THE AERIS MODEL - COMBINING PATHWAYS AND FATE INFORMATION TO ASSESS SOIL QUALITY

by

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1.0 INTRODUCTION

Wherever contaminated soil poses a concern to people or the environment, a series of questions inevitably emerges: Does the site need to be cleaned? What types of remedial measures or actions should be taken? When will the site be safe to use? What level of residual contamination is acceptable? These and other concerns often are expressed by the simple phrase "how clean is clean?". Unfortunately, the answer is not so simply stated and at the present time few jurisdictions have established acceptable soil concentrations or clean-up guidelines and those that have often address only a few parameters.

The process of deciding whether to reduce or remove soil contaminants and render a site suitable for use is a complex issue. Many factors need to be considered including the type of industry that used the site, the contaminants that are present, the age of the plant, site-specific characteristics such as its geography, geology, hydrogeology, and climate, past waste management practices, and the proposed future use of the site. The extent and costs of clean-up activities are largely determined by the level of contamination which, from environmental and human health standpoints, can safely be left on-site.

To provide direction and guidance to decommissioning efforts across Canada, the Canadian Council of Ministers of the Environment (CCME) established the Decommissioning Steering Committee (DSC). Members of the DSC include Environment Canada, the environment ministries of Alberta, Ontario, and Quebec, and several industrial associations. In 1987, the DSC awarded a contract to a consortium of companies to investigate various aspects of decommissioning. One of the tasks was to create a computer program capable of deriving clean-up guidelines for industrial sites where redevelopment is being considered. The result of this effort is the AERIS program, an Aid for Evaluating the Redevelopment of Industrial Sites. The version of AERIS described in this paper was submitted to the DSC in the fall of 1989.

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2.0 BASIC PROGRAM STRUCTURE

2.1 Underlying Premises and Constraints

While the broad objective of this study was to develop a model for establishing site-specific clean-up guidelines, the process of establishing guidelines is far more complex than can be represented by a mere computer model. As such, it was recognized from the beginning of the modelling effort that whatever program was developed, it should not be perceived or used as a sole arbiter in setting guidelines. Accordingly, the acronym AERIS was chosen to help users remember its intended use, that of being an aid for evaluating the redevelopment of sites. As an aid, AERIS can be used to identify the factors that are likely to be major contributors to potential exposures and those aspects of a redevelopment scenario with the greatest need for better site-specific information.

It was assumed that some users probably would use AERIS to study generic situations while others would be interested in specific scenarios. Those interested in specific scenarios might have some site-specific data but likely would be uncertain about some of the many factors that can be considered in such an evaluation.

Based on assumptions about the intended uses and users, together with the objectives and constraints noted above, a series of decisions was made at the outset of model development about basic model characteristics:

- AERIS would be structured so that each run evaluates one chemical for one receptor, one land use, and one environmental setting. This may require a user to run the model several times and base interpretations on the collective outcomes of those runs. Accordingly, AERIS would be designed so that adjustments to input parameters could be made relatively easily.

- The user should be given the opportunity to select default values for various parameters or provide site-specific inputs so that the redevelopment scenario in the program can resemble actual situations of interest. As a result, AERIS would include default values and various aids to help users select appropriate values.

- AERIS would consider only those exposures that are experienced on-site. Off-site populations would be considered indirectly by comparing concentrations in air, water, and produce with existing environmental criteria such as point-of-impingement criteria for air quality and drinking water objectives.

- AERIS would be designed to evaluate situations where the soil had been contaminated sufficiently long ago to establish equilibrium or near-equilibrium conditions between the various compartments of the environment. These conditions should apply to most sites that are being considered for redevelopment.

- It would be assumed that the concentration of the contaminant in soil is constant across the site and over the depth of soil that is contaminated. Furthermore, the concentration is assumed to remain constant over time (although there is the option to correct model results for degradation).

Based on many of these considerations, it was decided to design AERIS to run within an "expert system" programming environment. This facilitated the creation of a model in which the user has the option of entering either site-specific data or relying on default values. At each point where the user is asked for information, on-screen assistance can be invoked to help a user make decisions and understand how the choices can affect the outcome. The entire process has a relatively high degree of "friendliness" and provides some automatic error checking.

