Honda Foundation Report №100

Eco-Chemistry

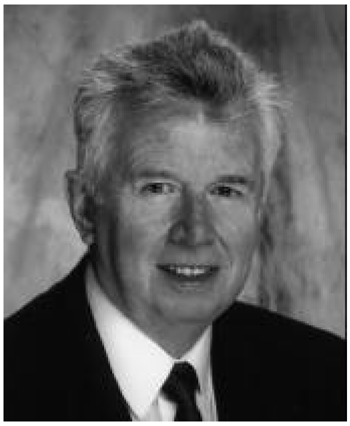
Achieving Harmony Between Chemical Use and Environmental Stewardship

Dr. Donald Mackay
Professor, Environmental and Resource Studies, Trent University Canada

On Friday,November 16,2001 at Hotel Okura in Japan

22th HONDA PRIZE Commemorative Lecture

HONDA FOUNDATION



Personal History

1936 Born in Glasgow, Scotland
1958 B.Sc. in Applied Chemistry, ARCST in Chemical Technology at Royal Technical College and University of Glasgow
1961 Ph.D. in Chemical Engineering at Royal Technical College and University of Glasgow
1961-64 National Research Council Postdoctoral Fellow at the Department of Chemical Engineering and Applied Chemistry, University of Toronto Working on shock tube research with Professor O. Trass
1964-67 Research Chemical Engineer with the Heavy Organic Chemicals Division of Imperial Chemical Industries Ltd., Billingham Co., Durham, England
1967-95 Professor, Department of Chemical Engineering and Applied Chemistry, University of Toronto
1995- Professor, Environmental and Resource Studies, Trent University,

Membership:

- Association of Professional Engineers of Ontario and Fellow (1972), Chemical Institute of Canada and Canadian Society for Chemical Engineering
- American Chemical Society
- Association of Environmental Engineering Professors
- International Association for Great Lakes Research

Awards: (from 1990 onward)

1990 The Chandler-Misener Award of the International Association for Great Lakes Research
1990 Francis W. Karasek Award of the University of Waterloo, Faculty of Science Foundation
1990 Founders Award SETAC
1991 Editor's Award, Journal of Great Lakes Research
1992 McLean Visiting Professor in Environmental Studies Trent University
1993 Varian Lecture, Carleton University Dept. of Chemistry
1998 International Association for the Exchange of Students for Technical Experience Award in recognition of outstanding service
2000 Mellanby Review Award, Elsevier Science Publishers and SETAC

2001 Gold Medal of the Professional Engineers of Ontario

Publications:
A total of about 520 publications of which over 400 are in the refereed literature.

" Eco-Chemistry" :Achieving Harmony Between Chemical Use and Environmental Stewardship

Commemorative Lecture at the conferring ceremony of the Honda Prize
on the 16th November 2001 in Tokyo

Dr. Donald Mackay
Professor, Environmental and Resource Studies, Trent University Canada

Acknowledgements

First, I would like to express my sincere appreciation to the Honda Foundation for this award. I accept it not only on my own behalf, but also on behalf of my colleagues with whom I have worked over the last 40 years. In particular, I am very grateful to Mr. Kawashima, President of the Foundation, to Mr. Inoue the Managing Director and to Mr. Ishihara the Secretary General.

I have been fortunate in having the continuing support of the Canadian Government, especially the Natural Sciences and Engineering Research Council (NSERC). They have achieved an enlightened balance between awarding public funds responsibly, with minimal bureaucracy, with an appropriate degree of direction, but leaving the researcher enough freedom to explore new ideas. Many of these ideas fail, but as I hope to show you later, some succeed.

I would also like to thank the many industrial chemical companies which have supported our research at the Canadian Environmental Modelling Centre (CEMC) at Trent University. As important as the funding, is the opportunity to exchange ideas with them, an exchange which is especially valuable for students. Without industrial contributions, our research on commercial chemicals in the environment towards a goal of "Eco-Chemistry" would be much less effective.

Finally, I thank the staff at the Canadian Embassy in Tokyo, especially Mr Kaneko and Dr Hicks, for their efforts on my behalf. They solicited independent letters of support for my nomination, and I am indeed grateful to those who must have written kindly about me.

Chemical Technology and a Humane Civilization

The general objective of the Honda Foundation is the "Creation of a humane civilization", a concept advanced by its founder Mr Soichiro Honda. The Honda organization has achieved a deserved reputation and success for promoting high quality in its many products. This conviction that high quality is inherently desirable is extended to our environment and society by the various activities of the Honda Foundation by its advocacy of "Eco-Technology". The concept that high quality technology can be immensely beneficial to society is one that I heartily support. Indeed, it has been a guiding principle in my career. In this address I would like to outline one aspect of the beneficial use of technology, namely the role of chemical substances for promoting human prosperity, health and well being. It can be called "Eco-Chemistry". It is an interesting aspect of technology because, as in other areas of technology, mistakes have been made in the past, largely through ignorance and lack of a full appreciation of how chemicals behave and what effects they may have on humans and other organisms which share our ecosystem. Regrettably, but understandably, many people now distrust chemicals and chemical technology. They are suspicious of pesticides and are willing to pay more for "organic" foods that are thought to be less contaminated with chemicals. There is a strong movement to regulate and even ban chemicals. This year the United Nations took a first small, but significant step to ban the use of twelve chemicals from production and use on this planet.

