rock formations has been the motivation behind some new and exciting developments in MR theory, experimental protocols, and measurement hardware. The NMR logging tool is one such technology and has been described as an "inside-out" measurement—that is, the sample to be characterized is actually placed outside the magnet (Kleinberg, 1996). A recent development by Hürlimann and coworkers (Hürlimann and Venkataramanan, 2002) allows "inside-out" measurement of a quantitative diffusion-relaxation time distribution function, in which full separation of the diffusion and relaxation analysis effects is achieved within a single measurement. This new measurement allows quantitative assessment of fluid composition, solid-phase wettability, fluid viscosity, and the distribution of the different fluid phases within the physical structure of the pore space of the rock.

There are many examples of MR applications at the R&D level. For example, MR is used in assessing the performance of filtration processes (e.g., Dirckx et al., 2000) and biofilm reactors (e.g., Beuling et al., 1998; Nott et al., 2001). Both of these applications exploit the capability of measuring the flow field within the process unit in combination with imaging the internal structure of the system to understand the interrelationship of the formation rate and deposited material structure with the local and macroscale hydrodynamics. Other applications include the visualization of flow within hollow-fiber bioreactors (Heath et al., 1990), and heat exchangers (Pangrle et al., 1992; Wang et al., 1999; Sun and Hall, 2001).

Building on the techniques used to study flow fields in process units, there is increasing activity in applying MR to help design fixed-bed separation and catalytic processes. Exhaustive studies of chromatographic column design and operation have been published by Tallarek, Van As, and coworkers addressing issues including quantification of the mass transfer between the intraparticle pore network of the porous particles and the interparticle void space comprising the column, as well as study of dispersion and electroosmotic perfusion phenomena (Tallerek et al., 1996, 1999, 2001). In studying catalytic processes, the ability to incorporate MR spectroscopy measurements into experimental protocols allows us to map chemical conversion in addition to the transport processes occurring within the reactor.