Because it runs within an "expert system" programming environment, AERIS consists of four basic elements - an "intelligent" preprocessor, a supporting data base, component modules, and a postprocessor.

2.2 The Preprocessor

The preprocessor takes the form of a series of questions that AERIS asks the user about the redevelopment scenario to be evaluated. These questions and answers collectively are referred to as the "Input Session". The answers are used to create a "context" file that describes the scenario of interest. Context files can be saved and recalled at the user's discretion.

The preprocessor is referred to as "intelligent" due to the utilization of expert system technology. The preprocessor uses a set of rules (collectively referred to as a "knowledge base") to establish a structure to the decision support offered; to aid the user in estimating unknown input parameters, and to control the flow of information between other program components. The preprocessor contains the "control modules" which are responsible for the user interface during the input and output sessions, the inference flow mechanism, the retrieval of information from the data base, and the management of information flow among the component modules.

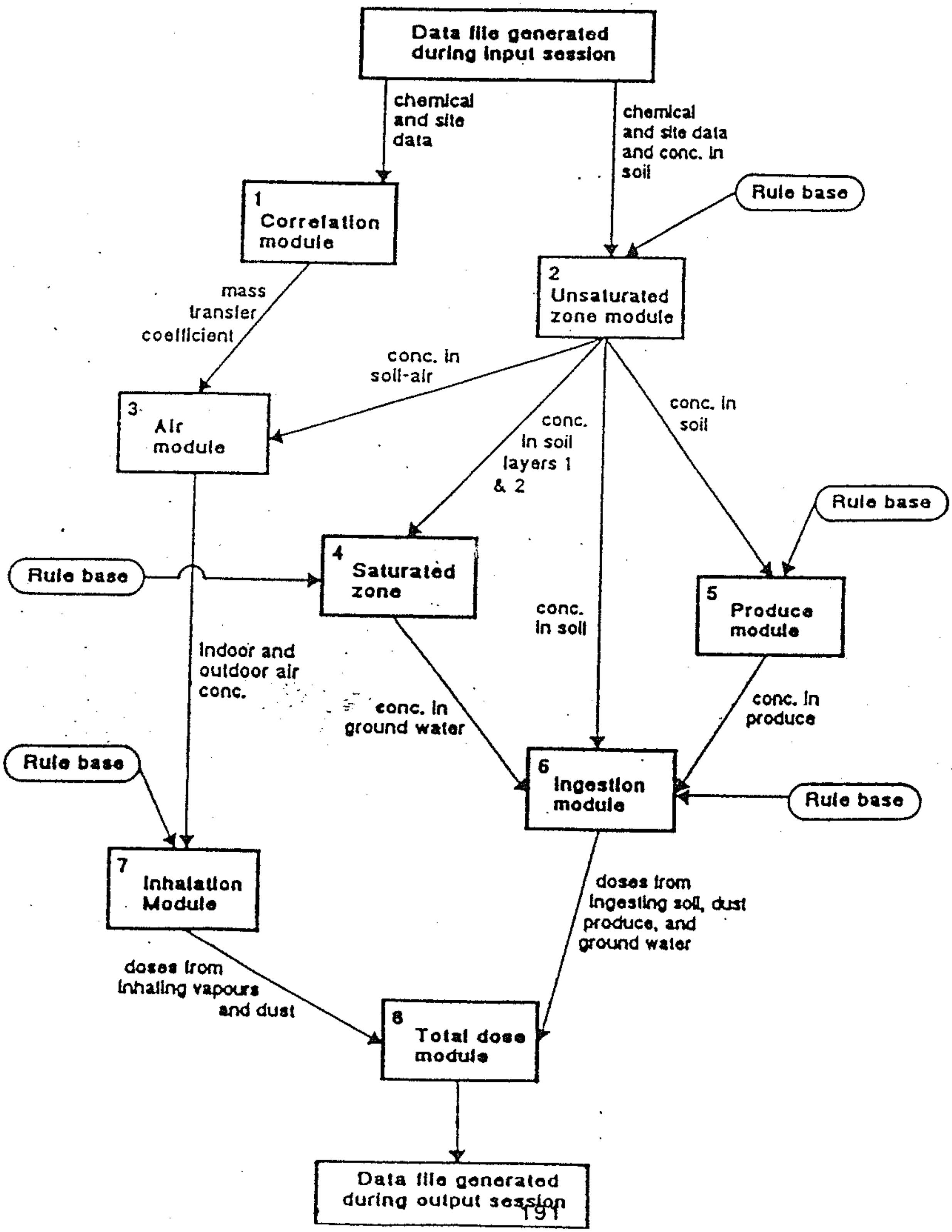
The preprocessor uses rules to determine if and when goals are met. Many of the rules are in the form of If... Then... Else statements which represent the decision making that an expert would consider when evaluating this type of scenario. The branched arrangement formed by the rules is similar to that of a decision tree. If sufficient information is gathered during the Input Session, the preprocessor passes the data to those component modules that are needed to evaluate a specific scenario.