There are about 20 million chemicals known to man. Of these perhaps 50,000 to 100,000 have been produced in commercial quantities. Currently in Canada about 24,000 chemicals are registered for use. We thus face an immense challenge evaluating them to identify the most troublesome ones, to apply appropriate regulations and encourage the substitution of safer, more environmentally capable chemicals.

As we embark on the 21st Century we have much improved knowledge of chemical substances and how they behave in the environment. As I hope to demonstrate, there is now no excuse for repeating past mistakes. Our aim must be to exploit the desirable properties of chemicals, but do so with an awareness of their potential to harm the environment, ourselves and our fellow creatures on this planet. This is the essence of "Eco-Chemistry".

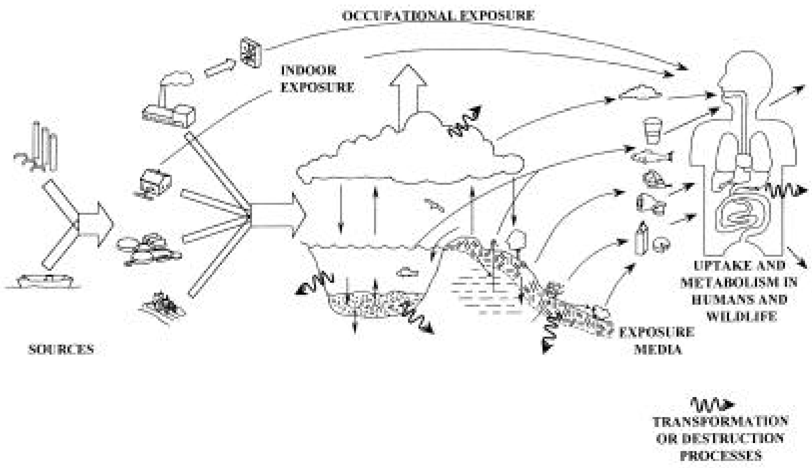


Figure 1: The chemical journey through the environment

Figure 1 illustrates my view of the journey which chemicals take from import and production, to discharge to the environment where they can undertake a long and tortuous journey, ultimately entering air, water and foods and our bodies. We have to be able to predict this journey quantitatively. The challenge is that every chemical behaves uniquely. It has its own preferred routes as it makes that journey.

In many respects the task of "Eco-Chemistry" is to design a new chemical eco-technology on this planet in which we use chemicals wisely to enhance the quality of life. Perhaps in doing so there is an analogy between designing engines and designing for the environment. When Honda engineers build a new engine, each component is designed to accomplish a specific task with negligible risk of failure, but economically and compactly. This is possible because these engineers have a full understanding of how the component behaves under the often stressful operating conditions of the engine. This behaviour can be expressed mathematically in the form of stress-strain relationships, or transmission of electrical signals or the complex chemical kinetic processes which occur during fuel combustion. Improvements in engine quality are possible only if these processes are fully and quantitatively understood and the effect of design innovations can be predicted, verified and implemented.

The early aircraft were designed and improved by trial and error. They are now designed on the computer. There is now confidence that the science of flight is understood and the prototype will fly.

The same principles apply to the design of chemical use in the environment. If we are to achieve maximum benefits with minimum adverse effects, we have to understand chemical behaviour and have the capability of simulating and predicting chemical fate mathematically. We have to be able to put numbers representing masses, concentrations and rates of flow on Figure 1.

During the 20th century, and especially since the advent of low cost, fast computing chemical engineers have built up a formidable capability of simulating and predicting how chemicals behave in the controlled conditions of chemical plants. These plants consist of vessels, pipes, pumps and other components which, like the Honda engine, are designed to operate under known specific conditions. Our environment, on the other hand is not designed by us. It is a very complex assembly of components such as the atmosphere, oceans, soils and organisms which are in a continuing state of change. Predicting how chemicals will behave in such complex systems is a huge challenge, but we have made great progress in recent decades. Our predictive abilities are now such that we can, I believe, predict their behaviour with acceptable accuracy. If we accept the principles of "Eco-Chemistry" we should be able to avoid repeating the mistakes of the past.

One of the greatest challenges is to achieve balance in society's response to managing chemicals. At the two extremes of society there are arrogant attitudes. First, there is a strong anti-chemical movement which sees the answer to the mistakes of chemical technology as being less technology and a return to the past. Chemicals and those who manufacture them are seen as evil. In my view this is arrogant. Given our present population, a return to the past is impossible, except for a small number of individuals. To maintain population numbers and densities require that we use chemicals as pesticides to support agriculture, as biocides to maintain sanitary conditions, as medicines, and as a wide variety of materials to support the quality we now demand in a modern lifestyle. The second arrogance is of those who regard the environment as a system to be exploited for immediate profit. Trees exist to be felled and turned into lumber. Animals and fish have value only as food for humans. The environment is viewed as so large that it can dilute all the chemicals we use and discharge to negligible concentrations. That arrogance has been responsible for many past mistakes. The answer must be a more balanced intermediate view to ensure the more careful use of chemicals, selecting them to ensure that they are used in a manner compatible with our hopes for environmental stewardship. It is part of the greater task of Mr. Honda's dream of assisting in the creation of a humane civilization.

In this address I would like to present a number of examples of "Eco-Chemistry" in practice in the form of simulations and predictions of chemical fate. I will end with some thoughts about how we can best ensure that chemicals are used such that "Eco-Chemistry" plays its role as an essential component of "Eco-Technology". But first a brief personal historical perspective.

