Recycled Materials Resource Center

Progress Report for the U. S. Environmental Protection Agency

- **Project Title:** Evaluation of IWEM For Non-Federal Users With Regard to Highway Applications
- **USEPA Contact** Mr. John Sager
- **Name of PIs:** Dr. Jeffrey S. Melton and Dr. Kevin H. Gardner
- **Affiliation of PIs:** University of New Hampshire
- **Project Dates:** October 1, 2004 to September 30, 2006
- **Progress Report Number:** Report #2
- **Progress Report Dates:** September 1, 2005 – February 28, 2006
- **Next Report Due:** May 31, 2006
- **Funds Expended to Date:** $20,966 of $35,000 Expended to Date.

1.0 Introduction: previous work and objectives

Comprehensive modeling has been performed with IWEM to determine how the model responds when simulating water and contaminant transport from heavy metal bearing secondary materials into the subsurface. The objective of this work is to evaluate whether IWEM can be used as a predictive tool to accurately determine whether leaching from materials will result in significant changes in groundwater concentrations when the materials are reused as a base or sub-base in a roadway.

Past modeling included evaluating how IWEM treats the behavior of heavy metal transport as a function of time and receptor well distance from the source. Additionally, simulations were performed with varying distribution coefficient values (K_d) and waste management unit (WMU) areas. Results and conclusions can be viewed in the previous progress report.

This phase of research involves comparing IWEM's results to those of other solute transport groundwater models using the same input. Doing so will allow for the analysis of whether IWEM can accurately predict groundwater concentrations at a point down gradient from a secondary material source. IWEM simulates 1-D flow in the unsaturated zone and 3-D flow in the saturated zone. A situation such as this requires the use of two models in order to effectively mimic the secondary material leaching scenario modeled by IWEM. After careful consideration, HYDRUS-1D/2D and Visual MODFLOW were chosen as the comparison tools to evaluate IWEM's solute transport prediction capabilities. Both models have been widely used and proven to be effective in simulating solute transport in the situations for which they were developed (e.g. flow dimension and level of media saturation) therefore providing the highest level of confidence in their output.

The remainder of the progress report discusses the HYDRUS-2D modeling portion of research. MODFLOW results will be presented in a subsequent progress report.

2.0 Methods

HYDRUS-2D was used to simulate one dimensional (1D) vertical solute transport from the secondary material source through the unsaturated zone down to the water table. Not only can HYDRUS provide 1D flow to mimic that modeled by IWEM, but it can do so through variably saturated media representative of the unsaturated zone. Input including initial metal concentrations and fluxes from the secondary material source, soil type, recharge rates, and hydrogeologic parameters (e.g. conductivity) has remained unchanged from those used for IWEM simulations. Upon running HYDRUS, output concentrations and fluxes were read from the lower boundary of the modeled domain which is representative of the top of the water table. These values will then be used for input into MODFLOW to complete the modeling process through the saturated zone.

Two scenarios were run using HYDRUS: (1) with a cross-sectional length of 14 meters (m) to mimic the arbitrarily chosen 200 m^2 WMU area ($(14\ m)^2 \sim 200\ m^2$) used for most of the previous IWEM simulations; and (2) with a cross-section length of 1000 m to represent a real life application of secondary materials along a stretch of highway. The purpose of using these lengths is to compare the output concentrations from both and determine if increasing the cross-sectional horizon has any dramatic effect on the concentration observed at the water table along the plume centerline. In previous IWEM work, it was observed that increasing the WMU area had an almost linear effect on the output groundwater concentrations. It was thought that this is an unrealistic result that may be attributed to the fact that IWEM assumes its WMUs to be squares which is not representative of roadway geometry (rectangular).

Both scenarios were run using average tabulated K_d values compiled by an extensive USEPA literature search (Table 1).

Metal	K_d (L/Kg)
Ag	398.1
Cd	501.2
Cr	6.3
Se	20

Table 1 – EPA tabulated K_d values based on literature search (EPA, 1999).