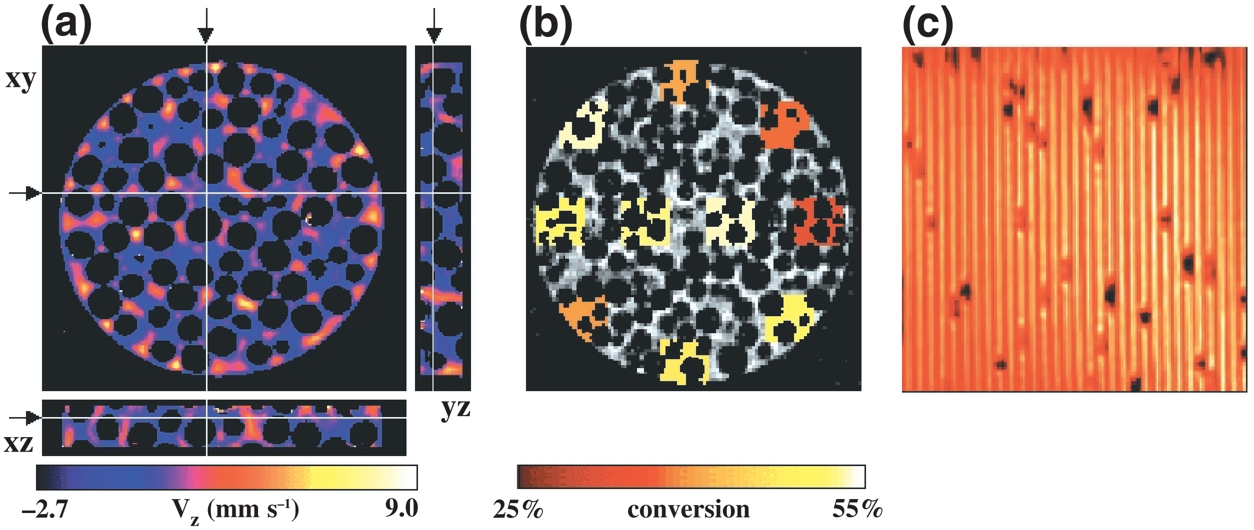

Figure 1. Different MR techniques probe quantitatively the internal structure, transport processes, and chemical composition within a system; these examples are taken from the field of reaction engineering.
(a) 3-D MR visualization of the z-component of the flow velocity (in the direction of superficial flow) of water within a packing of spheres (black). Flow fields through slices are taken in the xy, yz and xz planes through the 3-D image. Voxel resolution is 195 μm × 195 μm × 195 μm. The 5-mm-dia. ballotini are packed within a 46-mm-ID column. The superficial liquid velocity is 1 mm·s^{-1} (Sederman and Gladden, 2001b). Heterogeneities in flow within the bed can be studied as a function of catalyst shape and bed-loading procedure. (b) By combining MR spectroscopy with imaging, the chemical conversion within any specified region of the bed can be quantified noninvasively. Here, the extent of conversion of the esterification reaction of ethanol with acetic acid is studied in a fixed bed of ion-exchange resin catalyst (black pixels). The catalyst beads and reactor are of diameter ~700 μm and 10 mm, respectively. Local conversion within selected volumes (1.5 mm × 1.5 mm × 0.5 mm) is shown by the color scale. Fractional variations in conversion within a given transverse slice section through the bed can be of the order of 20% and correlate with the heterogeneity in transport processes characteristic of the bed (Yuen et al., 2002). (c) Ultrafast imaging allows us to follow in real time, Taylor flow of gas and liquid within individual channels of a ceramic monolith. This monolith is rated at 400 cpsi (i.e., channels of width ~1 mm); gas bubbles are visualized as the dark regions (Mantle et al., 2002).

Figure 1 shows some of the varied applications of MR in studying heterogeneous catalytic processes. Both single- and two-phase flows can be visualized, and in multiphase reactors such as trickle-beds, gas-liquid, and solid-liquid contacting areas are obtained directly from the images (e.g., Sederman and Gladden, 2001a). Such issues as the extent of film wetting, to which the technique is sensitive, still have to be resolved, but MR provides an invaluable new tool for the noninvasive study of contacting patterns in reactors. Even if the system has to be substantially scaled down to fit inside the magnet, useful information can be gained on the effect of particle size, shape and surface hydrophobicity on liquid flow velocity and gas-liquid-solid contacting. Furthermore, with the increasing interest in process intensification, many reactor configurations can now be studied at full operational scale within a standard MR magnet system. All the MR methods currently used in mainstream catalysis can, and almost certainly very soon will, be transferred to studying bioreactor design. For example, by making the image contrast dependent on molecular diffusion coefficient, the spatial variation of protein folding within a reactor can, in principle, be followed. Developments in gas-phase imaging are also going to extend the range of experiments accessible to study by MR.

Integrating MR, theoretical modeling, and numerical simulation

The ability of MR to provide 2-D and 3-D images at spatial resolutions of 10–200 μm in optically opaque environments offers exciting opportunities for the integration of MR with theoretical modeling and numerical simulation studies. MR data are used in two quite different ways. The first is to combine MR and numerical simulation codes as a single tool for problem solving. The key idea of using the MR image is to guide the description of the problem to be solved by using it directly in a pixelated form as the simulation lattice or by using it in a more qualitative way to identify the structural features to be represented within the simulation and to explore the accuracy of the numerical prediction.

This is an area of research in which work in the medical and engineering fields is at a similar development stage which is not surprising since both research communities require each other's skills. A good example of this research methodology is found in the work of Wang and Li (1998), in which they used MR images to develop a 3-D simulation lattice to be employed in numerical simulation of the mass transport processes relevant to drug delivery to a brain tumor. From this simulation, it was possible to predict the optimal location of a controlled release drug delivery implantation. Why is MRI so much more useful in this type of application compared to other tomographic techniques? Of course, the ability to image an optically opaque subject is key, but just as important is the fact that MR can also give a 3-D mapping of the transport processes occurring within the sample. If one needs the real diffusion coefficients of species within the sample to input to the model, one can measure them directly. This is enormously powerful, because we can develop models in which the simulation lattice, boundary conditions, and many of the transport parameters required by such models are not free variables, but parameters measured on the real system.