A Personal Historical Perspective

About 1970, there were proposals to produce oil and gas in the Canadian Arctic. This raised questions about the effects of oil spills on the Arctic ecosystem. Because of my background in the petrochemical industry I knew a fair amount about the properties of the hydrocarbons which constitute oil and gas, and I was able to start research on this topic, indeed this continued for nearly 20 years. We developed methods of predicting how oil slicks will move, how fast they evaporate, dissolve, disperse and emulsify. We also sought to demonstrate that in some cases a valuable remedial strategy is to burn the oil or disperse it using surface-active chemicals of the type used in household detergents. Many of these predictive methods are still used today. In 1988 I decided to stop this research because I predicted there would probably never be another major oil spill. Nor would production or transport of oil in the Canadian Arctic occur in my lifetime. In March 1989 the Exxon Valdez ran aground and now President Bush wants to develop Arctic oil reserves. I am not very good at predicting the future!

Our research convinced me that although it is impossible to predict where and when oil spills will occur, it is possible to predict how they will behave, especially because of the availability of low cost fast computers. I also became convinced that this predictive capability could be extended to other chemical substances such as pesticides which are much more toxic and persistent than crude oil.

This topic has been my major effort in the last 25 years.

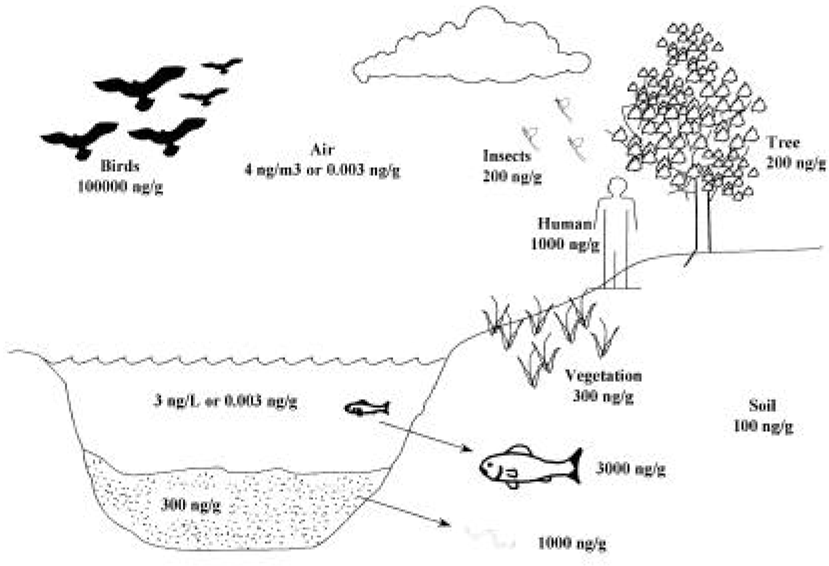


Figure 2: Typical concentrations of DDT in a contaminated ecosystem.
1 ng is 10^{-9} or 1 billionth of a gram.

To illustrate the approach we took, Figure 2 shows an ecosystem consisting of a lake, the surrounding terrestrial soils with their vegetation, the atmosphere above and sediments at the bottom of the lake. There is also a variety of animals resident in this ecosystem, fish in the lake, benthic creatures such as worms in the sediment, terrestrial animals, insects and birds, and even humans. Consider the possibility that the insects prove to be a nuisance, for example they could be mosquitoes which bite and possibly cause malaria, “river blindness” or transmit the West Nile virus. One option for improving the quality of life, at least for the humans, is to add an insecticide to the lake where the mosquitoes breed. This will be effective but it is likely that after a period of time the mosquitoes will return and more insecticide will be needed.

Situations very similar to this occurred in the 1950's, notably in Clear Lake in Northern California. The problem developed that the insecticide caused the death of other, non-target organisms such as birds and there was even contamination of humans. The obvious insecticide to use was DDT, the structure of which is shown in Figure 3. It, and other related substances into which it can be converted, are very potent insecticides. It lasts for a long time in the environment and it is relatively inexpensive. It saved many thousands of lives in Asia, the

Pacific, Africa and Central and South America. Ironically, it is one of the 12 substances which are scheduled for banning by the United Nations. It was a major issue in what is now regarded as the classic book "Silent Spring" by Rachel Carson published in 1961. That book alerted society to the problems caused by chemicals and it started a major environmental movement to seek less harmful chemicals and understand the environmental fate and toxicology of all chemicals of commerce.

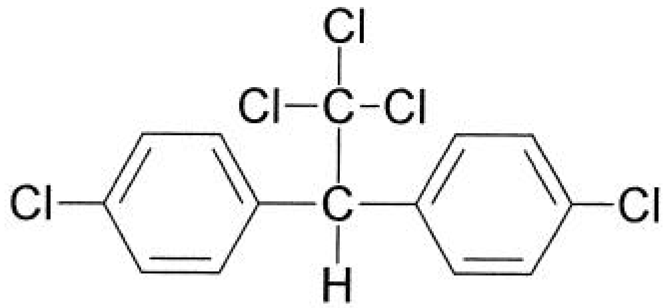


Figure 3: Chemical structure of p,p'-DDT

This problem arose because we did not fully understand the properties of DDT, nor how these properties influence the behaviour of DDT in the ecosystem and the effects it may have on the resident organisms. We now have that capability, at least in a primitive form, and if we use it properly we should be able to avoid repeating such mistakes.

