

What's in that bottle?

Michelle Espy, James Hunter, and Larry Schultz

Nuclear magnetic resonance and x-ray imaging combine to offer a powerful tool for identifying liquids in sealed containers.

Michelle Espy is the leader of the MagRay project at Los Alamos National Laboratory in Los Alamos, New Mexico. **James Hunter** and **Larry Schultz** are engineers on the MagRay team.

Imagine you have to quickly figure out just what liquid is inside a bottle. The container might be opaque, or even metal. You can't open it, and you can't trust what is on the label. That scenario is faced in airports, at border crossings, and in response to hazardous-material or bomb scares. Moreover, the need to accurately identify liquids is common in quality control of everything from medicine to cosmetics to foods.

It turns out that by combining nuclear magnetic resonance (NMR) and x-ray imaging, scientists can meet the challenge of liquid identification more reliably than with either technique alone.

Spinning atoms to look at tissue

Magnetic resonance imaging (MRI) is the premier noninvasive diagnostic for imaging soft tissue, in which changes in density are subtle. It works because, unlike density differences, chemical differences within the tissue are significant enough to strongly influence the NMR signal that is the basis of MRI. Figure 1 explains the technique.

When applied to obtain high-resolution images of anatomy, MRI requires large magnetic fields (typically 1.5–3 T) and expensive equipment. But it is possible to perform MRI with much weaker fields if high resolution is not needed (see the article by Micah Ledbetter and Dmitry Budker, *PHYSICS TODAY*, April 2013, page 44). From early on in NMR history, groups have demonstrated the technique in fields as low as that of Earth. More recent work has shown that sensitive detectors such as superconducting quantum interference devices (SQUIDs) can improve resolution. For liquid screening, we at Los Alamos National Laboratory “prepolarize” the sample with a field of about 50 mT, 1000 times Earth's magnetic field. We can then read out the precession of the magnetization (see figure 1) with a field comparable to Earth's. The low-frequency signal associated with such a weak read-out field can penetrate through metal. The weak fields are safe for the security checkpoint setting, since metal is not moved or heated—and as a bonus, the expense of generating the magnetic field is greatly reduced. In the newer version of our screeners, we have been able to dispense with SQUIDs, which greatly simplifies instrumentation.

Assay with x ray

If you've seen x-ray images in a doctor's office, you know that x rays behave differently as they pass through various materials. Denser or thicker materials like bones stand out in x-ray

images because they absorb a relatively large fraction of the x-ray intensity that strikes them. A quantitative measure of the absorption, or beam attenuation, is given by Beer's law for the intensity I of an x-ray beam that has passed through a thickness x of material: $I(x) = I_0 e^{-\mu x}$. Here I_0 is the initial intensity of the x-ray beam, which is the number of photons entering the material, and the material-dependent parameter μ is called the attenuation coefficient of the material.

Obtaining a complete understanding of x-ray attenuation is a complex undertaking, but some key general concepts are simply stated. First, attenuation depends on the energy of the x-ray beam; higher-energy beams generally attenuate less. Second, attenuation is linearly dependent on the density of the material—twice as many molecules of a material stop twice as many x rays. Third, attenuation is nonlinearly dependent on the atomic number of the material; at typical x-ray energies, materials with higher atomic number stop more x rays.

For a given material of specified thickness, analysis of an x-ray image will yield μ for the energy of the x-ray beam. If the identity of the material is unknown, one could try to find out what it is by comparing its μ against a library of attenuation values from known materials. Since specimen and library μ values depend on x-ray energy, running the comparison at two or more different energies will reduce the uncertainty in the characterization of the unknown material.

