VERIFICATION DOCUMENT
FOR
HWIR99 VADOSE ZONE MODULE

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Acknowledgments

A number of individuals have been involved with the verification of the vadose zone module. Dr. Zubair A. Saleem of the U.S.EPA, Office of Solid Waste, provided overall technical coordination and review throughout this work. The vadose zone module was verified using an independent fate and transport module, MODFLOW-SURFACT (HydroGeoLogic, 1996). Mr. Patrick Sullivan of HydroGeoLogic, Inc. performed the module verification tests and this report was prepared by Dr. V. Guvanasen and Mr. P. Sullivan.

1.0 BACKGROUND

The HWIR99 (U.S. EPA, 1999b) Vadose Zone module simulates infiltration and contaminant transport between the top of the vadose zone and the water table.

The flow in the vadose zone is steady-state and one-dimensional in the vertical dimension toward the water table. The upper boundary starts just underneath the waste management unit (WMU), the lower boundary of the vadose zone is the water table. The flow into the vadose zone is predominantly gravity-driven. Therefore, the vertical flow component accounts for all the fluid flux between the WMU and the water table. The flow rate is determined by the long-term average infiltration rate through the waste management unit.

Contaminants are transported in the vadose zone by advection and dispersion. The vadose zone is assumed to be initially free of contaminants, and it is assumed that contaminants migrate vertically downward. The Vadose Zone module simulates transient transport. Although the Vadose Zone module can accommodate single and multiple species chain decay reactions with linear or nonlinear sorption, a single species with linear sorption is simulated in the verification example.

2.0 VERIFICATION PLAN

The verification of the Vadose Zone module employed a flow and transport code, MODFLOW-SURFACT (HydroGeoLogic, 1996). The verification process focused on two main components:

1. Contaminant concentration.
2. Water pressure (saturation) profile.

The verification plan was executed using site and chemical specific SSF and GRF files for HWIR99 Setting LF0223504 (see Appendix A, Table 1).

MODFLOW-SURFACT (MS-VMS) (HydroGeoLogic, 1996) is a fully integrated groundwater flow and solute transport code that is based on the U.S. Geological Survey modular 3-D groundwater flow modeling code, MODFLOW (McDonald, 1988). Although the MODFLOW-SURFACT is a fully 3-D code, the verification problem is posed to simulate the 1-D vertical flow and transport that is simulated by the Vadose Zone module.

3.0 SOFTWARE VERIFIED AND DATA USED

The Vadose Zone module is written in FORTRAN 77/90 and extracted from the EPA's Composite Model for Leachate Migration with Transformation Products (EPACMTP)(U.S. EPA, 1996) code. EPACMTP is a fate and transport code that incorporates advection, hydrodynamic dispersion, linear or nonlinear sorption, branch-decay, and chain-decay reactions. A rigorous description and derivation of the code is summarized in The Vadose and Saturated Zone Modules Extracted from EPACMTP for HWIR99 (US EPA, 1999-a). The module input data and parameters used for the verification case were generated using FRAMES HWIR99 for Benzene with a landfill source type at site setting 0223504. The databases and software versions used were: beta 2 database Version 14, National database Version 0, Met data Version 2, lfo 7batch 1-11, and HWIR Update 56 (US EPA 1999-b).

4.0 VERIFICATION DESCRIPTION

4.1 PROBLEM DESCRIPTION

The Vadose Zone module simulates vertical flow and transport through unsaturated soil. The 1-D domain is basically a unit area tube with a top boundary at the bottom of the source zone and a bottom boundary at the water table. The top of the domain has a prescribed flow boundary where the water flux is the long-term average infiltration, as calculated from the source module. The mass loading to the top boundary is determined from the leachate flux from the source module. At the bottom boundary the concentration gradient and the hydraulic head are zero.

4.2 VERIFICATION OF CONTAMINANT CONCENTRATION

The module was run for Benzene with a landfill source at site setting 0223504 to generate the input parameter values for the verification model(MODFLOW-SURFACT) as well as the Vadose zone module output. Identical parameter values defining the site and chemical were used for Vadose Zone module and MODFLOW-SURFACT. The parameters values used by both codes is shown in Tables 1a-c of Appendix A.

The verification model employed a block centered grid discretization with the center of the top block at the top of the vadose zone and the center of the bottom block at the water table. The grid for MODFLOW-SURFACT was considerably more refined than the grid scheme in the Vadose Zone module, due to the fully 3-D solution of MS-VMS.