A major difficulty is that DDT molecules migrate among all the components of the environment. It establishes very different concentrations in different places. Figure 2 give some typical concentrations for a contaminated ecosystem. For example the concentration in fish is about a million times that in the water.

My research efforts in the last 25 years have been largely devoted to developing that capability. I would like to explain briefly some of the principles involved and give you some examples of successful applications.

The Multimedia Environment

First we must acknowledge that the environment is very complicated and its properties vary in time and space, so it is unlikely that we will ever be able to describe it mathematically with the same accuracy as Honda engineers can achieve in engine design. We must therefore simplify the environment and reduce it to its essential components as shown in Figure 4. In the ecosystem given earlier there are four basic components or compartments, the atmosphere, soils, water and sediments. Although living organisms (biota) are important (and we selfishly regard ourselves as particularly important) the quantity of biota is quite small, with the possible exception of vegetation. We argue that DDT will behave similarly in this ecosystem in the presence or absence of animals. We acknowledge that micro-organisms play an important role in degrading substances such as DDT, but relatively little of the DDT resides in these organisms.

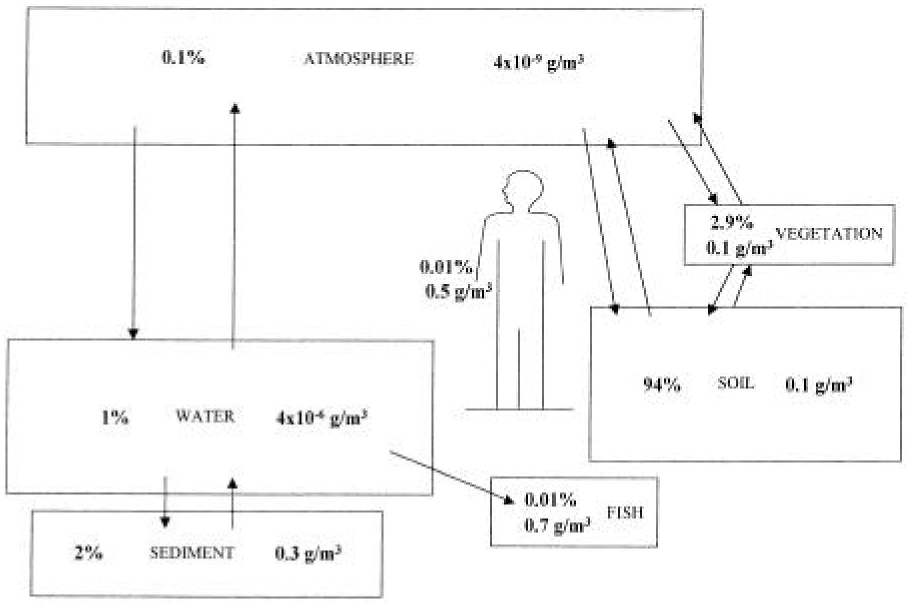


Figure 4: Calculated concentrations and distribution of DDT at a common fugacity of approximately 30 nPa.

In 1979 as a result of a collaboration with the US EPA, we introduced the idea of considering the entire "multimedia" environment as a set of connected compartments and then calculating how a substance such as DDT will behave in such systems. These are now referred to as "Mackay Models". They are used to simulate the behaviour of chemicals in "real" regions such as Japan or Canada, and in hypothetical or "evaluative" regions typical of a jurisdiction such as a Prefecture in Japan, a Province in Canada or a US State. The advantage of the evaluative or specimen region is that people in different countries can calculate how a chemical will behave in this specimen environment and compare their results internationally. They can then refine the calculation to apply to their own specific region with its unique areas of soil and water, vegetation, rainfall, temperature and biota.

It is relatively easy to define the areas, volumes, soil and water characteristics of a region, especially because much of this information is now readily available and accessible on the Internet in Geographic Information System form. The more difficult task is to determine how the chemical will be distributed between these compartments, i.e. the percentage of the total amount present in each. This is controlled by the chemical's properties such as its volatility or vapour pressure and its solubilities in water and in organic liquids or solids such as octanol, fats or lipids and the natural organic matter in soils and sediments. We can now measure these properties under controlled conditions in the laboratory and use them to estimate the partitioning phenomena.

For example, if we know the chemical's solubility in water and vapour pressure or boiling point we can calculate how the substance will partition between air and water. We can then measure this partitioning preference in the laboratory or in a small model ecosystem and confirm our predictions.

In the late 1970's we agonized over a philosophical question about this partitioning. What is the fundamental quantity which controls it? In the case of DDT in our ecosystem we can calculate the concentrations in each compartment at equilibrium, i.e. when the DDT has finally migrated through the environment and has settled out at constant concentrations and quantities in each compartment. From Figure 2 we saw that the concentrations differ greatly. The fish is nearly a billion times more contaminated than the air. Obviously concentration is not the common factor. The common factor proves to be fugacity.

Fugacity

Chemical engineers are also faced with this problem of multimedia distribution of chemicals when they design chemical and petrochemical plants. When they boil crude oil they have to predict how the various hydrocarbons distribute between the oil and its vapour. They use this information to design crude oil distillation columns. They use the concept of fugacity, a rather obscure thermodynamic quantity which was developed by G.N. Lewis in 1901. We had the idea of applying the fugacity concept to environmental situations.