More than the sum of the parts

An NMR signal is typically generated by hydrogen atoms because they readily respond to magnetic fields—that is, the more hydrogen atoms, the stronger the NMR signal. In secu-

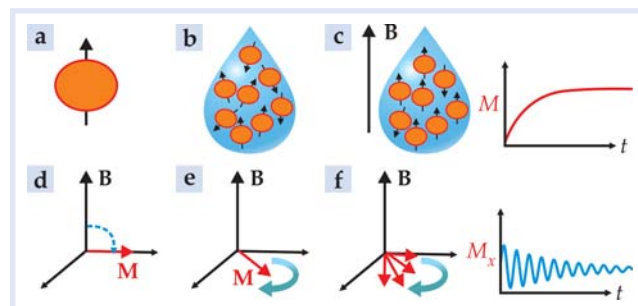


Figure 1. How magnetic resonance imaging works. (a) The protons in water's hydrogen atoms possess a quantity called nuclear spin, which gives them a magnetic moment. (b) In the absence of a magnetic field, the spins are oriented randomly and there is no net magnetization. (c) A net magnetization $\mathbf{M}$ develops in the presence of a magnetic field. It forms with a characteristic time T_1 that depends on the chemical environment of the protons. (d) The spins can be tipped by a short burst of RF waves at a characteristic Larmor frequency. (e) Once tipped, the spins precess at the Larmor frequency. A detector measuring a particular component of $\mathbf{M}$ produces a sinusoidal signal. (f) The magnetization decays with a characteristic time T_2 that, like T_1 , depends on the protons' chemical environment. When the applied magnetic field varies spatially, the position-dependent signal gives spatial information that can be used for magnetic resonance imaging.

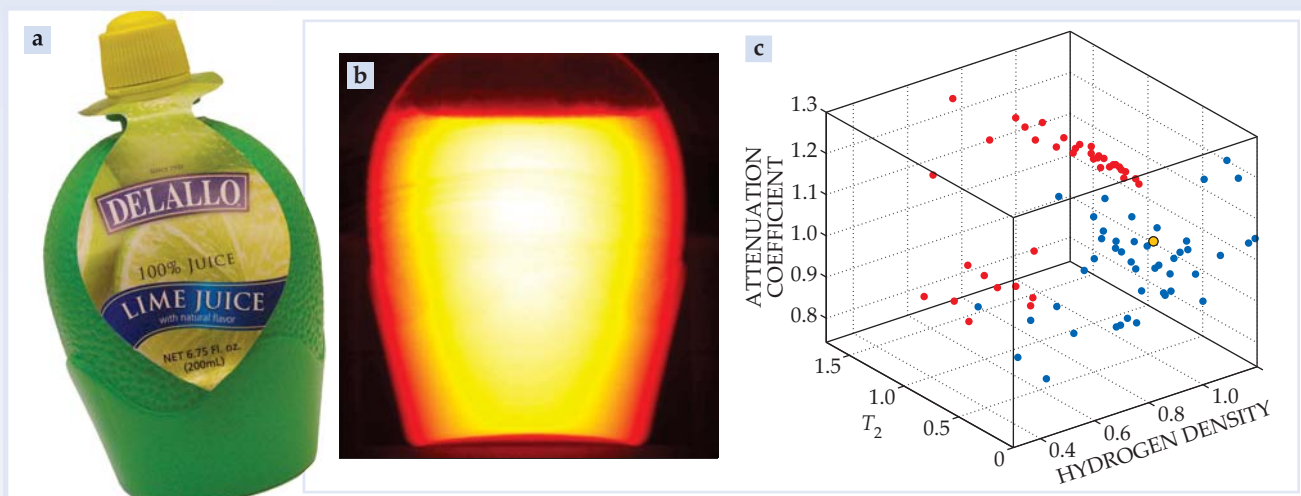


Figure 2. It says lime juice, but is it really? An off-the-shelf bottle of lime juice (a) generates an x-ray image, such as in (b), from which we can extract the volume and attenuation coefficient of the liquid. In the x-ray image, the white areas are those of greatest attenuation; the orange areas are of less attenuation. (c) We combined x-ray data with nuclear magnetic resonance data to get a signature of the juice (yellow point) in a three-dimensional space. (The meaning of the relaxation time T_2 is explained in figure 1.) The result can be compared against a library of safe (blue) and dangerous (red) materials. Our prototype system classified the lime juice as a water mix. The three axis variables are given relative to the values for water.

rity applications, for example, many benign liquids are water based and exhibit a characteristic NMR signal. On the other hand, many explosive liquids are packed with additional elements, so the density of hydrogen atoms goes down significantly. For those liquids, the NMR response is less than for water. Other types of explosive liquids have excess hydrogen atoms and provide an NMR response greater than for water.