2.3 The Component Modules

The component modules contain algorithms that estimate contaminant concentrations in various compartments of the environment. The estimated concentrations serve as the basis for estimating exposures via various routes of exposure or pathways. Figure 1 indicates the sequence that the modules are used in AERIS and shows how they are interrelated

FIGURE I

COMPONENT MODULES AND INFORMATION FLOW



by the information that flows between them. If concentrations of a contaminant have been measured in one or more compartments of a site, a user has the option to override the estimated concentrations with the site measurements.

The *Correlation Module* is used to predict mass transfer coefficients. The predictions subsequently are used in the *Air Module* which calculates the flux of chemical from the soil into outdoor air and into basements of buildings where it subsequently can be inhaled by a site user or visitor. The rate at which a chemical will be transported from soil into the outdoor air is influenced by properties of the soil, properties of the contaminant, and environmental conditions. Transport into indoor air is contributed by diffusion through foundation walls and/or floor and pressure-driven flow. The ratio of vapour concentrations on the main to those in the basement are a function of volumes and air change rates.

The *Unsaturated Zone Module* predicts concentrations in soil-water and soil-air in the soil above the water table. It assumes that there is a contaminated layer that starts at the surface and that the user can define the layer in terms of its typical or average depth and concentration of contaminant over that depth. If appropriate, there can be an underlying non-contaminated soil layer. The *Saturated Zone Module* predicts concentrations in ground water. Key factors it considers include the depth of contamination with respect to the depth to the local water table, and soil characteristics.

The *Produce Module* is used to estimate concentrations in produce grown on the site. The uptake of chemicals is assumed to be contributed by root uptake and foliar deposition of local soil particles. The extent of uptake is influenced by the type of produce, length of growing season, chemical properties of the chemicals, and soil characteristics.

While the five modules described above address concentrations of a substance in various environmental compartments, the final three modules translate those concentrations into exposures and doses that hypothetical site users could receive. The *Ingestion Module* can estimate the intakes of water, soil, and garden produce. Only those pathways that are appropriate according to the scenario described by the model user are addressed. The concentrations in the water, soil, and produce are determined in the Saturated Zone Module, Unsaturated Zone Module, and Produce Module, respectively.

The *Inhalation Module* estimates the amount of a chemical inhaled by the receptor while outdoors and indoors. Both the inhalation of vapours and particulate matter while the receptor is indoors and outdoors can be taken into account in accordance with the receptor characteristics assigned by the model user.

In the *Total Dose Module*, the exposures from all relevant pathways are converted into doses by taking into account bioavailability on a substance- and pathway-specific basis. The total dose is then compared to an "acceptable" dose level as defined by toxicological information. The user can decide whether all or some fraction of the "acceptable" level is to be used.

While human health often will be the most stringent basis for setting clean-up guidelines, a user has the option of specifying a concentration in any one of several environmental compartments as the basis for calculating an "acceptable" soil concentration.

2.4 The Post Processor

The results calculated by the component modules are passed to the postprocessor, which offers the user various ways of displaying the results during the "Output Session". Each run of the model concludes with tables that display dose estimates for each route and the identification of an "acceptable" soil concentration. Three types of graphical summaries can be displayed: a plot of soil concentration versus dose; pie charts that show the relative contributions of each route to total exposure; and diagrams that compare the calculated "acceptable" concentrations to guidelines or criteria issued by regulatory agencies.

