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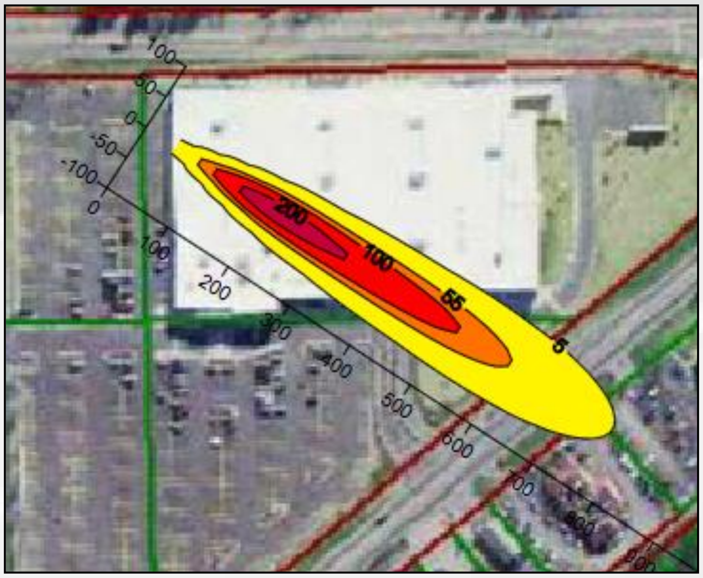
CASE HISTORY

Variation in Hydraulic Conductivity and Retardation Factor and its Effect on Numerical and Analytical Model Results

Challenge:



The project Site is the former CS & T Dry Cleaner located on the northeast side of Columbus, Indiana. Soil and groundwater contaminated with Perchloroethene (PCE) was discovered at the Site during a Phase I Investigation performed in 2002. Initial remediation activities using in-situ chemical oxidation were successful in removing a significant portion of the source area of the impacted groundwater plume. However, a significant dissolved plume of organic chemicals remained associated with the Site. In an effort to bring the remedial efforts to an effective closure, Mundell & Associates, Inc. (MUNDELL) was retained by a partnering consulting firm to evaluate the stability of the dissolved organic plume using groundwater flow and chemical transport modeling. Modeling activities were completed in 2007 utilizing published three-dimensional analytical transport solutions (Domenico and Robbins, 1985; Domenico, 1987) to model the transport of residual contamination in the plume. Using these calibrated results, a comparison between the computer software BIOCHLOR and the utilized 3D analytical transport solution was conducted. Numerous sets of simulations were completed using both modeling methods to determine if they yield comparable results using the same hydraulic inputs. In addition, attempts were made to duplicate the calibrated analytical model results varying solely hydraulic conductivity and the retardation factor (r-factor) within the BIOCHLOR solution.

Action:

Upon formulation of a calibrated 3D analytical flow model, identical hydraulic values were utilized in BIOCHLOR to predict center-line concentrations with increasing distance from the source area. Comparison between the simulated PCE concentrations (3D analytical and BIOCHLOR) and the observed PCE concentrations indicated that the fit of the 3D analytical model values to the observed PCE values is significantly better than that of the BIOCHLOR results.

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Point ID	Distance from Source Area (x)	Observed PCE Concentration	Analytical Model Values	BIOCHLOR Model Values
MW-17	55.3	9300	7848	4701
CL-1	72.7	5000	4836	4095
CL-2	190	1000	1119	2491
DG-1	281.4	600	698	1987
PGW-1	308.5	62	611	1848
CL-3	322.4	500	585	1770
CL-4	358.6	100	484	1548
CL-5	425	55	326	1049

The second set of simulations used identical input parameters as both the previously run 3D analytical and BIOCHLOR simulations with the EXCEPTION of the hydraulic conductivity and r-factor. Attempts were made to set the K value at a more reasonable level (140 ft/d vs. 9 ft/d) and then adjust the r-factor until results similar to the first BIOCHLOR runs were attained.

