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REPORT ON

APPROACHES AND METHODS FOR EVALUATION VERTICAL TRANSPORT IN GROUNDWATER- HYDROGEOLOGICAL ASSESSMENT TOOLS PROJECT

Submitted to:

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February 15, 2006

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1.0 INTRODUCTION

This report has been prepared for the Science Advisory Board for Contaminated Sites (SABCS) in British Columbia to evaluate approaches and methods that could be used by practitioners to evaluate the potential for transport of dissolved contaminants through complex hydrostratigraphic systems. Specifically, and for simplicity, the assessment considered vertical transport through an aquitard, followed by lateral transport via an underlying higher-permeability stratum. Simple groundwater pathway models, such as that currently proposed for the SRA-2 protocol, typically assume that, once the dissolved contaminants reach the water table, they will migrate horizontally towards a receptor such as a receiving body of surface water. At a large number of sites, this approach is valid, especially at locations close to groundwater discharge zones where hydraulic gradients favour upward flow, or where a shallow aquifer is underlain by a thick sequence of low permeability sediments. However, at some sites, contaminants migrate vertically from the shallow flow system to a deeper aquifer, and then move laterally in one or both systems towards a receptor. At some of these sites, contaminants moving along this deeper pathway may arrive at the discharge point earlier than the contaminants migrating in the shallow flow system. At those sites, the application of the SRA-2 protocol would not be straightforward.

The following text discusses approaches and methods that could be adopted to identify sites where the potential for vertical movement of dissolved contaminants from a shallow to a deep flow system exists. In addition this guidance can be used to identify sites where vertical transport is primarily from shallow to deep aquifers but in a manner that allows sufficient attenuation that receptor impact is not expected. First, a conceptual model is presented that includes a deeper flow system, as well as the shallow system that is currently implicit in the SRA-2 protocol. A discussion is provided on simple and practical methods that could aid in the identification of sites when the expanded conceptual model would need to be adopted. Finally, a series of quantitative approaches are outlined that could be used to evaluate a deep transport pathway.

2.0 CONCEPTUAL MODEL

The conceptual model proposed for the SRA-2 protocol is presented in Figure 1. This model incorporates the following processes: i) soil-water partitioning in the unsaturated zone; ii) mixing of contaminated water with groundwater at the water table; and iii) horizontal transport in the shallow aquifer resulting from advection, dispersion, retardation, and decay. Most important for this discussion is the assumption in Figure 1 of negligible vertical flow into the underlying strata.

Figure 2 shows the expanded conceptual model that is the focus of this discussion. This model includes the same components as the original model but, in addition, incorporates a deep confined aquifer that is separated from the shallow aquifer by an aquitard of relatively low hydraulic conductivity. The expanded model is loosely based on the hydrogeologic setting typical of, for example, the Lower Mainland in B.C. at locations in proximity to the Fraser River. The shallow aquifer represents surficial sediments that are underlain by overbank silts and clays. These silts and clays are typically present in the lowlands nearby the Fraser River and act as an aquitard. The underlying Fraser River Sands, a laterally extensive and relatively homogeneous sand unit, corresponds to the deep aquifer.

The expanded conceptual model assumes that both aquifers discharge to a nearby surface water body, and that groundwater flow in both units is nearly horizontal. Vertical leakage across the aquitard, including vertical flow through potential discontinuities, could be directed up or down depending on the difference in hydraulic head between upper and lower aquifers. Downward flow would occur if the hydraulic head in the deep aquifer is lower than the head in the shallow aquifer. These conditions are most likely if, for example:

- The hydraulic conductivity of the shallow aquifer is lower than the hydraulic conductivity of the deep aquifer. In this case, higher hydraulic gradients will be required to induce lateral flow in the shallow flow system than would be required for comparable flows in the deeper system. This may result in an elevated water table and corresponding downward leakage through the aquitard;
- The hydraulic conductivity of the aquitard is relatively low, and recharge from precipitation is relatively high. As above, this will result in an elevated water table and potential for vertical leakage through the aquitard;
- The shallow aquifer is not directly connected to the river but, instead, the discharge occurs via a seepage face located high on the river bank. If the deep aquifer is hydraulically connected to the river, a downward hydraulic gradient between these two units is likely;
- The source zone is located sufficiently distant from the discharge zone, away from the river, such that recharge to the deep aquifer is primarily from the shallow flow system; and
- Pumping is occurring in the lower aquifer. This may lower the hydraulic heads in the lower aquifer thus inducing vertical leakage through the aquitard.