2.5 The Data Bases

The AERIS data bases can provide much of the information needed for the calculations. Information is retrieved as the user answers questions concerning the scenario to be evaluated. The types of information that can be retrieved include physico-chemical data, "acceptable" dose levels, bioavailability factors, concentrations associated with other types of adverse effects, guidelines or criteria from various jurisdictions, receptor characteristics, meteorological data, and physical characteristics of soils and underlying formations. The data bases in AERIS have information for:

- two types of site users: an adult and a young child
- four future land uses: residential, commercial, recreational (park land), and agricultural
- more than 30 organic compounds and three inorganic substances
- the meteorology of six Canadian cities: St. Johns, NFLD, Montreal, PQ, Toronto, ON, Winnipeg, MN, Edmonton, AL, and Vancouver, BC
- physical characteristics of nine soil types and 14 underlying formations.

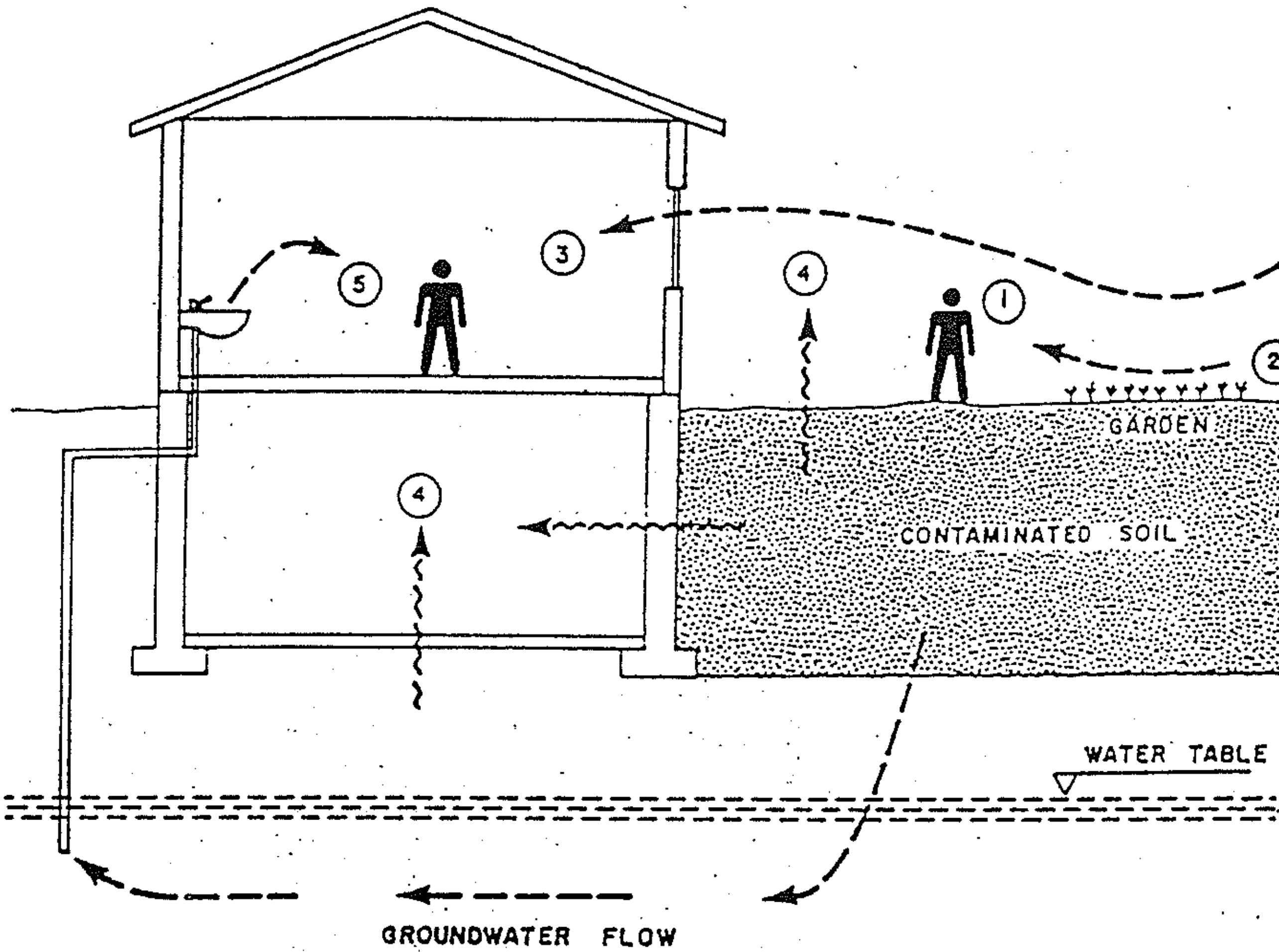
The user has the opportunity to edit all of the information retrieved from the data base so that the redevelopment scenario can be made to resemble the actual situation of interest. AERIS also includes default values and various aids to help users select appropriate values.

