



# MODEL BEHAVIOUR

Controlling the adverse effects of chemicals on the environment requires an understanding of how chemicals behave in the natural world. Environmental modelling developed at Trent University can predict chemical impact—and help engineers design solutions.

In the practice of engineering, mathematical models are used for simulation, design and prediction. Engineers construct and apply models that simulate the behaviour of physical, chemical, electrical and even biological phenomena. One area of modeling that has been relatively slow to evolve is environmental modeling applied to the behaviour of chemical substances in the environment. Two main reasons have slowed this application. First, conditions in the natural environment—air, water, soils, sediments, vegetation and animals—are highly variable in both space and time. Descriptions of such phenomena as atmospheric turbulence or lake currents can become very detailed and complex. The result is a high degree of specialization with relatively isolated professional groups addressing and regulating aspects, such as air pollution, water quality, or pes-

ticide fate in soils. Chemicals, however, migrate freely throughout the environment ignoring these specializations. The result is often that the “big picture” of chemical fate is not fully understood.

## Chemicals at large

A second reason is the large number of chemicals and the wide range in their properties. It is believed that some 100,000 chemicals of the more than 20 million identified substances have been mass produced. In Canada, the Domestic Substances List contains about 24,000 compounds and more are being introduced each year. Environment Canada and Health Canada have been mandated to evaluate all chemicals in the next few years—a formidable task. Other jurisdictions, notably the U.S., Japan and the European Union, have similar programs to identify and regulate substances that

have the greatest potential to harm the environment or human health. The list includes solvents, fuels, intermediates, soap and detergents, monomers and polymers, biocides, pesticides, drugs and by-products.

## Mission possible

This task of evaluating and predicting in broad terms how chemicals behave in the environment is the primary mission of the Canadian Environmental Modelling Centre (CEMC), established in 1995 at Trent University in Peterborough. The centre develops, tests and disseminates a variety of models, mainly through its website ([www.trentu.ca/cemc](http://www.trentu.ca/cemc)), from which models can be freely downloaded. The work is supported by grants from the Natural Sciences and Engineering Research Council (NSERC), a consortium of chemical companies, including Dupont, Dow,

by Donald Mackay, PhD, P.Eng.

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Procter and Gamble, 3M, Unilever and ExxonMobil, and such government departments as Environment Canada, Health Canada, Indian and Northern Affairs, and Fisheries and Oceans. The centre has collaborative links with other universities and research groups that share a common interest in modelling.

The models enable the user to input key chemical properties, such as vapour pressure, or solubility in water, and deduce into which environmental media a chemical is likely to migrate, the relative concentrations in such media as air, water and fish, and how long the chemical will survive. These depictions of “fate” in the form of “mass balance statements” are invaluable when assigning environmental priorities to chemical substances. Most regulatory agencies set priorities on the basis of four criteria: persistence, bioaccumulation, toxicity and potential for long range transport, i.e. the P, B, T and LRT criteria. Models available from the CEMC are widely used to assess P, B and LRT by regulatory agencies that include Environment Canada, the U.S. Environmental Protection Agency, the European Union and the United Nations Environment Program, and they have been applied in such countries as Japan, the U.K. and France. These models can be applied to “evaluative” environments that have hypothetical but typical properties. They can also be applied to region-specific condi-

tions with actual temperatures, wind speeds and dimensions.

#### **Human exposure**

Models for describing chemical behaviour in sewage treatment plants, river basins and lakes are also available. Many local applications include the waters of the Great Lakes Basin. The models also address the important task of establishing a comprehensive assessment of human exposure. Often, the key route to human exposure is not in drinking water or inhaled air; it is “natural” foods such as fish or vegetation that can accumulate chemicals directly from the environment and transfer them through food chains.