In FRAMES HWIR99, the mass loading from the source module is in the form of mass per area per time. The top boundary condition in the MS-VMS simulation required contaminant concentrations and fluid flux rates, so the mass loading rate was converted into discrete concentration using the long term average infiltration rate. The long term average infiltration rate was calculated as the time-average rate of annual average infiltration rates determined by the source module.

The breakthrough curves for the Vadose Zone module and the verification code are shown in Figure 1.

4.3 VERIFICATION OF PRESSURE PROFILE

The pressure profiles for the problem described above were obtained for the FRAMES (MMSP) Vadose Zone module by modifying the code to output the pressure heads at each grid node. This was an available feature in MODFLOW-SURFACT. The resulting pressure profiles are shown in Figure 2.

5.0 SUMMARY OF VERIFICATION RESULTS

The verification of the Vadose Zone module was performed in two parts: the verification of the transport, and pressure head profile. The transport was verified by producing similar breakthrough curve results with the Vadose Zone module and separate fate and transport code, MODFLOW-SURFACT. The Breakthrough curves from both codes is shown in Figure 1. The time of arrival of the peak concentration is the same and the Vadose Zone module is slightly conservative ($(C_{vadose} - C_{MS\text{-}VMS}) / C_{Max} \times 100 = 2.94\%$). The pressure head profile was verified in a similar manner, by plotting the pressure head at each grid node and is shown in Figure 2. The results from both portions of the verification process are in close agreement.

6.0 REFERENCES

HydroGeoLogic. MS-VMS Software (Version 1.2) Documentation. HydroGeoLogic, Inc., Herndon, VA, 1996.

McDonald, M.G. and Harbaugh, A.W. A moduler three-dimensional finite-difference groundwater flow model: U.S. Geological Survey Techniques of Water-Resources Investigations Book 6, chapter A1. 1988.

U.S.EPA. EPA’s Composite Model for Leachate Migration with Transformation Products, EPACMTP. Background Document, Office of Solid Waste, U.S.EPA, 1996.

U.S.EPA. The Vadose and Saturated Zone Modules Extracted from EPACMTP for HWIR99, Office of Solid Waste, U.S.EPA, 1999-a.

U.S.EPA. Office of Research and Development. FRAMES-HWIR Technology Software System for 1999: System Overview. July, 1999-b.

APPENDIX A

INPUT PARAMETERS AND VALUES

Table 1a Input Parameters and Values

Parameter Name	Description	Value	Type	Unit
ChemADiff	Air Diffusion Coefficient	0.083876343	FLOAT	cm^2/s
ChemAerBioRate	Aerobic Biodegradation rate	0	FLOAT	1/day
ChemAnaBioRate	Anaerobic Biodegradation	0	FLOAT	1/day
ChemHLC	Henry's Law Constant	0.003541062	FLOAT	(atm m^3)/mol
ChemHydRate	Catalyzed Hydrolysis	0	FLOAT	1/day
ChemKd	Partition Coefficient for Med	1.605821024	FLOAT	L/kg
ChemKoc	K_{oc}	51.56699019	FLOAT	mL/g
ChemKow	K_{ow}	107.7387131	FLOAT	
ChemSol	Solubility for each media	28091.53811	FLOAT	mg/L
ChemSolCw	Solid Waste Cw's for chemical	1, 10, 1000, 10000, 100000	FLOAT	ug/g
DISPR	Longitudinal Dispersivity	0.07368	FLOAT	m
NumChem	Number chemicals described	1	INTEGER	
POM	Percent Organic Matter	3.8	FLOAT	g/g
RHOB	Bulk Density of Soil	1.4575	FLOAT	g/cm^3
TermFrac	Peak output fraction for simulation termination	0.01	FLOAT	fraction
VadALPHA	soil retention parameter alpha	0.021061994	FLOAT	1/cm
VadBETA	soil retention parameter beta	1.407857344	FLOAT	unitless
VadID	Environmental Setting Id for Aquifer	LF0223504	STRING	
VadLWSIndex	LWS Index for vadose zone	1	INTEGER	
VadPh	Average Vadose Zone pH	6.203353939	FLOAT	pH units
VadSATK	saturated hydraulic conductivity	0.099139425	FLOAT	cm/hr
VadTemp	Average Vadose Zone Temperature	12.5	FLOAT	degrees Celsius
VadThick	Vadose zone thickness	2.44	FLOAT	m
VadWCR	residual water content	0.069926818	FLOAT	L/L
VadWCS	saturated water content	0.45	FLOAT	L/L
AnnInfil	leachate infiltration rate	see Table 1b	FLOAT	m/d
LeachFlux	leachate contaminant flux	see Table 1c	FLOAT	$g/m^2/d$