2.6 Pathways Considered

Site users can be exposed to substances present in site soil through various pathways (routes of exposure). AERIS allows all or any of the following pathways to be considered: inhalation of vapours and particulate matter when indoors and outdoors; direct ingestion of local soil and indoor dust; ingestion of plants grown on-site; and ingestion of ground water (see Figure 2).

FIGURE 2

PATHWAYS CONSIDERED IN AERIS



POTENTIAL PATHWAYS:

(1) DIRECT INGESTION OF SOIL
INHALATION OF PARTICULATE MATTER

(2) INGESTION OF GARDEN PRODUCE

(3) DIRECT INGESTION OF DUST
INHALATION OF PARTICULATE MATTER

(4) INHALATION OF VAPOURS (BOTH OUTDOORS AND INDOORS)

(5) INGESTION OF GROUNDWATER

The extent to which a person is exposed to a substance by any of these pathways is influenced largely by the physical characteristics of the person and the way(s) that they use the site. The AERIS data base contains information for two types of individuals (an adult and a young child) and four types of future land use (residential, commercial, recreational, and agricultural).

Model users have the option to use any or all of the default values that describe the site users (receptors) or can replace default values with specific values at their discretion. The default values for the adult receptor include a body weight of 70 kg, an inhalation rate of 23 m^3/d, a water ingestion rate of 2 L/d, and a consumption rate for fruits and vegetables of 0.6 kg/d. Similarly, the default values for the young child receptor include a body weight of 10 kg, an inhalation rate of 5 m^3/d, a water ingestion rate of 1 L/d, and a consumption rate for fruits and vegetables of 0.3 kg/d.

The characteristics associated with residential land use is directed towards estimating doses that result from the full-time use of the site. The receptor is assumed to live in a single-story house with a full basement located in the middle of the site. All of a receptor's time is spent either in the house or in the yard. While outdoors, receptors breathe outdoor vapours and can ingest soil particles during the summer. A garden on the property supplies a percentage of the fruits and vegetables that the receptors consume. When indoors, the receptors inhale indoor vapours and can ingest dust, a percentage of which originates from local soil. The water supply can be local ground water.

Commercial land use is intended to estimate doses that result from spending a substantial portion of most days on a site inside a building (i.e. 8 hours a day, 5 days a week). As such it is analogous to portraying an office worker or a child at a day-care centre. The building is assumed to have one story and no basement. Sources of exposure include direct ingestion of dust, the inhalation of indoor vapours and particulate matter, and ingestion of local ground water.

Recreational land use is intended to generate doses received by frequent visitors to a park or playground. While on-site, visitors are assumed to be engaged in vigorous, outdoor activities. The visits are more frequent and of longer duration during the summer than the winter. The visitors live off-site. Potential sources of exposure are limited to direct ingestion of soil, inhalation of vapours and soil particles, and ingestion of local ground water.

The characteristics of agricultural land use are similar to those of residential except that larger amounts of time are spent outdoors by the adult and particulate matter levels at elevated for a portion of the year as they would be during plowing.

3.0 SAMPLE RESULTS

To illustrate the relationships between the environmental fate of substances in soil and the contributions that individual pathways can make to total exposures and doses, the AERIS program was used to evaluate three compounds with distinctly different environmental behaviours: toluene, phenanthrene, and lead. Each of the substances was evaluated within the context of residential and commercial development of a hypothetical site that was assigned characteristics typical of those that might be encountered at a site in southern Ontario. Table 1 displays the information used to portray the two scenarios while Table 2 summarizes the results of the AERIS runs.

