Study offers recipe for global warming-free industrial materials

May 3 2010, by Greg Kline

Let a bunch of fluorine atoms get together in the molecules of a chemical compound, and they're like a heavy metal band at a chamber music festival. They tend to dominate the proceedings and not always for the better.

That's particularly true where the global warming potential of the chemicals is concerned, says a new study by NASA and Purdue University researchers.

The study offers at least a partial recipe that industrial chemists could use in developing alternatives with less global warming potential than materials commonly used today. The study was published in the Proceedings of the National Academy of Sciences.

"What we're hoping is that these additional requirements for minimizing global warming will be used by industry as design constraints for making materials that have, perhaps, the most green chemistry," says Joseph Francisco, a Purdue chemistry and earth and atmospheric sciences professor.

The classes of chemicals examined in the study are widely used in air conditioning and the manufacturing of electronics, appliances and carpets. Other uses range from applications as a blood substitute to tracking leaks in natural gas lines.

The chemicals include fluorine atom-containing compounds such as hydro fluorocarbons, per fluorocarbons, hydrofluoroethers, hydrofluoroolefins, and sulfur and nitrogen fluorides.

In a 2009 study, Francisco and NASA collaborators Timothy Lee and Partha Bera examined the molecular qualities that make fluorinated compounds even more powerful warming promoters than chemicals emitted in greater quantities, such as carbon dioxide and methane.

The fluorinated compounds proved to be far more efficient at blocking radiation -- or heat -- in the atmospheric window. The atmospheric window is the frequency range in the infrared region of the electromagnetic spectrum through which radiation from Earth is released into space. This helps cool the planet. When that radiation is trapped instead of being released, a greenhouse effect results, warming the planet.

The new study looked at a broader class of chemicals to identify molecular-level features that make them more or less efficient at trapping radiation in the atmospheric window. The study employed results from atomic-scale quantum chemistry calculations done on computers from NASA and Information Technology at Purdue (ITaP), Purdue's central information technology organization.

"We specifically looked at molecules that we felt would have potential for industrial use as replacements for chlorofluorocarbons," says Francisco, whose research focuses on the chemistry of molecules in the atmosphere.

Among other things, the study looked at how the number and placement of electronegative atoms in a molecule's structure affects its radiative efficiency. The number and placement of fluorine atoms proved to be a key factor because they're very electronegative and form highly polar bonds with carbon and sulfur.

Fluorine atoms thus tend to change the bond-polarity of the molecules -- modifying the bonds holding the atoms in the structure. This, in turn, affects how a molecule will absorb infrared radiation that normally passes through Earth's atmosphere and into space.

"The polarity change is what makes for an efficient absorber of infrared radiation," says Lee, chief of the Space Science and Astrobiology Division at NASA Ames Research Center.

One message from the study: Avoid allowing fluorines to bunch up in a molecular structure. "In other words, don't put them all on one atom," Francisco says. "Spread them out."

The fluorinated compounds also persist longer in the atmosphere than carbon dioxide and other major global warming agents, Lee and Francisco note. Even if emitted in lower quantities, fluorine-containing chemicals might have a powerful cumulative effect. Some don't break down for thousands of years.

Provided by Purdue University

Citation: Study offers recipe for global warming-free industrial materials (2010, May 3) retrieved 20 April 2024 from
https://phys.org/news/2010-05-recipe-global-warming-free-industrial-materials.html