The NMR signal is also affected by the volume of liquid in a bottle—twice the volume generates twice the signal. X-ray analysis can determine the volume of liquid, so bringing together x-ray and NMR techniques enables the volume effect to be removed in determining the hydrogen content of a liquid.

Figure 2 illustrates how NMR and x-ray analysis might be combined to determine whether a liquid passing through an airport security checkpoint is benign or harmful. We subjected a bottle of lime juice to a joint NMR and x-ray scan. From the x-ray image we extracted μ and the liquid volume. The NMR signal delivered hydrogen content and the relaxation time T_2 (see figure 1 for an explanation). In figure 2, μ , T_2 , and the hydrogen content (with volume effect removed) for various liquids are represented as points in a three-dimensional space. Some areas in that space are populated only by harmless liquids; others include liquids that are harmful in some way. The lime juice sits squarely in a benign region. Indeed, the benign and threat regions of the 3D space are well separated. As a result, in airport-security applications, both false alarms and missed detections of dangerous materials should be less than they would be if NMR or x-ray imaging were used individually.

In addition to addressing particularly difficult security issues, the combined NMR and x-ray technology can answer such questions as, Has food or medicine spoiled? Does a liquid meet quality control standards? Has a foreign chemical been added to water? Is this expensive bottle of wine really as advertised? In all those cases, the nondestructive imaging combination shows the promise to be more reliable and less costly than destructive statistical sampling techniques currently in use.

From the lab to the airport and back

X-ray imaging such as you may have seen in dental offices or airports is ubiquitous in the public domain. So is NMR, but

not at the low fields necessary for practical liquid scanning. Nowadays, groups worldwide are working to make low-field NMR a practical method for a variety of applications. With support and guidance from the US Department of Homeland Security, we and the rest of the MagRay team at Los Alamos have taken low-field NMR out of the laboratory and demonstrated that it can work in a public setting.

Two NMR instruments (not combined with x-ray imagers) were tested at the Albuquerque airport in New Mexico. The first was an imaging machine that examined trays of bottled liquids (see <http://www.youtube.com/watch?v=xT2zncrtU-s>). The second was a much more compact instrument for scanning individual bottles (see <http://www.youtube.com/watch?v=HQT5iAwodDc>). Those exercises showed that low-field NMR machines could operate in the electronically cluttered public-transportation environment. Now we've returned to the lab and are working to integrate safe x-ray machines and NMR instruments. A video record of our prototyping results can be found at <http://www.youtube.com/watch?v=nizjDxt3F5Q>.

Although NMR and x-ray imaging have been demonstrated individually in both public and industrial environments, the combined technology has not. Work still needs to be done to test materials, assess the influence of bottle shape and container material over the widest class of packaging, and figure out how to merge the techniques for rapid and cost-effective screening of multiple bottles. Whether combined NMR and x-ray screeners will appear in an airport near you is unknown, but already we have seen that the physics of two completely different imaging modalities can come together to provide new information for solving difficult problems.

Additional resources

- A. Macovski, S. Conolly, "Novel approaches to low-cost MRI," *Magn. Reson. Med.* **30**, 221 (1993).
- J. Clarke, M. Hatridge, M. Mössle, "SQUID-detected magnetic resonance imaging in microtesla fields," *Annu. Rev. Biomed. Eng.* **9**, 389 (2007).
- R. Austin et al., "MagViz: A bottled liquids scanner using ultra-low field NMR relaxometry," in *Magnetic Resonance Detection of Explosives and Illicit Materials*, T. Apih et al., eds., Springer, New York (2013), chap. 9.