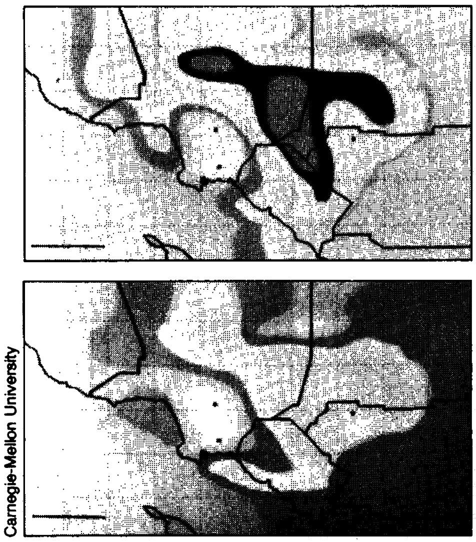

Carnegie-Mellon University

Ozone levels *in the Los Angeles basin drop if cars switch from gasoline (top) to methanol.*

McRae says: "Controlling hydrocarbons in the city just pushed the ozone out into the countryside." The key to the ozone level, the researchers discovered, was actually the amount of nitrogen oxide emissions. The hydrocarbons mostly affect the rate of ozone production, McRae says, so that lowering hydrocarbon emissions in the city slowed down the rate of ozone production but not the total amount produced. As a result, the city would get less ozone, but the areas downwind from the city would get more.

The two engineers ran simulations where gasoline-burning automobiles were replaced by methanol-using ones, and found they could decrease the ozone level significantly. The methanol by-products are much less reactive in their ozone-forming potential than are the gasoline by-products. As a result, changing half the cars over to methanol could cut peak ozone levels by 40%. These computer experiments played a big role in President Bush's recent decision to call for methanol-burning cars to be used in the nation's worst pollution centers, McRae and Russell say.

The best part about these simulations, McRae says, is that they are much cheaper than doing the actual experiments. Replacing all the cars in the Los Angeles area with methanol-mobiles and then seeing what happens would cost hundreds of millions of dollars. And then, "if it doesn't work, you're in a lot of trouble. If it doesn't work on the computer, you just put in a different set of numbers and try again.

Computer experimentation does have its limits, of course. The first and most obvious is that if one does not know the fundamental physical laws governing a system, one cannot use a computer to learn them. And many systems that do behave according to known physical laws may forever defy accurate simulation. "Living systems," Abdulla says, "may never be modeled on a computer because they are too complex."

Also, computer experimentation is not an end in itself; in fact, researchers say that it is most valuable when done in conjunction with physical experiments. Testing of the space shuttle was done both in wind tunnels and on computer, Holst says, because the two methods complement each other. They are prey to different types of errors, he explains—while the wind tunnel falls short in trying to mimic the features of the real world in a small, enclosed space, numerical experiments make mistakes because of the limits of the model or the limits to the computational power of the computer. A wind tunnel is vital, for example, in testing the effect of turbulence, something that no computer can yet simulate accurately.

But the power of supercomputers continues to increase, and with it the ambition of computer experimenters. Right now, Bob Dick at ALCOA has enough confidence in his simulated drop tests that he will design a can for a customer without ever having built a physical model, but no one is ready to do that with an aircraft wing, for instance. Bailey at NASA-Ames says that once computer simulations narrow a wing design down, the final work must still be done in the wind tunnel. "Basically, the wind tunnel goes into much greater detail, down to the rivet head," he says. "We don't have computers powerful enough to do that, yet." He estimates that a computer a million times faster than those now available would be necessary to get results as accurate as in the wind tunnel.

As each new generation of computers comes along, not only will researchers be able to do their old experiments with greater accuracy, but entire new lines of experimentation will open up. "We can't wait to get our hands on the next generation with several orders of magnitude more computing power," says McRae at Carnegie-Mellon. With these powerful machines, he envisions such experiments as controlling acid rain over entire regions or designing the most economically efficient strategies to curb air pollution. With enough computing power, researchers could experiment with the formation of the Milky Way galaxy, earthquakes in California, or chemical interactions between complicated organic compounds. All without getting their hands dirty.

■ Robert Pool

Putting the Squeeze on Hydrogen

It was hydrogen, the lightest of gases, that floated the great zeppelins across the Atlantic Ocean 60 years ago, but in the hands of Ho-Kwang "Dave" Mao and Russell Hemley, hydrogen is something else altogether.

In Mao and Hemley's lab at Carnegie Institution of Washington, hydrogen is a solid, crystalline substance with metal-like properties. As reported on page 1462 of this issue, the two researchers have squeezed hydrogen with pressures of more than 2.5 million atmospheres (2.5 megabars), and their optical measurements of hydrogen at these pressures indicate that it becomes a semimetal—a substance that conducts electricity, although to a much smaller degree than normal conductors.

Ten years ago, Mao and colleague Peter Bell at the Carnegie Institution were the first to create solid hydrogen, at about 57 kilobars. At this pressure the hydrogen is an insulator, but as the pressure increases, theory predicts it will go through a series of transformations from an insulator to a semiconductor to a semimetal and finally, somewhere between 2.5 and 4 megabars, to a metal. Checking these experimental predictions is important not only to physicists interested in bonding in solids, but also to planetary scientists. Metallic hydrogen is likely to constitute a large portion of the mantles of such gaseous planets as Jupiter and Saturn, and thus could greatly influence their electromagnetic properties. It is also possible that metallic hydrogen could be a high-temperature superconductor.

Mao, a geophysicist, and Hemley, a physical chemist, used a diamond-anvil pressure cell to put tremendous pressure on the hydrogen, and as they squeezed, they made optical measurements through the transparent diamond. At 2.5 to 3 megabars, the hydrogen becomes "virtually opaque," Hemley said. This implies that some of the electrons bound to the individual hydrogen molecules are moving into new energy levels to become conduction electrons, creating a semimetal. At some point, all of the electrons should come loose from the nuclei and the material should become fully metallic, but Hemley does not believe they have reached that point.

Unfortunately, the researchers may have trouble seeing the metallic hydrogen if they do achieve it. Above 2 megabars, the diamonds begin to glow bright red, making it hard to do optical measurements. So far, they have managed to overcome the interference, but it may get worse with increasing pressure.

■ Robert Pool