It would give me great pleasure to give you a series of lectures on fugacity, but this would take several days, so I will spare you that enjoyment. The key point is that fugacity is a pressure, an escaping tendency that expresses the desire of the DDT to move from compartment to compartment, e.g. from fish to water and from water to air. It can be related to concentration if we know the properties of the substance.

In the case of Figure 4 we have calculated how DDT will become distributed when it has settled out at a common fugacity or pressure of 30 nano Pascals, i.e. its fugacities in all compartments are the same, so its escaping tendency from air to water is the same as from water to air and there is no net transfer. 30 nano Pascals is the pressure or escaping tendency exerted by the DDT molecules in all the media. A nano Pascal is a billionth of a Pascal. The atmosphere has a pressure of about100,000 Pa or 100 kPa. In many respects fugacity is like temperature. Heat moves from hot to cold until the temperatures settle out at the same value. Chemicals move from high to low fugacity and attempt to reach a common value. The pressure or fugacity in Figure 4 is very low, but it is sufficient to cause ecological problems.

Using fugacity greatly simplifies calculations of how DDT will behave in the ecosystem. More important, it explains a number of puzzling phenomena. Still more important, once the calculations have been done successfully for few chemicals (and if the predictions prove to be correct) then they can be repeated for other substances. We are then able to predict with some confidence how these substances will behave in the environment and determine if they are likely to cause problems such as occurred with DDT. Chemical companies such as Sumitomo, Dupont, Dow and Procter and Gamble use these fugacity calculations when developing new chemicals. There is little economic benefit in developing a chemical which is later banned. It is better to find a more benign substitute which will have a longer life on the market and wider uses. Eco-Chemistry can bring real economic benefits. To many business people the prefix “eco” spells trouble. This is wrong. It can spell profit. The eco-performance of a modern Honda four stroke engine is one of its most attractive features.

Recently the 3M company withdrew from the market a series of fluorine-containing substances used in fabric coatings such as Scotchgaurd because it transpires that these substances are converted in the environment into rather troublesome chemicals which tend to accumulate in fish, birds and humans. The economic penalty has been severe. We must therefore not only be vigilant about the chemicals of commerce, but also about the chemicals produced when they degrade in the environment into other chemical species. We should have appreciated this possibility, because DDT degrades into a "daughter" DDE which is as toxic as its "parent".

Adaptations of these models are now used by regulatory agencies to evaluate chemicals. One of the most advanced is the European Union System for Evaluation of Substances (EUSES) which uses a multimedia model describing the fate of chemicals in Europe. Similar models are used by other national and international agencies such as he United nations and OECD. These models are available as computer programs, some free, some sold commercially.

The Role of Industry

Earlier, I mentioned the desirability of collaboration with industry. I conceived of the idea of using fugacity for environmental purposes as a result of my experience working as an engineer in the chemical industry. Those of us in the academic world and in government usually greatly underestimate the depth of knowledge and experience that exists in industry. The scientist or engineer in industry who is responsible for environmental or ecological issues related to the industry's chemical products is thus in a particularly important and challenging position. Often they have detailed information available about the properties of the chemicals and how they may enter the environment.

An example is the development of a very successful and innovative fugacity model describing the fate of pesticides in the indoor environment by Dr. Yoshihide Matoba and his colleagues at the Sumitomo Chemical Company.

“ Explaining the Inexplicable” A Lesson from Fish

The simple DDT calculation suggests that if the fish and water reach the same fugacity, i.e. they are allowed to remain in contact long enough to achieve an equilibrium state, the concentration in the fish will be about a million times that of the water. When this was first observed it was puzzling. It was proposed that it was caused by the fish absorbing DDT from its food and then being unable to release it. It was thought to be a kind of one-way accumulation process. Applying the fugacity models showed that this process of “concentration” is inevitable for reasons of physical chemistry and fugacity. It is not now puzzling. As a result we are now able to predict which chemicals will bioaccumulate and which will not. If that predictive ability had existed some decades ago, we would not have developed troublesome pesticides such as toxaphene or industrial chemicals such as polychlorinated biphenyls (PCBs). We would have sought to minimize releases of substances such as dioxins from incinerators. The tragedy of mercury poisoning at Minimata could have been avoided. We should acknowledge these past mistakes and work to ensure that they are not repeated.

Human Exposure

This bioaccumulation process is not only important to animals such as fish and whales, it is important to humans who consume fish. If an individual lives in the ecosystem of Figure 2, they will be exposed to DDT by breathing air, by drinking water and by eating fish. A typical person may during an average day breath 20 m^3 of air, drink 3 litres of water and eat 20 grams of fish. Knowing the concentration in air, water and fish we can calculate how much is consumed. It proves to be 40 ng (billionths or 10^{-9} gram) from air, 6 ng from water and 60,000 ng from fish. We suffer exposure to toxics, not only from our air, water and soil, but also from our diet. Clearly it is fish consumption which is most important. In many cases the large concentration increase or “bio-magnification” from water to fish can cause high human exposure and toxic effects. We must strive to predict such situations in advance and prevent problems of this type.