Toluene is a relatively volatile compound and poses a moderate level of toxicological concern. Without running the model, it would be anticipated that the inhalation of vapours would be the dominant pathway. The AERIS model results indicate that for the residential land use scenario the inhalation of vapours pathway accounts for 75 to 90% of the total dose. In the commercial land use scenario, the inhalation of vapours represents 65 to 90% of the total dose. The remainder of the dose is due to the ingestion of local ground water in both the residential and commercial setting.

Based on human health considerations, the soil guidelines for toluene recommended by AERIS are 150 to 250 mg/kg for the residential setting and 600 to 900 mg/kg for the commercial setting. The Province of Quebec has recommended concentrations of 3 mg/kg as the threshold at which detailed site investigations may be needed and 30 mg/kg as a level above which may be necessary to take prompt remedial action.

Associated with the soil guidelines derived by AERIS are outdoor air concentrations well below the air quality criterion from Ontario and those reported to cause odours in air. Adverse effects on plants have been reported at concentrations as low as 200 mg/kg in sand and 2000 mg/kg in loam. For the soil type assumed in this evaluation, phytotoxic effects do not seem likely at the recommended toluene concentrations and therefore would not be as cause for modifying the AERIS recomendations.

Associated with the soil guidelines derived by AERIS are local gound water concentrations above those recommended by the Province of Quebec and the odour threshold for toluene in water. If local ground water is to be used as a water supply, it might be necessary to reduce the health-based guidelines identified by AERIS.

Phenanthrene is less volatile than toluene and has a stronger tendency to sorb onto organic matter in soil. Without running the model, it is difficult to anticipate which pathways will dominate. The AERIS results indicate that the ingestion of locally-grown produce and ground water are the major pathways in the residential setting. The ingestion of soil and dust are secondary pathways. In the commercial setting, the two major pathways are the ingestion of ground water and the ingestion of indoor dust.

The recommended soil concentrations for phenanthrene are 1,500 to 6,000 mg/kg for residential use and 5,500 to 30,000 mg/kg for commercial use. The Province of Quebec has recommended 5 mg/kg as the threshold at which detailed site investigations may be needed and 50 mg/kg as a level above which it may be necessary to take prompt remedial action. The same values are interim guidelines recommended by the Canadian Council of Ministers of the Environment (CCME) for abandoned coal tar sites.

There are no air quality guidelines for phenanthrene and there are no published accounts of concentrations in soil associated with other types of adverse effects such as odours, staining of phytotoxicological effects. It is likely that better information about concentrations that could cause odours or adverse effects on plants would provide a basis for setting soil guidelines lower than those based on health considerations.

Associated with the soil guidelines derived by AERIS are local gound water concentrations of phenanthrene well above those recommended by the Province of Quebec. If local ground water is to be used as a water supply, it probably would be necessary to reduce the guidelines identified by AERIS.

For **lead**, the inhalation pathways are obviously not of concern. Ingestion of soil or dust often are the pathways that receive the most attention. The AERIS results indicate that the consumption of local ground water accounts for more than 90% of the exposure. In the residential setting, the ingestion of locally-grown produce is a secondary contributor while the ingestion of soil and dust are relatively small contributors. In the commercial setting, local ground water accounts for more than 99% of the exposure.

The recommended soil concentrations in these settings (0.5 to 1.5 mg/kg for residential and 1 to 4 mg/kg for commercial land use) are considerably lower than the soil guidelines from several Canada provinces which lie in the range of 200 to 1000 mg/kg; however, the inclusion of site ground water as a source of exposure is an unlikely condition especially in urban areas. If that pathway had not been included, the recommended soil guidelines would be 6 to 25 mg/kg for residential settings and 175 to 1250 for commercial settings. Ingestion of produce would be the major exposure pathway in the residential scenario. The ingestion of soil and dust would account for about 10% of the total exposure.