Point ID	Distance from Source Area (x)	K	BIOCHLOR Model Values using fixed R (ug/L) (1st BIOCHLOR simulations)	Variable R (for 2nd BIOCHLOR simulations)	BIOCHLOR Model Values using varied R (ug/L) (2nd BIOCHLOR simulations)
MW-17	55.3	140	4701	1.03E-03	4733
CL-1	72.7	140	4095	8.92E-02	4092
	72.7	140		1.04E-01	4088
CL-2	190	140	2491	6.50E-04	2666
	190	140		9.80E-01	2495
DG-1	281.4	140	1987	4.83E-03	1993
	281.4	140		4.13E-02	1917
PGW-1	308.5	140	1848	3.75E-02	1808
	308.5	140		1.00E+01	1904
CL-3	322.4	140	1770	4.43E-02	1728
	322.4	140		1.88E+01	1763
CL-4	358.6	140	1548	8.35E-02	1487
CL-5	425	140	1049	5.00E-01	1079
	425	140		1.57E+01	1066

3.31 = Averaged secondary r- factor

Indicates point location with secondary r-factors

As displayed above, several calibration points had multiple r-factor/K combinations that produced PCE concentrations similar to those calculated in the first BIOCHLOR simulations. Unfortunately, variation of the r-factor within a single transport model is not realistic, nor is it supported in either the 3D analytical model or in the BIOCHLOR spreadsheet. Averaging the secondary r-factors to create a single representative value was attempted and input into BIOCHLOR (R = 3.31). Use of this averaged r-factor did not duplicate the earlier BIOCHLOR results, and produced error values in excess of 43%.

An additional attempt to obtain a secondary r-factor was completed by comparing BIOCHLOR simulated PCE concentrations to PCE concentrations observed in the field.

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Point ID	Distance from Source Area (x)	K	Observed PCE Values (ug/L)	R	BIOCHLOR Model values using varied R (ug/L)
MW-17	55.3	140	9300	1.29E-06	9389
	55.3	140		5.55E-06	9346
	55.3	140		8.10E-06	9337
	55.3	140		9.85E-05	9332
CL-1	72.7	140	5000	5.85E-07	4838
	72.7	140		6.50E-06	4911
	72.7	140		6.70E-05	5039
	72.7	140		1.01E-04	5014
	72.7	140		5.40E-04	5048
	72.7	140		7.50E-04	5114
CL-2	190	140	1000	6.90E-06	1022
	190	140		9.70E-03	1017
	190	140		1.15E-02	1062
	190	140		3.70E+01	1000
DG-1	281.4	140	600	2.54E-03	616
	281.4	140		2.55E+01	582
PGW-1	308.5	140	62	8.90E-07	49
	308.5	140		6.90E-06	75
	308.5	140		2.18E-03	65
	308.5	140		2.58E+01	62
CL-3	322.4	140	500	9.10E-07	490
	322.4	140		6.25E-06	484
	322.4	140		1.13E-02	545
	322.4	140		2.48E-02	531
	322.4	140		2.77E-02	503
	322.4	140		2.23E+01	508
CL-4	358.6	140	100	7.90E-07	81
	358.6	140		5.80E-06	96
	358.6	140		3.45E-03	103
	358.6	140		2.15E+01	101
CL-5	425	140	55	6.70E-07	45
	425	140		1.07E-06	47
	425	140		5.10E-05	61
	425	140		1.83E+01	53

15 = Averaged secondary r- factor

Indicates point location with secondary r-factors

As in the previous analysis, no single r-factor was attained that consistently reproduced similar results to the initial r-factor/K combination, with error values again extending above 40%.

Results:

Examination of both BIOCHLOR simulations showed similar error values when using the secondary r-factor values. However, the difference between the BIOCHLOR simulation errors and the 3D analytical solution errors are significantly different (an order of magnitude or more) and support the use of the 3D analytical solution as the best predicative method for the Site.

Based on these variations, it does not appear that multiple unique solutions can be attained for a single model solely by adjusting the K and r-factor.