Table 1b AnnInfil Values

Year	Infil (m/d)	Year	Infil (m/d)
1	0.002514828	9	0.002794619
2	0.002028211	10	0.002424609
3	0.001668433	11	0.002448446
4	0.002843175	12	0.002697006
5	0.002569474	13	0.002203096
6	0.002945244	14	0.002119414
7	0.002860521	15	0.002746304
8	0.002481776	16	0.004581293

Table 1c LeachFlux Parameter Values

Year	Leach Flux ($g/m^2/d$)	Year	Leach Flux($g/m^2/d$)	Year	Leach Flux ($g/m^2/d$)	Year	Leach Flux ($g/m^2/d$)
1	4.86E-07	51	0.712844483	101	0.61206551	151	0.513377349
2	0.003145479	52	0.709150057	102	0.610393199	152	0.51068356
3	0.037011696	53	0.704882674	103	0.609253656	153	0.508223079
4	0.099960279	54	0.70133243	104	0.607378802	154	0.505769673
5	0.168120682	55	0.697776656	105	0.606248839	155	0.503031788
6	0.231113468	56	0.694216619	106	0.604414828	156	0.500761838
7	0.286446647	57	0.6913152	107	0.603048095	157	0.497870477
8	0.338369707	58	0.687807994	108	0.601463355	158	0.495589294
9	0.385122548	59	0.685292354	109	0.599754919	159	0.492752929
10	0.430577553	60	0.682054858	110	0.59843058	160	0.490268131
11	0.472895287	61	0.67960452	111	0.596460595	161	0.487651498
12	0.514041625	62	0.676866443	112	0.595205393	162	0.484896935
13	0.553798039	63	0.674291259	113	0.593193562	163	0.482496205
14	0.591808993	64	0.67210324	114	0.591753161	164	0.479556665
15	0.629735293	65	0.669420873	115	0.589933812	165	0.477209072
16	0.665577017	66	0.667596614	116	0.588158949	166	0.474272186
17	0.701840196	67	0.664998219	117	0.586606439	167	0.471777798
18	0.73635911	68	0.663236885	118	0.584529698	168	0.46902795
19	0.770959429	69	0.660978587	119	0.583102688	169	0.466283327
20	0.804722494	70	0.659051653	120	0.580911433	170	0.463766799
21	0.837762636	71	0.657264815	121	0.579361654	171	0.460816713
22	0.870956249	72	0.655135308	122	0.577299825	172	0.458410144
23	0.902772982	73	0.65371209	123	0.575441394	173	0.455414781
24	0.935274983	74	0.651529555	124	0.573638893	174	0.452922175
25	0.966363946	75	0.650198135	125	0.571456408	175	0.450072483
26	0.997949359	76	0.648218688	126	0.569828438	176	0.447359879
27	1.025587169	77	0.646721048	127	0.567471176	177	0.444745649
28	1.022274154	78	0.645135712	128	0.565788761	178	0.441818043
29	0.989959012	79	0.643379096	129	0.563495381	179	0.439360264
30	0.951449408	80	0.642157167	130	0.561546287	180	0.436346285
31	0.918811413	81	0.640242338	131	0.559490726	181	0.433863517
32	0.892584278	82	0.639152499	132	0.557212647	182	0.430949016
33	0.870469172	83	0.637317488	133	0.555369777	183	0.428285509
34	0.852662509	84	0.636085765	134	0.55287036	184	0.4255943
35	0.836260032	85	0.634561484	135	0.551042211	185	0.422716859
36	0.822921173	86	0.633042923	136	0.548542491	186	0.420216272
37	0.810079456	87	0.631872586	137	0.546502547	187	0.417219734
38	0.799252723	88	0.630116135	138	0.544206459	188	0.414752034
39	0.789058146	89	0.629119643	139	0.541848722	189	0.411807776
40	0.779750597	90	0.627332958	140	0.539789889	190	0.409205366

Table 1c LeachFlux Parameter Values (continued)