3.0 IDENTIFICATION OF POTENTIAL FOR VERTICAL TRANSPORT

The following sections present a set of simple and practical methods that could aid in the identification of sites where the potential for vertical transport through an aquitard could exist. This proposed approach is based primarily on methods routinely used in site characterization that are utilized in the field of physical hydrogeology. The potential presence of DNAPLs is not specifically addressed by this approach. Where DNAPLs may be present, added caution beyond measures discussed in this report should be taken to avoid possible drag-down of DNAPL into the subsurface during efforts to characterize deeper strata and chemical conditions.

The approach is centered on a set of questions that would need to be answered in sequence. Any answer in the negative would provide a stopping point in establishing whether or not the deep flow pathway potentially exists. For example, in the absence of a deep aquifer (Question 2), it would not be necessary to evaluate the vertical gradient in the strata underlying the shallow aquifer (Question 3). The evaluation process would stop. Figure 3 provides a flowchart of the proposed approach.

Q1: How thick is the shallow aquifer and does the plume extend to its base?

The thickness of the shallow aquifer controls, to a large degree, the potential for vertical transport through the underlying aquitard. If this aquifer is relatively thin, it is more likely that, due to vertical dispersion occurring between the source zone and the discharge point, the base of the contaminant plume will extend to the bottom of the aquifer. This is even more likely if the source zone is deep relative to the thickness of the aquifer. Once the contaminants reach the bottom of the aquifer, the possibility for vertical transport increases. On the other hand, if the shallow aquifer is of considerable thickness and the source zone is relatively shallow, the resulting plume is more likely to remain in the upper part of the aquifer.

The shallow aquifer is typically investigated during initial site characterization activities, which commonly include drilling, well installation and test-pitting. Unless the base of the shallow aquifer is located relatively close to the ground surface (*e.g.*, within 5 m or less), test pits are of limited use in establishing its base. The same applies to shallow boreholes and monitoring wells that do not penetrate the entire thickness of the aquifer. To investigate the potential of vertical transport through the underlying aquitard, it is important that some of the boreholes extend to the base of the shallow aquifer. Monitoring wells completed in these boreholes should have relatively short screens set just above the contact between the aquifer and aquitard. Groundwater samples collected from these wells downgradient of the source will aid in the assessment of the vertical extent of the contaminant plume. If it is found that the shallow aquifer is of limited thickness and/or the plume extends to its base, then the site investigations should be expanded to address the next question.

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Q2: Is a deep aquifer present?

The presence of a deep aquifer or multiple deep aquifers is necessary for the alternate pathway for contaminant transport to exist. During routine site investigations, it is uncommon to advance boreholes beneath the first permeable horizon where most of the contamination is typically present. Thus little site information is typically available to make this assessment.

The potential for the existence of a deep unit should be first investigated using available hydrogeologic data, including published geologic maps, reports of previous investigations, and water well and aquifer database information maintained on-line (http://wlapwww.gov.bc.ca/wat/gws/index.html) by the Ministry of Environment (formerly Ministry of Water Land and Air Protection). Of particular importance is the water well database, which may contain logs of deeper boreholes completed nearby during water supply investigations. Review of these logs will yield stratigraphic data at depth beyond the range of local site investigation. Even if the borehole logs for the nearby water supply wells are not available, the total depth of these wells (if reported) can provide information on the average depth of more permeable units. Well yields reported for these wells may provide indication of hydraulic conductivity of the deep aquifer.

If the available hydrogeologic data suggest that a deeper aquifer may be present, consideration should be given to the installation of at least one, and preferably three deep boreholes. Three boreholes are recommended at locations where other hydrogeologic data suggest that groundwater flow direction in the deep aquifer may be different from that in the shallow aquifer. These boreholes should be located downgradient of the source of contamination, and each should be completed as a monitoring well with a screen set in the deep aquifer. The wells should be located near monitoring wells completed in the shallow aquifer. During installation, care should be taken to prevent cross-contamination between shallow and deep aquifer. If warranted (for example, to prevent downward migration of DNAPLs), drilling techniques that employ dual casing and grouting should be used.

Q3: Is the vertical hydraulic gradient down?

Once the presence of a deep aquifer is confirmed, it is important to establish the direction and magnitude of the vertical hydraulic gradient across the aquitard that separates these units. If a strong downward gradient is present, the potential presence of a deep pathway for contaminant transport becomes more significant. The vertical gradient should be assessed by simultaneous measurements of hydraulic heads in the deep wells and nearby wells completed in the shallow aquifer (the deep and shallow wells should not be more than few meters from each other). These measurements should be repeated quarterly over a full year to establish seasonal trends in vertical gradient. At locations where groundwater flow varies seasonally or is strongly influenced by ocean tides, such as many sites located in the Lower Mainland and other coastal regions of B.C., specialized techniques (for example refer to Zawadzki et al., 2002) should be employed to establish the average direction of the vertical gradient.