AERIS makes no allowance for reductions of concentrations in produce that result during food preparation such as washing, peeling, or boiling. As a result, the estimated doses for eating produce likely exceed actual doses. This becomes an important consideration in interpreting the output for scenarios in which the consumption of produce is a major pathway. If information was available for a scenario that supported the lowering of exposures from the ingestion of produce, the recommended soil guidelines for residential land use would become similar to but slightly lower than those for commercial settings. Ingestion of soil and dust would become the important pathways.

Another aspect of the evaluation that is hindered by a lack of published information concerns the bioavailability factors. It is suspected that lead-specific bioavailability factors (rather than the default values) would increase the recommended soil concentrations.

4.0 CONCLUSIONS

AERIS has achieved many of the original objectives set for this project: it is highly user-friendly; it can be used even if various pieces of site data are missing; it is highly flexible in the types of contaminants and scenarios it can evaluate; and it generates site-specific clean-up guidelines. During the development of the model, it also was realized that with increasing ease of use also came the increasing possibility of misuse. While the original goal was to create a product that even a novice could use to develop guidelines, the developers have come to regard the model as being better suited to assisting experts to evaluate situations expeditiously and consistently. That AERIS should not be perceived to be a substitute for expertise is evident in the cautionary notes that should be applied to the interpretation of model results:

- The conservative, risk-based philosophy and default values that are used when health concerns are the basis for evaluating a site make it possible to recommend soil guidelines lower than those that regulatory agencies may be using or considering. Conversely, relatively high guidelines can be identified when using AERIS if the scenario being evaluated generates very small dose estimates or the important exposure pathways are relevant for chemicals with certain physico-chemical properties or environmental behaviours.

- The algorithms used to estimate environmental fate and concentrations in environmental compartments as a function of the concentration in soil have been verified but not calibrated (that is, the predictions of the algorithms have not been compared to concentrations measured at sites in various environments). An assessment of the model's worth may only be possible once it has been used to evaluate several real situations.

- Some of the algorithms represent processes that are not well understood (such as plant uptake) and the model may require site complexities to be replaced with generalizations.

- Soil guidelines recommended by AERIS should not be taken as absolutes but rather as being indicative of appropriate concentrations. Scenarios should be evaluated by running AERIS several times with key parameters adjusted between runs to develop an appreciation of the sensitivity of the output to input data or assumptions.

Table 1

SCENARIO CHARACTERISTICS

meteorology	Toronto
soil type	stiff, glacial clay
underlying formation	unweathered marine clay
depth to ground water	1.5 m
soil pH	7.4
aquifer thickness	5 m
K_{di} for lead	0.04 m^3/kg
depth of contamination	1 m
organic carbon content	2.5 %
hydraulic gradient	0.01

Assumptions

- dissolution dominates over desorption for lead
- all bioavailability factors set to 100%

- soil allowed to contribute 50% of the reference dose for toluene
  90% of the reference dose for phenanthrene
  75% of the reference dose for lead

- duration factor of 3 used for toluene (half-life in soil < 10 days)
- duration factor of 2 used for phenanthrene (half-life in soil ≈ 30 days)

Summary of AERIS Results

Land Use Scenario/Receptor	Toluene	Major Pathways
Residential		
Adult	250 mg/kg	Vapours: 90% Drinking Water: 8%
Child	150 mg/kg	Vapours: 75% Drinking Water: 20%
Commercial		
Adult	900 mg/kg	Vapours: 90% Drinking Water: 10%
Child	600 mg/kg	Vapours: 65% Drinking Water: 33%

Land Use Scenario/Receptor	Phenanthrene	Major Pathways
Residential		
Adult	6,000 mg/kg	Produce 45% Drinking Water: 35%
Child	1500 mg/kg	Produce 40% Drinking Water: 30%
Commercial		
Adult	30,000 mg/kg	Drinking Water: 60% Ingestion of Dust: 35%
Child	5,000 mg/kg	Drinking Water: 50% Ingestion of Dust: 45%

Land Use Scenario/Receptor	Lead	Major Pathways
Residential		
Adult	1.5 mg/kg	Drinking Water: 90% Produce 6%
Child	0.5 mg/kg	Drinking Water: 90% Produce 6%
Commercial		
Adult	4 mg/kg	Drinking Water: 99%
Child	1 mg/kg	Drinking Water: 99%