A related example is the accumulation of toxic chemicals in marine mammals such as whales. It has been shown by researchers, notably Dr. Tanabe of Ehime University, that whales have remarkably high concentrations of toxic chemicals, especially males. We have been able to build models describing the uptake and loss of toxics by whales during their entire lifetime. What this shows is that whales take up toxics from their food, but because of their large reserves of fat and because they breathe air, they have great difficulty losing them, whereas fish breathe water. DDT is much more soluble in water than in air so a fish can rid itself of DDT in a year or two, but for a whale this may take nearly 100 years, well beyond its lifetime. Female whales are more fortunate because they can lose toxics in their milk, a loss route not available to their male companions. It is one of the few instances in which females have an advantage! The problem is, of course, that the infant whale suffers.

Since whales are often much more contaminated than fish, this is a good reason not to catch and eat them. It is better to leave them alone and hope the population can recover from both our toxic insults and over-exploitation.

We live in a global village.

We were privileged to collaborate with Dr. Katsuya Kawamoto of Kanto Gakiun University in Yokohama in his study of some 68 chemicals in the air, water and soils of Japan. Dr. Kawamoto gathered data on the emission rates of these chemicals from the Japanese Environmental Agency's Pollutant Release and Transfer Registry, he obtained information on the prevailing concentrations in the Japanese environment as a whole and in Kanagawa Prefecture. He then applied the European EUSES Simplebox model and we applied our ChemCAN model (which we use in Canada) but adjusted to describe the environmental characteristics of Japan. This study, depicted in Figure 5 which was published earlier this year yielded several interesting results.

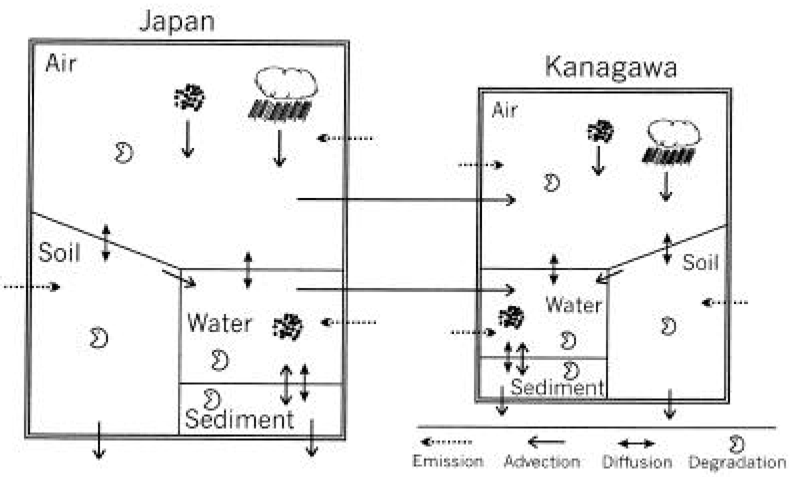


Figure 5: Evaluative elements of Japan and the Kanagawa Prefecture.

First, both models gave similar predictions which is encouraging. It is of course possible that we are both equally wrong!

Second, when Dr. Kawamoto calculated concentrations resulting from Japanese emissions the results were fairly good but generally the calculated concentrations were too low. Apparently much of the toxic chemical that is experienced in Japan is imported in the winds from the west. The same problem exists in Canada where much of our pollution is imported from the U.S. The implication is that Japan and Canada are limited in their ability to create a clean environment. We are, to an extent, the victims of those who live upwind and upstream. We also lose contaminants in air and water, but it is those who live downwind or downstream who suffer. It is thus necessary to view ourselves as part of a contaminated global village in which we all affect each other.

When Dr. Kawamoto includes an estimate of imported contaminants in his model calculations he gets good agreement. This is very satisfying, because if, for reasons of health it is desired to reduce concentrations of these chemicals in Japan it is now possible to determine by how much emissions must be reduced. Essentially Dr. Kawamoto is providing the tools to help design a cleaner, more healthy Japanese environment.

Emissions

When we run models, such as those for Japan or North America, one of the principal difficulties we face is not scientific, it is the lack of enough complete and accurate data on emission rates of chemicals to the air, water and soil environments as well as waste disposal facilities.

These emission rates "drive" the model. The concentrations and exposures which we calculate are entirely dependent on having reliable, quantitative emission data. For example it is believed that in the Kanagawa Prefecture the emission rate of benzene to the environment is about 500 tonnes per year. These emissions result in a calculated concentration in air of about 0.1 micrograms per cubic metre. A resident then inhales about 2 :g per day. If this emission estimate is wrong and emissions are actually twice that value or 1000 tonnes per year then the concentration will also be about twice the original estimate or 0.2 micrograms per cubic metre and exposure to residents is 4:g/day. Emissions thus directly control concentrations which control exposures and we presume toxic effects. In practice, benzene also enters the Prefecture from neighbouring Prefectures and from abroad.

If we are to use chemicals responsibly we must have reliable emission information. In Japan there is the Pollutant Release and Transfer Registry (PRTR). In the U.S. there is a Toxics Release Inventory (TRI) and in Canada there is a National Pollutant Release Inventory (NPRI). These are very enlightened programs, but regrettably they are often not given the priority they deserve, nor are they as complete and accurate as is needed if we are to use them fully.

One reason for this is that governments do not fully appreciate how the information can be used for the benefit of the public. The multimedia mass balance models I have described play the role of using this information to estimate concentrations and public exposure to chemicals. Of course we sample and analyse the environment to detect these chemicals, but there are too many chemicals, too many locations and too many occasions for us to achieve complete monitoring. Modelling, in which we predict chemical concentrations and exposures is much cheaper, faster and it can be more complete in coverage spatially and temporally, but we need assurance that the predictions are reliable. What is then needed is a purposeful, designed partnership between those who gather emission data, those who monitor and analyse the environment, those who model and predict, those in governments who manage and regulate and finally those in industry who synthesise these chemicals and are in the best position to find more benign substitutes. Together they can implement the principle of Eco-Chemistry.