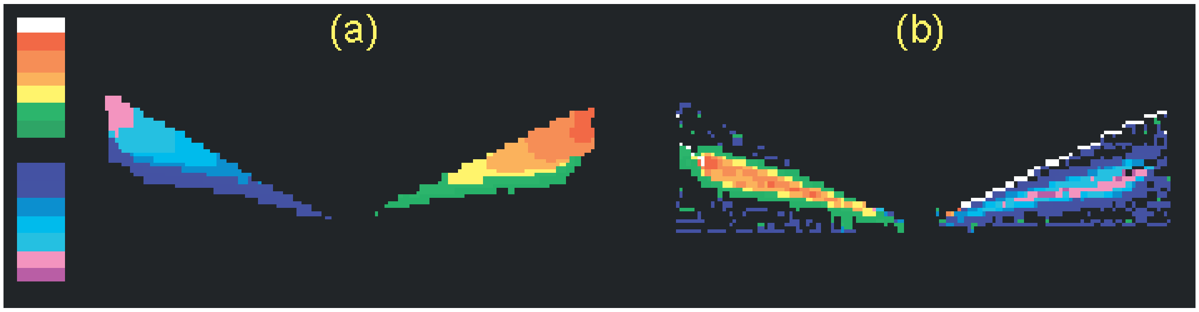

Figure 2. (a) Velocity image and (b) shear rate map for a wormlike surfactant in a 4° cone gap, at a shear rate of 16 s^{-1} (above critical shear rate).
A distinct deviation from a linear velocity gradient and shear banding are observed. The velocity scale lies between the limits ±12 mm s^{-1} and the shear rate between ±57 s^{-1} (Britton and Callaghan, 1997).

The second, but quite different, use of MR is to provide 3-D datasets for the validation and development of numerical codes. Looking to the future, many of us expect to exploit developments made in computational physics to provide an alternative strategy to using scale-up rules and correlations in process design. To achieve this goal, these "predictive" codes must be validated rigorously, and MR has an important role to play in this. Again, the key attribute of MR is its ability to give you spatially resolved information on structure, transport and, as appropriate, chemistry within the system of interest. If the numerical code is able to predict at high spatial resolution the experimentally-determined chemical composition, diffusion, dispersion, and flow behavior, there is compelling evidence that the code is capturing the correct chemistry and physics, and, hence, should be able to predict the performance of the scaled-up system. Of course, strategies are still required for modeling heterogeneities in macroscale systems on length-scales greater than those probed in the MR experiments.

An example of this methodology is the validation of a lattice-Boltzmann code for low Reynolds number flow of water through a packing of spheres reported by Manz et al. (1999b). Of course, many comparisons have been made between a numerical prediction and experimental data. However, the point being illustrated in this work is that the simulation lattice fed to the lattice-Boltzmann code was the *actual* 3-D MR image of the packed bed for which the MR visualization of flow was also recorded. The comparison of the experimental data with numerical prediction shows the ability of the code to reproduce the correct physics of the system. If the simulation lattice itself is only an approximation to the system to be modeled, one is not only testing the code, but also the quality of the simulation lattice. Consideration of the finite size of the image voxels is important in such studies, and, if MR images are to be used in this way, the 3-D images must be acquired with as high a spatial resolution as possible.

Emerging Areas of MR Research

Gas-phase imaging

Conventional MR measurements rely on the "thermal" polarization of the atomic nuclei within the magnetic field. Since the interaction energy of the nuclear "magnets" with the applied magnetic field is about 10^4 times smaller than the thermal energies of the system, the resulting polarization of the nuclear magnets is very weak and the inherent sensitivity of MR measurements is lower than other spectroscopic techniques. This characteristic of MR measurements is particularly limiting in studying systems of low nuclear spin density such as gases. Despite this, MR studies of so-called thermally polarized gases are successfully performed using ^{3}He, ^{129}Xe, and ^{19}F observation (for the case of the ^{19}F nucleus, the molecules CF_4, C_2F_6 and SF_6 are studied). Outside of medical applications, thermally polarized gases have been shown to be a powerful probe of inorganic porous media (e.g., rock cores) (Mair et al., 2002). ^{3}He and ^{129}Xe are particularly well suited for such studies given their rapid diffusion, inert nature, low surface interactions that reduce relaxation time effects, and the ability to tailor the diffusion coefficient by altering the gas pressure in the sample. In particular, the faster diffusivities of gas-phase species compared to liquid-phase probes of the pore space, have made it possible to extend the length scales that can be probed in a porous media by more than an order of magnitude. A further demonstration of the potential application of thermally polarized gas has been the ^{1}H imaging studies of acetylene, propane and butane gas flow in monolithic catalysts (Koptyug et al., 2000).