#### **The dirty dozen**

Recently, the United Nations Environment Program identified a “dirty dozen” chemicals that are subject to bans or severe regulation. The dozen includes PCBs, “dioxins” and certain pesticides, such as DDT. This marks the first small, but very significant, step to control chemicals on a global scale. It acknowledges that society has recognized that certain chemicals are better not synthesized or used on this planet. Attention is now focused on the next dozen. Mass balance models of chemical fate on a global scale are under development at the CEMC and elsewhere to identify and regulate the chemicals of greatest concern prior to widespread use. The old

system of identifying problem substances by finding them at high levels in the environment is no longer acceptable. A proactive rather than reactive approach is needed in which the fate and effects of chemicals are assessed. For example, it has become clear in recent years that brominated fire retardants are quite persistent, so that levels throughout the environment are increasing steadily, even in remote locations.

Inadvertent contamination of distant locations is of particular interest to Canadians. There is slower degradation of chemicals in the Arctic, by virtue of its low temperatures, and contaminants survive longer. As a result, several food advisories are in place to protect humans from exposure to chemicals that were never used locally, but have migrated there in atmospheric and oceanic currents. Human exposures in the north are often much higher than in the more temperate, industrial south.

#### **Science first**

Recent actions by such municipalities as Halifax and Toronto to ban pesticide use in urban areas are responses to public demands for more vigorous regulation of chemicals to ensure negligible exposure. These decisions can be made on the basis of qualitative perceptions or “gut feelings” –or they can be based on sound quantitative assessments of chemical fate and effects. Regrettably, there is often extreme “chemophobia.”



Engineers have the opportunity to contribute to enlightened management of chemicals in the environment. Given their quantitative skills, surely they have an obligation to do so? They have the basic understanding of mathematics, the physics and chemistry of the environment, and they can acquire the necessary biological and ecological knowledge to develop and apply comprehensive models of chemical fate in the environment. These capabilities can form the foundation for sound, enlightened and economic decisions on how we can use the chemicals of commerce to our benefit without adverse effects on human or environmental health. ❖

**Donald Mackay PhD, P.Eng., is director of the Canadian Environmental Modelling Centre (CEMC) at Trent University. Mackay is renowned worldwide as the originator and developer of an environmental modelling system that provides valuable insight into the behaviour of chemicals in the natural environment, as well as a framework for future projects.**

**In 2001, Mackay was awarded the PEO Engineering Medal in the category of Research and Development for his work on environmental modelling, and he has received other awards, notably the Honda Award for Eco-Technology in 2001 and the Kalev Pugi Award of the Society of the Chemical Industry in 2003.**

## **Green power: Ontario engineers and the environment**

**A**s members of PEO, Ontario's 65,000 professional engineers have a responsibility to safeguard public health, safety and welfare. This includes taking action to protect and sustain the environment. Engineers work to harmonize human activities with conservation, environmental protection and restoration strategies. Understanding the broader implications of engineering practice, including the potential environmental impacts of engineering projects, is recognized as an important element of professional engineering practice.

Professional engineers, given their professional responsibilities as individuals and as corporate decision makers, have an important role to play in protecting the public from the potential health impacts of climate change. They understand the link between energy use, air quality and human health, and will need to consider how climate change will affect air quality to develop new technologies to solve environmental problems.

Dubbed by government as "the most profound economic challenge since the Second World War," the Kyoto Protocol requires Canada to reduce its greenhouse gas emissions to a level 6 per cent below those produced in 1990. In practical terms, this means that Canada must reduce carbon-based emissions by nearly one-third (240 megatonnes of carbon) by 2012. The federal government, after the December 2002 ratification of the accord, is planning its implementation and is embarking on discussions with provincial governments, industry and the public.

Through their leadership in the development of Ontario's infrastructure, individual professional engineers and the companies they lead, have been vital to the province's economic growth and prosperity. This was especially true during the years of economic expansion following the Second World War when our world-class transportation and power infrastructures were planned and initiated. Through their professional accountability and innovative creativity, individual professional engineers can assist Canada achieve and reap the economic and social benefits of reducing carbon-based emissions.

As the Ontario government continues to adopt more stringent environmental laws and standards, engineers will be challenged to develop new solutions to reduce pollution, clean up the environmental problems of the past, and preserve what's left for future generations.

*by Ken McMartin, P.Eng., President, Professional Engineers Ontario  
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