One problem about emission estimation is commercial confidentiality regarding the nature and quantities of chemicals used and discharged. I believe that an environmental ethic is emerging that anyone who discharges a chemical into the public environment has an obligation to make that information fully available. When a chemical is discharged all control is lost over its fate. In the oil spill business it is said that there are three primary needs, prevention, prevention and prevention. When oil is spilled we are lucky if we can recover 10% of it. By analogy in eco-chemistry the primary needs when addressing persistent, bioaccumulative and toxic chemicals is discharge prevention, prevention and prevention. Released chemicals behave like leaves in a typhoon - totally beyond our control. We can not retrieve them.

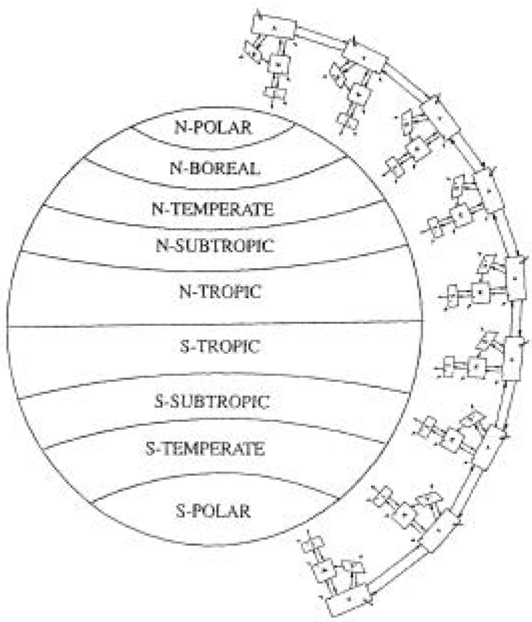
We at Trent are currently working with colleagues at the University of California at Berkeley and the Harvard School of Public Health to build up a capability of predicting the behaviour of chemicals in the entire North American continental environment of Canada, the U.S. and Mexico. Figure 6 shows how we divide the continent into compartments in the BETR (Berkeley-Trent) model. We attempt to predict, for example, how a chemical used in Mexico will journey to the Canadian Arctic.

Figure 6: The Berkeley-Trent (BETR) North American continental model.

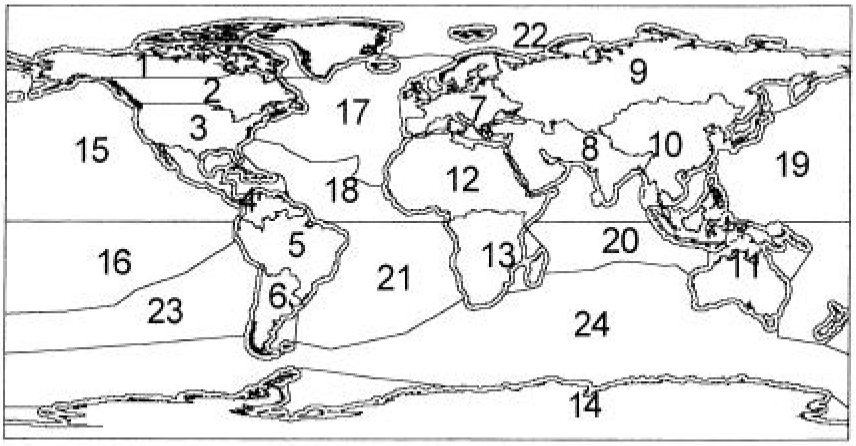
A surprising observation is that fish in Lake Superior are badly contaminated with toxaphene, despite the fact that very little toxaphene has been used in the vicinity. Most has been used on cotton crops in the Southern U.S. Over the years since toxaphene was banned, we believe that the residues in soils in states like Alabama, have evaporated and been transported north to be deposited in the cold waters of Lake Superior in sufficient quantities to contaminate its fish. It is likely that the journey involved a series of hops, evaporation then deposition some hundreds of kilometres north, then repeated evaporation-deposition. This has been called the “grasshopper” effect. In Australia it is called the “kangaroo” effect. The BETR model actually “predicts” that this has occurred. If the model had been available in the 1960's this toxaphene problem could have been avoided.

Ultimately, we believe, there will be reliable predictive models for not only North America, but all continents and indeed the entire global environment.

My colleague Professor Frank Wania at the University of Toronto has developed a model for the entire global environment as shown in Figure 7 by dividing the planet into nine meridional segments each of which contains air, water and soil. Each has its own seasonal variations in temperature. This model has been successfully applied to alpha hexachlorocyclohexane (∀HCH) which was for many years a contaminant in the pesticide lindane which has been widely used, especially in Asia. It is now not used but its legacy remains in the oceans. Concentrations in the Western Pacific Ocean increase from south to north with the highest values in the Arctic Ocean. It has not been used in the Arctic to any significant extent, so why are levels there so high? It seems that Arctic regions are particularly vulnerable to contamination.



Figures 7: Meridional global model.



Figures 8: Geographical global model.