Q4: Is the horizontal flux in the deep aquifer high? Is the vertical flux in the aquitard significant?

Even where a deep aquifer and a strong downward gradient between this aquifer and the shallow aquifer are present, the deep transport pathway may not be significant. For example, if the hydraulic conductivity of the deep aquifer is relatively high and groundwater flow in this unit occurs under a relatively steep hydraulic gradient, the resulting horizontal flux may provide sufficient mixing with contaminants leaking from the aquitard to reduce the downgradient concentration to acceptable levels. This condition would be even more likely if the aquitard was relatively thick and of low hydraulic conductivity, thus resulting in low vertical flux.

The hydraulic conductivity of the deep aquifer should be measured in the deep well(s) using standard aquifer testing techniques. This should involve single-well-response tests or pumping tests conducted using, for example, portable pumps. Additional estimates of hydraulic conductivity should be made based on grain size analysis of soil samples collected from this unit. Preferably, horizontal hydraulic gradients in the deep aquifer should be estimated based on hydraulic head measurements from at least three monitoring locations. If only one monitoring well is installed in this aquifer, an approximate estimate of the horizontal gradient could be made based on hydraulic head measured in this well and the water level in the receiving water body. The measured values of hydraulic conductivity and horizontal gradient, together with an estimates of cross sectional area available for groundwater flow, can be used to calculate horizontal flux in the deep aquifer.

The vertical flux in the aquitard is mainly controlled by its hydraulic conductivity. This parameter can be measured in situ using single-well-response tests conducted in monitoring wells completed in this unit. Although these tests measure horizontal hydraulic conductivity, it is considered conservative to use the resulting values as the vertical hydraulic conductivity is commonly less than horizontal one. Additional laboratory tests can be performed on undisturbed soil samples recovered from the aquitard using a constant-head or falling-head permeameter. These measurements, together with measured values of vertical hydraulic gradient (Q3) and estimates of the source horizontal area, will allow calculation of vertical flux through the aquitard. In addition, the effects of aquitard discontinuities (e.g., natural features related to sedimentation or erosion, anthropogenic features associated with abandoned wells) on vertical flux in the aquitard should be evaluated. This evaluation should be based on the results of site investigations, data available from the Ministry of Environment well database, and aquifer vulnerability mapping (where available). Site-wide geophysical survey should be considered were aquitard continuity is questionable, particularly at sites where aquitard thickness is less than 5 m.

4.0 QUANTITATIVE METHODS

Quantitative methods may also be used to assess the potential for deep transport pathways at a contaminated site. These methods have varying degrees of complexity, ranging from "back of the envelope" calculations based on Darcy's Law to computer simulations that utilize numerical modelling codes. The former methods are suggested for screening the site under investigation for the potential for a significant deep pathway, whereas the latter methods may be used for more detailed assessment of potential travel times and contaminant concentrations at a receptor.

4.1 Simplified Approaches Based on Darcy's Law and Mixing

An order-of-magnitude estimate of the significance of the deep transport pathway can often be made using, for example, Darcy's Law, as discussed below. This method focuses on an assessment of the mixing of contaminated groundwater that is moving vertically through an aquitard, with non-contaminated groundwater that is flowing laterally in the deep aquifer. If the mixing ratio is low, then the resulting concentration at the mixing zone (near the aquitard-deep aquifer interface) may be sufficiently low to reduce the concentration of the dissolved contaminant to acceptably low levels.

The mixing calculations are based on the following equation:

$$r = \frac{Q_{aquitard}}{Q_{aquifer} + Q_{aquitard}}$$

$$Q_{aquitard} = K_{aquitard} \dot{i}_{aquitard} A_{aquitard}$$

$$Q_{aquifer} = K_{aquifer} \dot{i}_{aquifer} A_{aquifer},$$

where r is the mixing ratio, O indicates groundwater flux (m^3/s) , K is hydraulic conductivity (m/s), *i* is hydraulic gradient (-), and *A* is cross sectional area assumed for flow (m^2) . The estimates of hydraulic conductivity and gradient should be based on field measurements, as discussed in the preceding section. The area $A_{aquitard}$ should be based on the approximate area of the dissolved phase plume in the shallow aquifer. This is the area over which contaminated groundwater may enter the aquitard via leakage. The area $A_{aquifer}$ is more difficult to estimate, as the thickness of the portion of the deep aquifer that mixes with water entering via the overlying aquitard is often uncertain, and must be estimated. If the distance from the source zone to the receiving surface water body is large relative to the total thickness of the deep aquifer, it is possible that this mixing occurs over the entire thickness of the deep aquifer as a consequence of vertical dispersion along the flow path. At the other extreme, if the distance to the receptor is short, then little dispersion may occur and vertical mixing may be limited to the upper part of the deep aquifer prior to discharge. Better understanding of the mixing zone thickness may be gained by installing monitoring wells in the lower aquifer with screens completed at different elevations. Overall, the selection of the an appropriate value for A_{aquifer} requires careful consideration and professional judgment.

