Urban smog control: A new role for trees?

Trees can serve as a major source of the hydrocarbons contributing to smog ozone (SN: 9/17/88, p.180). But trees can also help cool the air, thus slowing the heat-driven photochemical reactions that brew ozone from hydrocarbons and nitrogen oxides. Indeed, because smog production is so temperature-sensitive, trees that cool cities may do more to limit ozone than to foster it.

This conclusion, drawn from new computer simulations, suggests that sprawling urban growth may take an unnecessarily large toll on air quality if planners don't spare as many trees as possible, says study coauthor William L. Chameides, an atmospheric chemist at the Georgia Institute of Technology in Atlanta. He believes city planners and air-pollution-control managers should join forces to "think about how they want their [region] to grow" — and especially "where they want to leave green spaces."

Noting that most U.S. ozone-mitigation strategies focus on limiting hydrocarbons, Chameides says the new findings also reinforce the importance of shifting to approaches that place at least as much emphasis on nitrogen oxides.

Growing cities sacrifice many trees to development. Atlanta, whose population has increased 30 percent each decade since 1970, has lost about 20 percent of its trees over the past 15 years, Chameides says. During that same period, average summer temperatures have climbed steadily in both the city and its surroundings. But Atlanta's increase, totaling almost 4°F, dwarfs those of its rural neighbors — in one case by a factor of about 5. In a paper to appear in the JOURNAL OF GEOPHYSICAL RESEARCH later this summer, Chameides and Georgia Tech colleague Carlos A. Cardelino argue that the urban temperature increase probably stems from a deforestation-fostered "heat-island effect," in which asphalt and dark-roofed structures become massive heat reservoirs.

On the basis of Atlanta's 1985 tree cover of about 57 percent, Chameides and Cardelino computed likely ozone concentrations for a typical summer day in Atlanta under a range of scenarios. Each scenario explored some facet of the city's changes over the past 15 years, such as tree loss or an estimated reduction of as much as 50 percent in hydrocarbon emissions from human activities, including traffic and industrial facilities.

Comparisons of these simulations suggest that the sharp, steady rise in Atlanta's summer temperatures over the past 15 years has resulted in a large net increase in hydrocarbon emissions from vegetation — despite the loss of one-fifth of the city's tree cover. This apparent contradiction reflects the fact that a tree's hydrocarbon-emission rate increases dramatically as temperatures climb. Indeed, Chameides and Cardelino say the estimated vegetative-hydrocarbon increase from Atlanta's remaining trees would have canceled the city's decrease in automobile and industrial hydrocarbon emissions.

Arthur H. Rosenfeld, a leading analyst of urban heat-island effects, has long advocated tree planting to reduce urban heating and to sequester the carbon dioxide emissions that threaten to initiate a global warming (SN: 5/7/88, p.297). "But I hadn't even thought about that [vegetative-hydrocarbon feedback on ozone from tree cutting], so I'm happy to have [the Georgia Tech team] publish it," says Rosenfeld, who directs the Center for Building Science at Lawrence Berkeley (Calif.) Laboratory.

The new simulations make "an important contribution," adds John R. Holmes, director of research at California's Air Resources Board (CARB) in Sacramento. The results also dovetail with observations made by CARB — a state agency responsible for some of the toughest auto-emissions regulations in the nation. During the 1970s, when CARB's vehicle-emissions controls focused on hydrocarbons, Los Angeles experienced a reduction in ozone, but only downtown, where traffic was highest and vegetation was lowest. Ozone levels continued to increase in the areas where they had always been highest — downwind. It wasn't until "we had large reductions in both hydrocarbons and nitrogen oxides that ozone levels went down rapidly all over," Holmes says.

Gary Z. Whitten, who models urban ozone at Systems Applications, Inc., in San Rafael, Calif., says the Atlanta report makes a good argument for controlling nitrogen oxides, but he points out that the computer model failed to account for several factors that could greatly affect ozone production, such as a heat-driven increase in atmospheric mixing. Whitten views the analysis as "interesting" but only a "first start" at defining the complex interactions among trees, temperature and smog. *— J. Raloff*

Simulated liquids point to new solutions

Detergents lifting dirt from clothes, paint disappearing into a turpentine-soaked rag and cellular proteins folding into their biologically active shapes all depend on the way chemicals dissolve in various liquids.

Two theoretical chemists have run new computer simulations of water and nonwater liquids that help clarify why some liquids dissolve specific solutes better than others. They say their work could give molecular biologists a better understanding of how proteins fold and function, while helping materials scientists predict how various ingredients will behave in new mixtures.

Liquids fall into two broad categories — polar (such as water) and nonpolar (such as turpentine) — which differ in the abilities of their molecules to form hydrogen bonds among themselves and with other molecules. Although the intermolecular attractive power of a hydrogen bond reaches only about one-tenth that of the covalent bonds that link the atoms within a molecule, the weaker bonds help determine such important properties as a liquid's boiling point, viscosity and ability to dissolve specific solutes.

Any chemistry student can explain why table salt dissolves well in water but not so well in hexane, a nonpolar organic solvent. Electrically polar water molecules, with their segregated regions of positive and negative charge, cluster around the salt's charged sodium and chloride ions. Hydrogen bonding then helps the ion-centered clusters to merge into the surrounding water. Because the nonpolar hexane molecules do not form such clusters, they don't pull salt into solution as readily.

But even professional chemists have difficulty accounting for why nonpolar liquids outdo water in dissolving electrically neutral gas molecules such as methane. Lawrence R. Pratt of Los Alamos (N.M.) National Laboratory and Andrew Pohorille of the NASA Ames Research Center in Mountain View, Calif., set out to answer this basic question.

Using computer simulations of water and five nonpolar solvents, they calculated "the likelihood of finding, at an arbitrary point in the solvent, an atomic-sized cavity that could accommodate the solute." Though water has more overall cavity space than the nonpolar solvents, its spaces are distributed in smaller, less flexible packets, the chemists report in the June 20 JOURNAL OF THE AMERICAN CHEMICAL SOCIETY. Thus it appears that water, compared with a nonpolar solvent such as carbon tetrachloride, would have more difficulty rearranging its molecules to make room for small solute molecules such as methane.

Most previous models of solubility based on solvent cavities have portrayed molecules as hard spheres, a simplification that works well for nonpolar solvents such as hexane, notes theorist Frank H. Stillinger of AT&T Bell Laboratories in Murray Hill, N.J. But for probing subtle differences between the dissolving powers of water and nonpolar solvents, models that include the effects of hydrogen bonds on cavity size should prove more fruitful, Stillinger and Pratt assert. *— I. Amato*