It is still not clear how we can best simulate and predict how chemicals will behave globally. What is certain is that we must try and we must succeed. Figure 8 shows the structure of a model on which we are currently working in which the globe is divided into continents and oceans rather than meridional bands. Some believe that the best approach is to use as a basis existing global circulation models of the atmosphere which are used for weather and climate research. Unfortunately this task may take a decade or more. Given the uncertainties about how we can best proceed, perhaps the best approach is to try all these alternatives and see which proves most useful.

The Arctic

Canada is a northern country and we Canadians have a particular interest in the Arctic environment. The Arctic, its ecosystem and its human residents (the Inuit) play an important part in the Canadian identity, even if most Canadians never visit the North.

To our surprise and despair, the Arctic is quite contaminated not only by HCH but also with substances such as PCBs and certain pesticides such as toxaphene despite the fact that they have never been used there. They have been imported in winds and water. The Inuit have remarkably high levels of PCBs, often much higher than residents of southern Canada. We believe there are three reasons for this. Their diet is high in fat because they need the extra energy to survive the cold. They eat the meat from marine mammals such as seals and whales as an important part of their diet. That meat is contaminated. Second, the Arctic is cold, indeed it can be thought of as a huge household freezer in which the low temperatures preserve not only food but also contaminants. As a result, contaminants survive longer and can build up higher concentrations. It also appears that there is a global condensation or distillation effect in which these chemicals migrate in a grasshopper-like fashion preferentially to the cold polar regions as shown in Figure 9. On the planet Mars, carbon dioxide migrates to the poles and condenses as carbon dioxide snow. Water vapour condenses on the surface of a bottle of cold beer. It seems that the same phenomena may occur to certain chemicals on Earth. These chemicals must do so because they have certain properties. They must be able to survive long enough to make the journey, i.e. they must be chemically stable or persistent. They must be sufficiently volatile that they can evaporate into the winds which carry them to the Arctic, or they must be sufficiently soluble in seawater that they can be conveyed in ocean currents, generally from the Pacific Ocean into the Arctic Ocean.

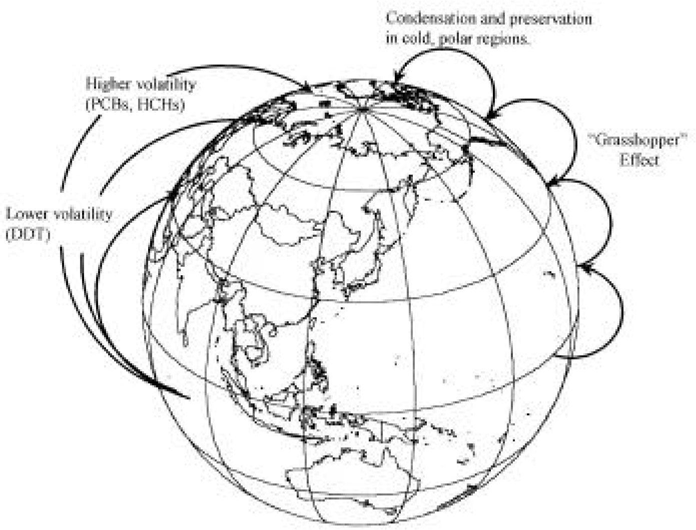


Figure 9: Transport of chemicals on a global scale.

It is only recently that the international community has acted together through the United Nations Environmental Program to regulate such chemicals. On May 22, 2001, 127 countries adopted the Stockholm Convention on persistent organic pollutants which will reduce and eliminate certain pesticides and industrial chemicals, presently 12 in number. This was a historic moment for human society. We decided to rid our planet of these substances and never again produce them. The challenge now is to review and assess some 100 or more suspect chemicals. Ultimately we have to assess all the many thousands of chemicals of commerce. I am convinced that multimedia models of chemical fate must play a significant role in this process. No doubt, most will be found harmless, but I suspect that there are surprises in store. For example, it appears that certain bromine-containing chemicals used as flame-retardants in clothing and plastics are emerging as problems as global contaminants.

Concluding thoughts

I am convinced that the "Eco-Technology" of chemicals or "Eco-chemistry" must play a key role in advancing society towards a "humane civilization". We have made technological mistakes in the past and many people and ecosystems have suffered as a result. In most cases the mistakes were the result of lack of knowledge, they were not the result of malice. We owe it to those who suffered to acknowledge that they were the victims of these mistakes. We must use the information gained to avoid repeating the same mistakes.

As a result of the advances in environmental science, in computing power, and more effective information technology we are well down the road towards understanding quantitatively how chemicals behave in the environment. If we can simulate and predict chemical fate, we can use this information to avoid repeating past mistakes, to select more benign chemicals and solve many of the problems of the past.

This task presents many challenges to Universities, Industry, Governments and the Public, but the rewards will be substantial. We should avoid the extreme arrogant attitudes that chemicals are all harmful or all harmless. The truth is that some are harmful and we should manage or even ban them from this planet. Some are potentially harmful but have valuable uses and, like explosives, must be used with care. Most are fairly harmless, especially if we use them with appropriate environmental sensitivity. We will then be able to assert that we use chemicals for the benefit of society with a full awareness of possible hazards and with assurance that the environment on which we and our fellow creatures depend for our survival is fully protected.

Let me end by thanking again the Honda Foundation for this prestigious Prize, those who have supported our work and especially the large number of students and staff who have worked with me towards the goal of building an "Eco-Chemistry".