The advent of hyperpolarized ^{3}He and ^{129}Xe for use in MR has given further impetus to gas-phase studies. Brunner et al. (1999) reported a continuous flow system that circulates laser-polarized

^{129}Xe through the sample, yielding an enhancement of signal intensity of 3–4 orders of magnitude compared to the equilibrium ^{129}Xe signal–gas-flow displacement profiles of ^{129}Xe flowing through polyurethane foams of different densities and pore sizes were reported. Another exciting area of potential development is the use of laser-polarized gases to provide enhanced sensitivity to study species at surfaces (Pietraβ et al., 1998).

Fast imaging techniques

The use of ultrafast MR techniques is well established in medical applications, and there is increasing effort in applying these methods in chemical engineering research. The motivation is strong, because a reduction in data acquisition times from several minutes to a few milliseconds opens up the transient world to us. MR visualization of turbulence during single-phase flow of water in a pipe was reported as long ago as the early 1990s, with Reynolds numbers of up to ~9,500 having been studied. Various imaging strategies can be used (Fukushima, 1999), the fastest of these being the echo planar imaging (EPI) technique originally developed by Mansfield (Mansfield, 1977), in which 2-D image acquisition times can be as short as 30 ms. EPI-methods have been used to image the velocity distribution in a cross-sectional plane perpendicular to the direction of superficial flow at a Reynolds number of 2,250; clear visualization of a turbulent 'puff' was recorded (Kose, 1991). Ultrafast techniques are now being applied to various other fluids problems; applications include mapping spatio-temporal structures formed in Taylor Couette flow (Kose, 1994), the velocity pattern within a falling liquid film (Heine et al., 2002), and a free-falling drop (Han et al., 2001), and two-phase Taylor flow through a ceramic monolith (Mantle et al., 2002).

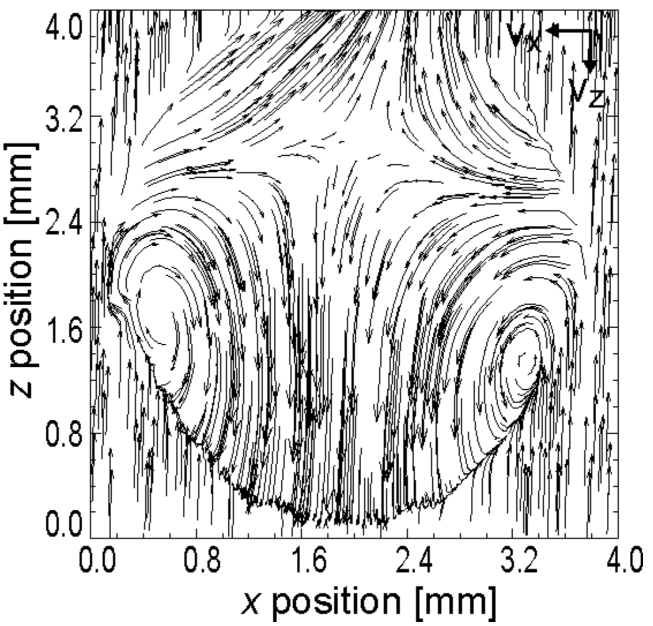

Figure 3. Another example of ultrafast imaging techniques. Velocity components v_z, v_x are shown within a drop of pure water falling at 2.0 m·s^{-1} as a function of position along the zx plane, averaged over the y dimension of the drop. The v_z component is scaled relative to the average falling velocity of 2.0 m·s^{-1} (Han et al., 2001).