Once the mixing ratio is calculated, it can be used to provide an order-of-magnitude assessment of the reduction of contaminant concentrations along the deep pathway. This is accomplished by multiplying the average concentration of dissolved contaminants measured in the shallow plume by r. If the resulting value is below the regulatory standard, it is likely that the significance of the deep transport pathway is low, and further consideration of the deep transport pathway is not required.

The above method can be considered very conservative in that it does not account for contaminant attenuation due to dispersion, retardation, biochemical degradation, and/or decay either in the aquitard or along the flowpath in the deep aquifer. As such, these types of calculations are probably best performed early during site characterization for screening purposes.

4.2 Calculations Based on Composite Analytical Models

More detailed assessment of the deep pathway for contaminant transport can be made using analytical models that are combined to simulate various components of the site conceptual model. An example of such a composite model is the SRA-2 Groundwater Module, which is based on a series of analytical calculations that include the Bear $(1979)^1$ solution for transport of dissolved contaminants in groundwater. The Bear (1979) solution represents transport of dissolved chemicals in the shallow aquifer in one dimension, resulting from advection, dispersion, biochemical degradation, and decay. Although somewhat limited in its application (*e.g.*, assumption of uniform flow field may not be applicable at some sites), this solution is an invaluable tool for assessing organic contaminant attenuation along the groundwater pathway. The solution could be adopted for simulation of contaminant transport in the aquitard and deep aquifer.

It is relatively easy to envision an extension to the SRA-2 Groundwater Module that would include degradable contaminant movement via an alternate, deep pathway. This extension could be incorporated into the existing model framework as an option that could be activated for applications where the deep transport pathway may be of concern. The extension would necessarily consist of three modules comprising: 1) vertical transport through the aquitard; 2) mixing at the aquitard-deep aquifer interface; and 3) horizontal transport in the deep aquifer.

The starting point for the first module would be the contaminant concentration in the shallow aquifer calculated at the watertable as the result of mixing of fresh groundwater with leachate originating from the source. This approach is conservative in that it assumes that the concentration at the base of the shallow aquifer, where the contaminant may enter the underlying aquitard, is the same as that at the watertable. In reality, this concentration may be less due to various transport mechanisms operational in the shallow aquifer. The contaminant source at the top of the aquitard would be represented by the above concentration and applied over the footprint of the shallow plume. Transport processes in the aquitard would be simulated using the Bear (1979) solution based on measured values of aquitard hydraulic conductivity and gradient, and published values of other transport parameters representative of the contaminant under consideration. The arrival time and contaminant concentration predicted by this module at the base of the aquitard would be used as input in the mixing calculations at the aquitard-deep aquifer interface.

¹ Section 10.6.1, page 627 to 633.

The next module, representing mixing of aquitard leakage with fresh groundwater in the deep aquifer, would be based on a similar equation as the one presented in Section 4.1. The main difference would be that the resulting mixing ratio would be applied to the contaminant concentration at the base of the aquitard, as predicted by the aquitard module, and not to concentration in the shallow aquifer. Thus, the potential attenuation of contaminants along the vertical flowpath in the aquitard could be taken into account.

The last module would represent transport of contaminants horizontally in the deep aquifer. Transport processes in this aquifer would be simulated using the Bear (1979) model, based on measured values of hydraulic conductivity and gradient in the deep aquifer, and on published values of other transport parameters representative of the contaminants under consideration. The source term in this model would be simulated using concentrations predicted by the mixing module at the aquitard-aquifer interface. The contaminant concentrations predicted by this model at the receptor would account for attenuation resulting from dispersion, degradation and decay mechanisms along the flowpath in the deep aquifer.

Alternatively, in the case of non-degradable compounds, the proposed protocols for modeling metals transport could be applied in a similarly linear fashion (*i.e.*, vertical flow through aquitard, mixing, and then horizontal flow through lower aquifer).