41	0.771598819	91	0.626235677	141	0.53717837	191	0.406460006
42	0.763387361	92	0.624670544	142	0.535199555	192	0.4036548
43	0.756668852	93	0.623282592	143	0.532528396	193	0.40112075
44	0.749470805	94	0.622049273	144	0.530401602	194	0.398172852
45	0.743600688	95	0.620366938	145	0.527889796	195	0.395723403
46	0.737485144	96	0.619345076	146	0.525471149	196	0.392782929
47	0.732045895	97	0.617537697	147	0.523205934	197	0.390248839
48	0.727008332	98	0.61646719	148	0.520514986	198	0.387473615
49	0.721843296	99	0.614789891	149	0.518387132	199	0.384757132
50	0.717662946	100	0.613446291	150	0.515584845	200	0.38220017

FIGURES

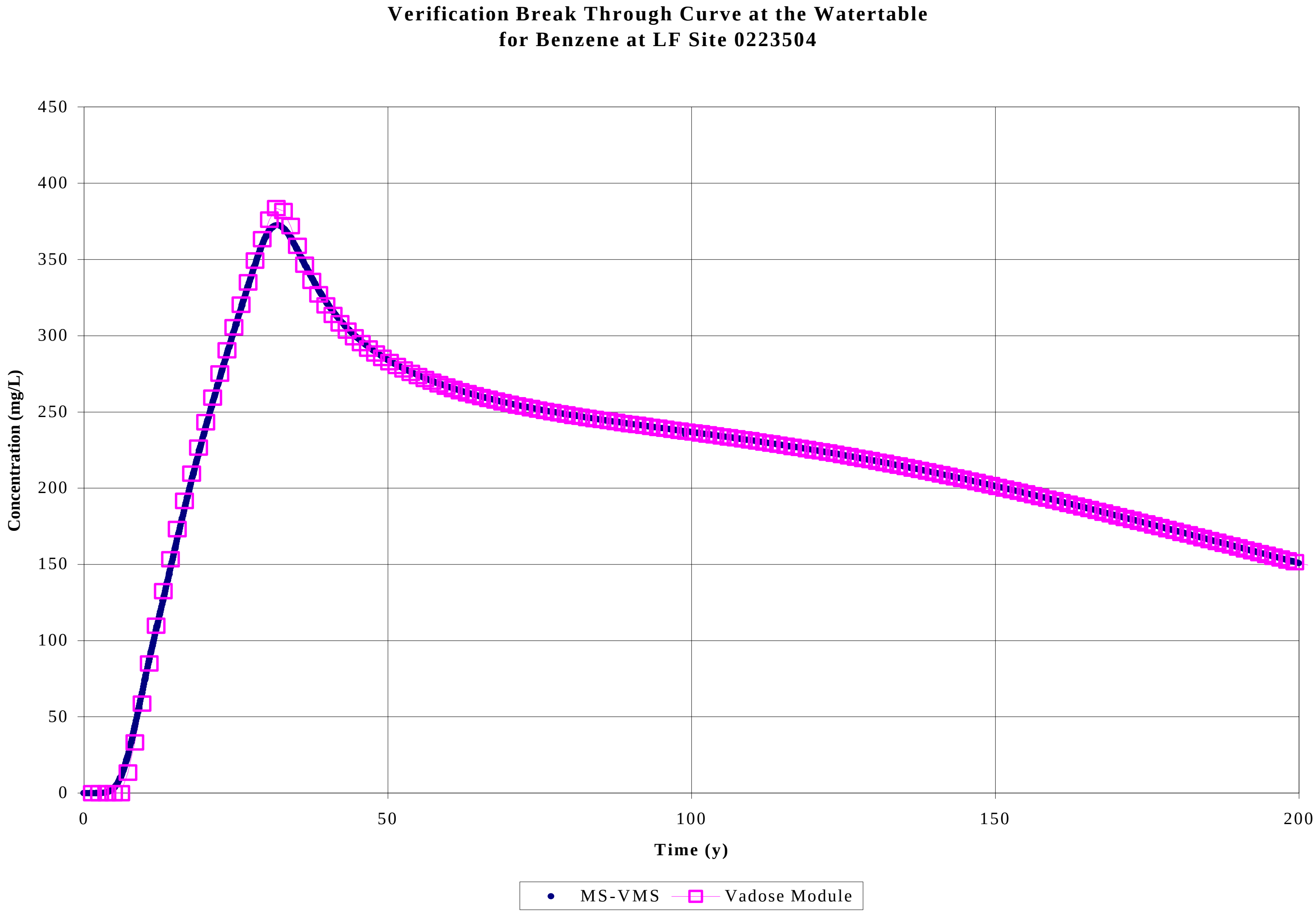

Figure 1. Breakthrough Curve at the Water Table for Vadose Zone Module and Verification Code (MS-VMS) at site LF0223504 for Benzene (source was terminated after time = 200 years).