Additionally, the 14 m cross-sectional scenario was run using a K_d value of zero for each solute (Ag, Cd, Cr, and Se). The majority of the IWEM simulations run to date have relied upon K_d values drawn from the MINTEQA2 database incorporated into the software. Earlier work has demonstrated that these values are relatively low (on the order of magnitude of one) and this allows for a good comparison between the models. Moreover, IWEM had been run as a function of time using the tabulated EPA values allowing once again for effective comparisons.

All HYDRUS simulations were run for 100 years using bottom ash data, which had the highest leachate concentrations. No runs were performed for the other materials in the research (e.g. foundry slag) under the assumption that these would yield identical trends. The unsaturated zone was represented by a simple rectangular geometry. The boundary conditions (BC) of the modeled domain were set up such that the top was defined by a daily *constant flux BC* representing the incoming water leaching from the secondary material as reported by Sauer et. al; the bottom as a *constant pressure head BC* set equal to zero which is characteristic of the water table; and the vertical sides as *no-flow BCs*. Additionally, five observation nodes were set along the center of the domain extending from the surface to the water table. Solute concentrations and fluxes, as well as water fluxes could be read from these nodes.

3.0 Results and Discussion

Solute concentrations from the five nodes for the 14 and 1000 m scenarios using the EPA K_ds were compared for 100 years. Table 2 shows the concentrations at node 5 (bottom boundary) for select years.

Table 2 – Comparison of output concentrations (mg/l) at node 5 (groundwater table) for 14 and 1000 m cross-section scenarios.

	Cd		**Cr**		**Se**		**Ag**	
Time (yrs)	14m	1000m	14m	1000m	14m	1000m	14m	1000m
1	0	0	8.35E-15	9.12E-15	7.38E-17	8.01E-17	0	0
10	4.70E-20	5.07E-20	1.04E-10	1.12E-10	8.48E-13	9.15E-13	8.27E-20	8.92E-20
40	4.78E-17	5.21E-17	9.58E-08	1.04E-07	8.38E-10	9.14E-10	8.40E-17	9.17E-17
100	4.64E-15	5.09E-15	7.60E-06	8.25E-06	7.69E-08	8.43E-08	8.15E-15	8.95E-15

Review of Table 2 clearly shows that increasing the cross-sectional length of the domain has minimal effect on the solute output concentrations along the centerline. This is in contrast to the large increases in concentration as a function of WMU area observed with IWEM from earlier work as shown in Figure 1. Figure 1 clearly demonstrates increases in concentration up to an order of magnitude (see Section 4.0).