4.3 Simplified Cross Sectional Models Based on Numerical Solutions

The most complex methods to address the potential for deep transport pathways at a contaminated site involve the application of cross sectional groundwater flow and transport models based on numerical solutions. Although development of such models requires a substantial amount of data and is more time consuming, this approach is capable of achieving the most realistic simulations of transport of dissolved contaminants from the source to the receptor. For example, the composite analytical model discussed above is limited in that it cannot easily account for transient changes in contaminant concentration at various "junctions" between model components. That is, in the composite model the source concentration in the deep aquifer would have to be kept constant whereas, in reality, its concentration would vary in time as the contaminant front moves across the aquitard. In addition, the vertical flow component in the shallow and/or deep aquifer could not be simulated by the composite model as it assumes a uniform horizontal flow field in both units. A numerical model that simultaneously simulates flow in the shallow aquifer, the underlying aquitard, and the deep aquifer would remove these limitations.

The simplified cross sectional model would represent an expanded conceptual model of the site (Section 2.0) and would be oriented along the dominant flowpath. Boundary conditions would be set according to hydrogeologic boundaries established in the conceptual model. A contaminant source at the water table would be represented using mass-flux calculated based on soil-water partitioning. If practical, limited model calibration to the observed hydraulic heads and measured concentrations of dissolved contaminants would be conducted. However, at many sites calibration of a cross sectional model would not be possible due limitations inherent in a two-dimensional simulation when applied to a three-dimensional groundwater flow field. For example, model calibration could not be conducted if groundwater flow directions in the shallow aquifer and deep aquifer were not the same. Nevertheless, the simplified cross sectional model is considered to be the most advanced predictive tool that could be used at the screening level analysis.

Several numerical codes are available for construction of a cross sectional flow and transport model. The most widely used codes include:

- MODFLOW/MT3D These codes were developed by the United States Geological Survey (Harbaugh et al., 2000) and United States Environment Protection Agency (Zheng, 1990) to simulate saturated groundwater flow and transport of dissolved contaminants in three-dimensions in heterogeneous and anisotropic porous media. Both codes solve the groundwater flow and transport equation using method of finite differences. They are the most widely used modelling codes in North America, and are well recognized by the professional and regulatory communities. Several graphical pre- and post-processor are available for the preparation input and output files required by these codes, including Groundwater Modelling System, Visual MODFLOW, Groundwater Vistas, Processing MODFLOW, and ArgusOne. Although features of MODFLOW/MT3D allow for the development of very complex three-dimensional model, they are easily adopted for two-dimensional cross sectional simulations.
- FEFLOW This modelling code has been in continuous development since 1979 in the WASY Institute in Germany (Diersch, 2005). It uses the method of finite elements to simulate groundwater solute and heat flow in three dimensions in variably saturated porous media. FEFLOW has been widely applied in Europe and, in recent years, its use in North America has gradually expanded. Similarly as for MODFLOW/MT3D, FEFLOW features extend far beyond the requirements of the two-dimensional model. However, it can easily be adapted for this task. In addition, method of finite elements employed in FEFLOW allows for somewhat greater flexibility in constructing two-dimensional model compared to MODFLOW/MT3D.

- SEEP/W-TRANS/W This modelling package was developed by Geo-Slope (Geo-Slope, 2004)) to simulate two-dimensional groundwater flow and transport of solutes using method of finite elements. The code has been extensively used in Canada, primarily by geotechnical and mining professionals. Two-dimensional cross sectional models discussed in this documents could easily be developed using this code.
- SVFlux-ChemFlux This modelling package was developed by SoilVision Systems (SoilVision, 2005) and has similar capabilities as SEEP/W-TRANS/W. Of particular interest for development of simple cross-sectional models is the extensive database of soil parameters that is included with the code.
- VS2DT This code has been developed by United States Geologic Survey (http://wwwbrr.cr.usgs.gov/projects/GW_Unsat/vs2di1.2/index.html) for simulation of variably saturated flow and solute transport in two dimensions. Similar to MODFLOW, this code uses method of finite difference to solve groundwater flow and transport equations. It is well suited for the construction of a simplified cross sectional model as it is relatively easy to use and is available with a built-in graphical interface. In addition, VS2DT is a free public domain software, whereas FEFLOW, SEEP/W-TRANS/W, SVFlux-ChemFlux and graphical pre-processors for MODFLOW/MT3D are only available commercially.

The development of three-dimensional groundwater flow and transport models is not recommended at the SRA-2 level. However, use of such models is a recommended Hydrogeological Assessment Tools option for pathway analysis. These models require much more extensive collection of hydrogeologic data than is typically conducted at the screening-level stage of site assessment. Without sufficient data necessary for model construction and calibration, a three-dimensional model would not be capable of providing more realistic predictions of contaminant transport than those which could be provided using more simplified two-dimensional models.

Yours very truly,

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