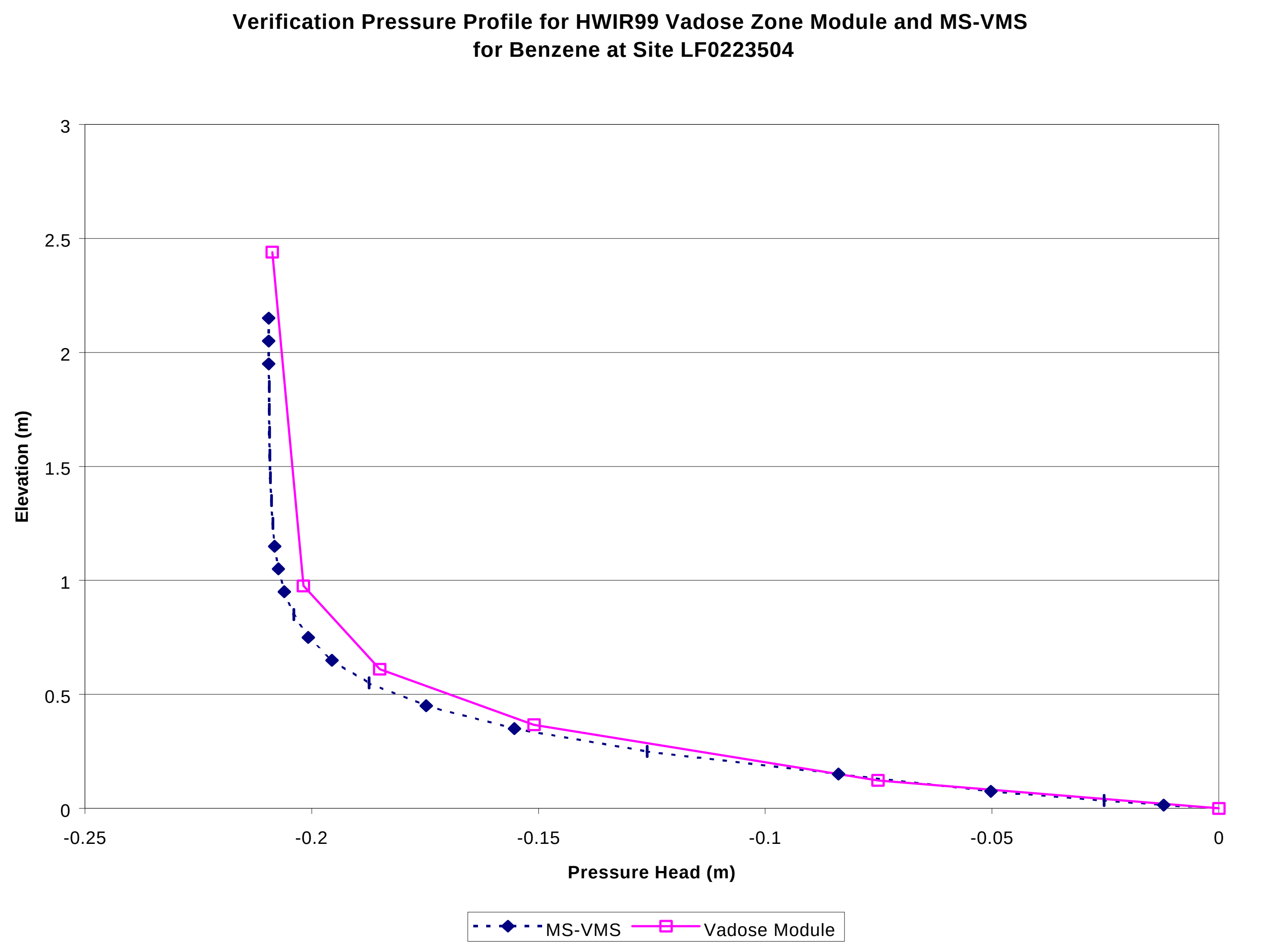

Figure 2. Pressure Head Profile for the HWIR99 Vadose Zone Module and verification code (MS-VMS) at site LF0223504 for Benzene.