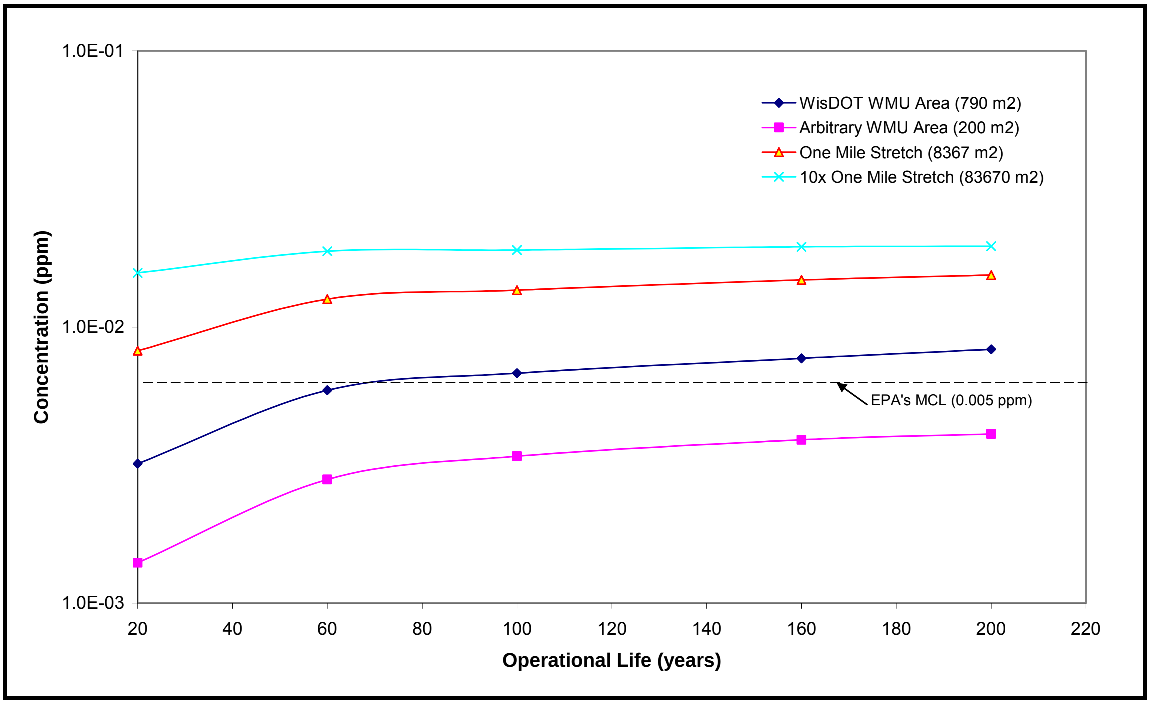

Figure 1 – Plot of Cd concentration with time for differing IWEM WMU areas.

Next, a comparison between HYDRUS-2D and IWEM results was performed with both models using USEPA reported K_d values. Again, concentrations of interest from HYDRUS were taken from the bottom node. Results can be viewed in Table 3.

	Cd		Cr		Se		Ag	
Time (yrs)	**IWEM**	**Hyd**	**IWEM**	**Hyd**	**IWEM**	**Hyd**	**IWEM**	**Hyd**
1	0	0	0	8.35E-15	5.65E-06	7.38E-17	0	0
10	0	4.70E-20	4.53E-06	1.04E-10	5.65E-05	8.48E-13	0	8.27E-20
20	0	1.50E-18	7.24E-05	3.21E-09	1.00E-04	2.68E-11	0	2.64E-18
40	0	4.78E-17	7.24E-05	9.58E-08	3.22E-04	8.38E-10	0	8.40E-17
80	0	1.52E-15	7.24E-05	2.67E-06	5.06E-04	2.58E-08	0	2.68E-15
100	0	4.64E-15	7.24E-05	7.60E-06	6.00E-04	7.69E-08	0	8.15E-15

Table 3 – Comparison between HYDRUS-2D and IWEM results for bottom ash concentrations (mg/l) with time using USEPS tabulated K_d values.

Analysis of Table 3 shows that the models predict similar concentrations for Cd and Ag. Because HYDRUS is only simulating transport through the unsaturated zone, it is likely the concentrations presented here would decrease due to dispersion and further retardation in the saturated zone, bringing them closer to the zero values reported by IWEM.

However, for Cr and Se, concentrations predicted by HYDRUS are considerably lower than those of IWEM. This raises concern because, again, HYDRUS is only representing transport through the vadose zone and one would expect the concentrations to be larger because the solutes have not yet been subject to further transport, dilution and attenuation through the saturated zone. Additionally, IWEM does not allow for user-defined K_d values for Cr. Thus, it is assumed that MINTEQA2 is being used to provide this parameter. As mentioned before, previous work with IWEM has observed that the model draws upon very low K_d values when MINTEQA2 is used. This could very well be the cause for such high Cr concentrations observed at the receptor well (50 meters from source) because retardation due to soil sorption is minimal.

Finally, a comparison was made with IWEM results using MINTEQA2 K_d values and HYDRUS results using K_d values equal to zero (Table 4).

