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What Models Can (and Can't) Tell Us About Risk

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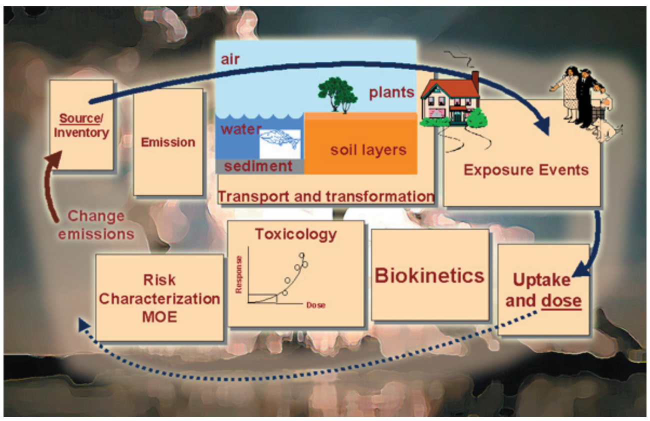
Scientists use computer models to estimate how pollutants distribute themselves in the environment. How far can we trust these models? How much can they tell us about health risks, and what are their limits?

Thomas McKone leads the Environmental Chemistry, Exposure, and Risk Group in Berkeley Lab's Environmental Energy Technologies Division; the group studies the physical processes by which pollutants migrate through the environment and use computer models to help policymakers regulate chemicals that pose threats to human health.



EETD's Environmental Chemistry, Exposure, and Risk Group studies how pollutants migrate through air, water, and soil and expose humans to risk.

What is a risk? What is a hazard?

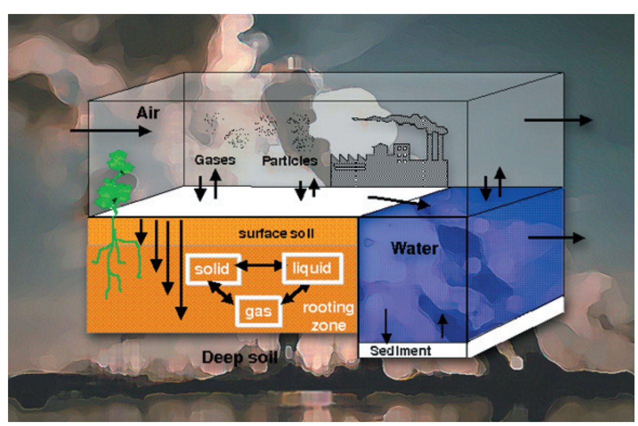
Everyone is at risk of getting cancer, some more, some less. Exposure to a cancer-causing chemical is a hazard. "Science can measure exposures and set up experiments to demonstrate hazard, based on occupational or other exposed groups or based on animals studies," McKone says, "but you cannot do a scientific experiment to assess human risk. Risk assessment is not a science."

Chemicals are characterized by half-lives, the time it takes for their concentration to decrease by half. Computer models estimate where chemicals go, how much get into the air, the water, or the ground, and how long they last before breaking down or combining with other chemicals. The half-lives of persistent organic pollutants (POPs) are so long that they can diffuse all over the earth, increasing human exposure.

"Because of complexity, you can relate things in a model that you couldn't in your mind, because there is too much to keep in your head," says McKone. "A model puts all these pieces together."

But just understanding how the pieces fit together doesn't guarantee correct results. "You can still get results that don't correlate to the real thing. You need observations to confirm the model and move it closer to a representation of reality." This can be a problem for policymakers, who don't like uncertainty. "A danger is that they may just use model results to tell them what to do."

Says McKone, "Our group's goal is to ask 'how do decision makers use models? What is it that they need to do their work effectively? Then we determine what it is you can do to make the models more effective." With continuing support from the Environmental Protection Agency, McKone and his group conduct regular research and development to improve models' usefulness for risk assessment and experimental studies. The goal is parsimony, "making the model as complicated as needed to solve a problem but not more so."