Future Prospects

How will MR develop over the next few years? Developments are most likely in the following areas:

- Increasing use of proven imaging, relaxation, transport and spectroscopic measurements to solve process-related problems. MR will be used as a routine "tool" in research laboratories, particularly in the research areas of combining spectroscopy and flow visualization to study reactive flows and to aid design of chemical and biochemical reactors. To date, most MR studies have focused on the ^{1}H nucleus because of its high natural abundance and MR sensitivity. Increasing use of multinuclear observation (e.g., ^{13}C, ^{31}P, ^{23}Na and ^{19}F) will allow a wider range of reactions to be studied *in situ*.
- In industrial, and to some extent, academic, laboratories there is potential for developing problem-specific experimental setups to enable the MR user, but nonexpert, to perform routine experiments (Fukushima, 1999). MR as a research tool has huge flexibility, but data are open to misinterpretation if the user does not fully understand the relevant principles of MR phenomena and their practical implementation during the experiment. Therefore, there could be an increase in MR spectrometer systems designed for a particular type of data collection and optimized to measure flow fields in particular process units so that the operator does not have freedom to change all possible acquisition parameters and, hence, introduce unknown influences to the contrast levels in the image. Precedents already exist in clinical medicine, downhole tools in oil exploration, and food quality control. In each of these applications, MR hardware and software are designed to perform a restricted set of measurements to readily interpret the resulting data in terms of specific characteristics of the system. In addition to this simplified user interface, the hardware design for a single specific function can also reduce hardware costs considerably. There is also potential for using dedicated, single-function MR hardware for process control applications. For example, droplet size distributions in emulsions can be characterized *in situ* under flowing conditions thereby enabling MR to be used as part of a process control strategy. This measurement technique also avoids the introduction of errors into the droplet-size determination caused by extracting samples from a process line for *ex situ* analysis (Johns and Gladden, 2002).
- There is much to be gained by thinking of MR as a research tool that can be used in combination with other tomographic and sensor technologies. For example, X-ray micro-tomography (XMT) can probe structures at higher spatial resolution than MR, but does not readily give information on transport processes. By combining MR and XMT, a greater range of spatio-temporal correlations may be accessed. Opportunities also exist in using MR to identify and understand, at the laboratory scale, the occurrence of particular phenomena that may have a detrimental effect on product quality or process performance, but using a cheap, robust measurement on the plant to identify when such phenomena occur in the real process. For example, in trickle-bed operation, the detailed nature of transitions in hydrodynamics between different flow regimes may be identified and their signature in terms of the variation in pressure drop measurements identified. The pressure drop

measurements may then be used on the full-size operating unit to provide a much more accurate assessment of trickle-bed operation.

- Specialist research groups will become experts in developing new MR measurement techniques that fully exploit the tremendous range of MR phenomena to be probed, to yield new insights into chemical engineering problems at a fundamental level. Particularly exciting future prospects include:

Combining new MR experiments with theoretical analysis to maximize the learning that can be obtained from MR studies of spatio-temporal correlations of transport and reaction processes

Using "thermal" and "hyperpolarized" gas-phase MR to study gas flows and to probe interfacial processes including the study of protein configurations and heterogeneous catalytic processes

Developing further "inside-out" MR techniques (e.g., Eidmann et al., 1996, Kimmich and Fischer, 1994; McDonald, 1997), in addition to well logging technologies, to overcome the problems of samples having to be placed within the bore of commercial magnetic systems

The majority of the applications identified in this article would not have been considered possible even ten years ago, and, as more chemical engineers become conversant with MR methods, the field is sure to expand. However, we must not be complacent. Takeup of MR methods has been slower across a wide range of possible applications in chemical engineering than it might have been. In contrast, the food industry has been quick to exploit MR in food science, processing, and quality control applications. MR has the potential to provide completely new measurements of the fundamental transport and chemical processes that are key to process and product design. To fulfill this potential, more chemical engineers need to be sufficiently conversant with the theoretical principles and experimental implementation of MR spectroscopy, imaging, relaxation and transport measurements so that they can operate beyond the simple "picture taking" mode of an MR imaging experiment. Every image voxel can be encoded with a quantitative measurement of a parameter of interest. If we engage fully with MR, we can expect exciting and deep insights into long-standing and new problems.

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