	Cd		Cr		Se		Ag	
Time (yrs)	**IWEM**	**Hyd**	**IWEM**	**Hyd**	**IWEM**	**Hyd**	**IWEM**	**Hyd**
1	0	1.24E-07	0	9.70E-08	1.80E-03	2.41E-07	1.67E-05	6.90E-08
10	7.00E-04	1.07E-03	4.53E-06	8.40E-04	7.30E-03	2.10E-03	7.00E-04	6.01E-04
20	1.40E-03	1.12E-02	1.84E-05	8.17E-03	8.30E-03	2.18E-02	1.30E-03	6.24E-03
40	2.30E-03	2.29E-02	3.54E-05	1.61E-02	9.40E-03	4.45E-02	1.90E-03	1.28E-02
80	3.10E-03	2.11E-02	8.68E-05	1.52E-02	9.50E-03	4.11E-02	2.30E-03	1.18E-02
100	3.40E-03	2.15E-02	2.00E-04	1.50E-02	9.80E-03	4.17E-02	2.50E-03	1.19E-02

Table 4 - Comparison between HYDRUS-2D and IWEM results for bottom ash concentrations (mg/l) with time. Results based on using K_d values of zero and MINTEQA2 derived for HYDRUS and IWEM respectively.

Observations from Table 4 show similar results in magnitude between the models for each solute and time. This appears to confirm the notion that IWEM is drawing upon very low K_d values (less than or equal to 1 L/Kg) from MINTEQA2 which contradicts the EPA tabulated data.

4.0 Conclusions

Based on the data presented in the previous section, several preliminary conclusions can be made. The major conclusion is that, based on HYDRUS 2-D data, it appears IWEM is very conservative in its modeling and thus is overestimating output concentrations at the receptor well. This may be the result of several factors.

K_d values derived from MINTEQA2 appear to be extremely low (less than or equal to 1 L/Kg) when compared to the EPA tabulated data (Table 1) and those from other literature sources. The use of these small K_d values seems to be accounting for the lack of retardation being observed, thus allowing the contaminants to move freely through the aquifer with minimal sorption. This is likely resulting in the higher observed concentrations at the receptor well when compared to HYDRUS-2D outputs. Furthermore, HYDRUS is only simulating flow/transport within the unsaturated zone while IWEM accounts for the entire aquifer. This raises further concern that IWEM may be too conservative it its predictions.

Another concern is the lack of output files with respect to non-user defined input values. For instance, if MINTEQA2 is used, the modeler can not view which K_d values were selected due to the absence of such a file. The same is true for Monte Carlo derived aquifer parameters. While there is a file listing national averages, it is not clear whether these are the values being used in the simulations. Such output files would allow for the modeler to determine whether the chosen values are realistic, and if not, to make the necessary adjustments.

Finally, because IWEM assumes WMUs to be square it does not allow the modeler to accurately portray the true geometry of a roadway (rectangular). It seems likely that IWEM is contributing more solute to the centerline line of the plume than would realistically be seen with a rectangular cross-section of the same area. The further you move away laterally from the plume centerline, the less likely it is that contaminants at those distances would be introduced into the groundwater that is seen at the receptor well down gradient (located along the plume centerline). Factors such as advection, dispersion, dilution and sorption would all act to counter any significant contributions from contaminants outside a certain lateral extent from the centerline.

5.0 Future Work

Upon completion of the HYDRUS-2D modeling portion of this research, MODFLOW will be used to simulate 3-D groundwater flow and solute transport in saturated media at an observation well down gradient of the secondary material source. Input will include the metal concentrations and fluxes obtained at the lower boundary of the corresponding HYDRUS simulation. Several layers in the MODFLOW domain will be created so that multiple concentrations can be obtained at various intervals along the observation well screen. The average of these concentrations will be compared to that obtained from IWEM in order to evaluate its predictive accuracy.

Additionally, arbitrarily selected high concentrations of solute (e.g. 10 x MCL) will be input into MODFLOW to observe the magnitude of dilution encountered along the pathway to the receptor well. These determinations will be compared to IWEM to make a conclusion on its transport accuracy.

6.0 References

Sauer, J.J., Benson, C.H., and Edil, T.B. (2005). "Metals Leaching from Highway Test Sections Constructed with Industrial Byproducts." Geo Engineering Report No. 05-21, Dept. of Civil and Environmental Engineering, University of Wisconsin-Madison.

U.S. EPA (1999). "Partition Coefficients for Metals in Surface Water, Soil, and Waste, Washington, D.C.