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# Technical Update

## Use of BIOCHLOR v.2.2 in risk assessments submitted under the Record of Site Condition Regulation (O. Reg. 153/04)

### What is BIOCHLOR v.2.2?

BIOCHLOR v.2.2 is software programmed in the Microsoft EXCEL™ spreadsheet environment designed to solve the problem of solute transport in uniform (one dimensional, steady-state) groundwater flow. Mechanisms for the transport of solute include advection and three-dimensional dispersion, sorption of the solute onto soil, and bio-transformation of the solute from parent to daughter compound via first order decay. By virtue of its user interface, the model is specifically intended to model the fate and transport of chlorinated solvents through sequential decay (e.g., PCE, TCE, DCE, VC sequence), and to evaluate natural attenuation via reductive dechlorination.

BIOCHLOR is free from the US EPA (<http://www.epa.gov/ada/csmos/models/biochlor.html>). The associated user's manual provides a useful summary of the input parameters, with suggested values for a variety of contaminant hydrogeologic conditions. The software includes help menus and macros to assist the user in the selection of input parameters and in the calibration of the model to measured contaminant concentrations.

### How is BIOCHLOR v.2.2 used in Risk Assessment?

The anticipated use of the model in the context of brownfields risk assessments (RAs) submitted under Ontario Regulation 153/04 is to estimate future dissolved-phase concentrations (i.e., extrapolation in time) or down-gradient dissolved-phase concentrations (i.e., extrapolation in space) of chlorinated solvents given known concentrations of such compounds and the proven or assumed existence of a source. Such dissolved-phase concentrations could then be incorporated into further pathway models (such as vapour intrusion models), and/or exposure models, for risk calculations.

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## **What are the Limitations of BIOCHLOR?**

The main limitation of BIOCHLOR v.2.2 is its limited applicability to the wide range of physical and contaminant hydrogeological conditions often encountered at contaminated sites. Simply stated, in order for the model to be applicable, the following three conditions must be met:

### Uniform Flow

The plume (existing and predicted) must be contained within a volume of porous media such that the groundwater velocity and the dispersivity are relatively constant. In general, these conditions will be met when the plume is contained within a single “aquifer” unit of homogeneous properties, and when transport is uni-directional (*i.e.*, horizontal or vertical, but not horizontal followed by vertical).

The flow path does not necessarily have to be straight, so long as the magnitude of the hydraulic gradient is unchanging between source and receptor (*i.e.*, a curved flow path that follows a zone of enhanced permeability is acceptable so long as the total flow distance is accounted for).

Conditions causing non-uniform groundwater flow, and thus precluding the use of BIOCHLOR in RAs include, but are not limited to:

- The existence of a significant change in geologic conditions over the transport distance (*e.g.*, a source within sandy soils and a receptor within clayey soils);
- The existence of pumping or injection wells causing radial flow;
- The existence of a significant natural source/sink of water over the transport distance, such as a river or a opening in a confining unit situated between the source and receptor;
- Non-uniform flow geometry such as a confined aquifer of non-uniform thickness (*e.g.*, a sand layer that pinches out), or an unconfined aquifer of non-uniform saturated thickness (*e.g.*, a water table aquifer with significant recharge and with a fixed bottom elevation).

Uniform flow can be demonstrated by contouring hydraulic heads measured in monitoring wells situated between the source and the receptor, and screened within the target aquifer. Contour lines with a fixed contour interval should be straight, parallel, and equally spaced. Uniform geologic conditions should also be demonstrated from available sources such as geological maps, existing reports, and/or borehole drilling.

### Known Source Configuration

A source of fixed size must supply sufficient mass to the groundwater flow field so as to maintain a constant concentration. This is a reasonable assumption for DNAPL sources, but the determination of the size and concentration of the source is not straight-forward, and generally requires a comprehensive subsurface assessment. BIOCHLOR v.2.2 does allow for a decaying source concentration, with the decay rate best demonstrated from source concentrations measured over a significant time frame, relative to the time frame for predictive simulations. An appropriate ratio for duration of the “history-matching” period to “forecasting” period might be between 1 and 2. That is, if the decay coefficient is demonstrated using solute concentrations

collected over the last three years, then solute concentrations should be predicted no further than three to six years into the future.

#### First Order Decay Kinetics

The compounds under consideration must transform as a decay chain with first-order kinetics, which is a reasonable assumption for chlorinated solvents. Coefficients can be selected via the process of model calibration to measured solute concentrations, or from tables assuming a sufficient understanding of environmental conditions (size of dechlorinating microbial population, availability of hydrogen as an electron donor, and oxidation-reduction potential of the groundwater).

Another limitation of BIOCHLOR is related to the fact that it relies on an approximate analytical solution ("Domenico" model) rather than an exact mathematical solution. Based on the available research, it appears that BIOCHLOR should be used only in situations where advection is the dominant transport mechanism. Practically, this means that the longitudinal dispersion coefficient should not be greater than ten percent of the distance from source to receptor.

#### **What are the Reporting Requirements?**

RAs submitted under O. Reg. 153/04 that use BIOCHLOR v.2.2 should include the following:

- A clear statement as to the applicability of the assumption of uniform flow between the source and the receptor;
- A clear statement on the evidence supporting the assumption of reductive dechlorination or chemical decomposition scenario, including the assumed source compound or compounds, and the members and order of the decay-chain;
- Justification for seepage velocity relative to site specific information on hydraulic conductivity, hydraulic gradient, and porosity;
- Justification for chosen dispersivities, and a discussion on whether the site is an advection dominated or dispersion/diffusion dominated system (BIOCHLOR should not be used in the latter case);
- Justification for choice of retardation coefficient, including values calculated for each of the considered dissolved compounds, and a statement on how the differences among them was accounted for in the single value input into the model;
- Description of location, concentration and size of source term, along with discussion of source zone decay, if applicable;

- Justification for chosen decay coefficients based on the size of the dechlorinating microbial population, availability of hydrogen as an electron donor, and oxidation-reduction potential of the groundwater. A description of the method (based on published values or via model calibration) used to ascertain decay coefficients should also be provided.
- Description of model calibration efforts, with figures, tables or text to indicate the agreement between simulated and observed solute concentrations, both as a function of time (if multiple sampling events have been completed) and space (if multiple locations have been sampled);
- Description of efforts to ascertain the sensitivity of the solution (e.g., the concentration of the contaminant(s) of concern at the location of concern) to the various parameters. Parameters should be adjusted up and down from the best estimates, and the magnitude in variation should consider the physical setting, and the quality of the data;
- Description of the level of uncertainty in each of the selected parameters, and how the model results are utilized in the RA in light of these uncertainties.

**For further information, contact:**

Ecological Standards Section  
Standards Development Branch  
Ministry of the Environment  
7<sup>th</sup> floor, 40 St. Clair Avenue West  
Toronto, Ontario, M4V 1M2

[SDBRARReview@ontario.ca](mailto:SDBRARReview@ontario.ca)