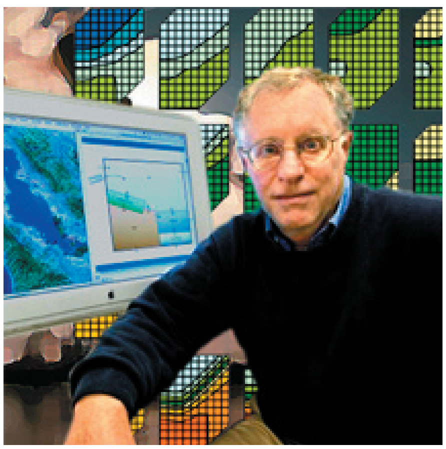
Models like CalTOX estimate where pollutants go and how long they persist in parts of the environment.

A model model study

In a unique study aimed at making models of POP persistence and long-range transport more useful to policymakers, McKone and Matthew MacLeod, formerly of Berkeley Lab's Earth Sciences Division and now at the Swiss Federal Institute of Technology in Zurich, brought together researchers from Canada, France, Germany, Italy, Japan, Switzerland, and the United States.

"To my knowledge, no study of this kind has been undertaken before," says McKone. "We worked with nine groups in all, each with their own model." To compare them, "we created 4,000 'chemicals'—not real ones, but imaginary chemicals with idealized properties—and we ran all the models through this 'space' of chemical properties." By learning which models produced consistent or conflicting results, the goal was to develop a consensus model that captured the minimum set of essential components.

"There were areas where the models had the same results, and areas where they diverged from one another," McKone says. The teams used elements of all nine models which led to common results and resolved the elements that produced divergent results, emerging with "the simplest model possible for solving the problem, that nonetheless had enough detail and complexity to accurately model the result properly."



Tom McKone in front of a page of chemical space plots from the CalTOX model, showing that the persistence of chemicals in the environment depends on the ratios of their water-to-air solubility and their octanol-to-water solubility.

Four chemical properties determined the behavior of POPs in all nine models. Two were solubility ratios: the chemical's solubility in air divided by its solubility in water, and its oil-water solubility ratio, which indicates mobility based on how much it sticks to soils, sediments, and lipids (fats) in biological organisms. A POP that accumulates rapidly in fat is a cause for concern, since human beings will build up high levels over a lifetime.

Two other properties were half-life in air and half-life in water, the latter a good measure of persistence in surface waters, soils, and sediments. Some POPs are volatile and cycle rapidly through different media. While both are perseistent, a volatile POP needs to be treated differently from a stable POP.

Their study not only demonstrated that the nine models could produce similar results but showed that policymakers should single out real POPs with the four specific qualities that emerged as determinant, the keys to their behavior in the environment.

What makes a good model?

In addition to parsimony, McKone mentions two other qualities that make a useful model: "One of the things decision makers want is transparency. They need to know how the model works—the method has to be transparent to the world."

Finally, McKone says, "models need fidelity. So in addition to making the model transparent and as simple as possible, you must incorporate all the processes that are important in linking the final result to the factors that, if changed, will alter that result. You are always walking a fine line between how much detail you need to get fidelity, while not incorporating so much detail that it overwhelms the final users."

It's a problem that comes up in plenty of other questions about how to make scientific models useful to nonscientists. Forecasting the weather, for example: there are plenty of sophisticated, supercomputer-based weather models, says McKone, but many daily forecasts are based on judgment, perhaps augmented by simple PC-based plug-ins that incorporate rules of thumb. "The bottom line is that no one wants to be overwhelmed with data. We all want just the few basic results that are useful to us."

This is an edited version of an article appearing in the January 2007 edition of Science@Berkeley Lab, the online science magazine of Lawrence Berkeley National Laboratory. The full-length version, including links to further information, may be accessed at http://www.lbl.gov/Science-Articles/Archive/sabl/2007/Jan/pollutant-models.html].