Application of heuristic optimization techniques and algorithm tuning to multi-layered sorptive barrier design, Supporting Information

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Summary of text pages, figures, and tables

S.1 Multi-Layer Sorptive Landfill Liner Optimization In general, landfill leachate is composed of one or more contaminants that have a range of sorptive and chemical properties. As shown in Figure S1, leachate transport is mitigated by a sequence of one or more layers that form the landfill liner. The goal of liner design is to determine the liner configuration that minimizes leachate transport (preventing migration to human and/or animal receptors) at the lowest financial cost. In such problems, design variables include the number, ordering, and material composition of the layers; and in the considered problems, multiple sorptive layer amendments were considered.

[Figure S1 goes about here]

S.2 Taguchi DOE Method Figure S2 contains example factor interaction plots. In Figure S2a, factors A and B interact and the optimal factor-level settings would be A_2 and B_2, corresponding to the peak point of the four interaction lines. In Figure S2b, none of the lines intersect, suggesting that no interaction is occurring. In this case, the optimal factor-level settings for C and E would be assigned using main-effects analysis.

[Figure S2 goes about here]

S.3 Views of the Design Space A primary justification for the use of heuristic (global search) algorithms to solve the considered multi-layer sorptive landfill liner problems is the presence of multiple local minima, as illustrated by the one-dimensional slices of design space plotted in Figure S3.

[Figure S3 goes about here]

S.4 Solute Transport Model The movement of leachate through a multi-layered sorptive landfill liner can be modeled as transient one-dimensional solute transport through low-permeability sorptive material(s). Assuming equilibrium sorption, the governing

advective-dispersive-reactive (ADR) equation for transport of a single solute through a single layer is given in Equation S1.

$$\frac{\partial C}{\partial t} = -v\frac{\partial C}{\partial z} + D\frac{\partial^2 C}{\partial z^2} - \frac{\rho_b}{n}\frac{\partial S}{\partial t} \quad \text{(S1)}$$

where C is the aqueous phase leachate (either TCE, Benzene, or 1,2-DCB, depending on liner problem) concentration [mg/L], t is time [s], z is the distance from the top of the layer [m], v is the fluid velocity [m/s], D is the dispersion coefficient, incorporating both hydrodynamic dispersion and molecular diffusion [m^2/s], ρ_b is the bulk dry density of the layer material [kg/m^3], n is the porosity of the layer material [dimensionless], and S is the sorbed phase leachate concentration [mg/kg]. As written, the ADR equation contains two unknowns (aqueous and sorbed concentrations) and isotherm expressions describing the partitioning of solute between these two phases are used to close the system. For a given combination of sorptive amendment and solute, isotherm selection (e.g. Langmuir, Freundlich or Linear) and configuration of relevant isotherm parameters is accomplished by regression against experimental data, as reported in Bartelt-Hunt et al. (*1*). When multiple layers consisting of different sorptive material compositions are considered, the sorption isotherms and parameters are spatially variable and numerical solution of the ADR equations is required. Therefore, leachate transport was solved numerically using a version of the MOUSER (*2*) software, modified to support multiple layers. The following boundary and initial conditions were applied: the top of the liner was treated as a constant 10 mg/L source of leachate while the concentration just below the liner and the initial concentration within the liner were set to 0 mg/L. Usage of a zero concentration boundary below the liner induces a maximum diffusive gradient, corresponding to a worst-case transport scenario in a diffusion-dominated system, and results in conservative

liner designs (*3*). Due to differences in the material properties of their respective contaminants (benzene, 1,2-DCB or TCE), the three considered problems yielded different optimal liner configurations. Relevant characteristics of these contaminants are: sorption behavior with respect to each sorptive amendment (defined in terms of empirical isotherm parameters), solubility, and liquid diffusion coefficient. Assumed values for these characteristics were taken from previously published studies (*1*, *4*).

S.5 Overview of experimental approach Figure S4 provides an overview of the numerical experiments performed in the study. As shown in the figure, a given heuristic algorithm searched for the optimal liner design by performing repeated executions of a solute transport model. Transport output was forwarded to a constraint-integration step that determined whether the given design violated constraints, in which case the design was considered infeasible and a penalty was assessed to the overall liner cost. Overarching the optimization process was a set of Taguchi DOE tuning experiments, where analysis of algorithm performance provided the optimal configuration of algorithm and penalty parameters. After completing the DOE experiments, tuned algorithms were utilized in a set of confirmation optimizations and these results facilitated a rigorous comparison and evaluation of the various algorithms with respect to each of the three organic solutes.

[Figure S4 goes about here]

S.6 Summary of Numerical Experiments Transport simulation was performed using an explicit finite-difference time-step formulation coupled with an operator splitting technique, and in which each layer is spatially discretized into 10 grid cells. Equilibrium sorption was assumed in all simulations, and a typical simulation of 100 years of leachate

transport required 0.8 seconds of computation time and had a mass balance error of less than 5%. All optimizations were performed using OSTRICH (*5*) and experiment samples were run in parallel on Linux-based computing clusters maintained by the University at Buffalo Center for Computational Research (CCR). Access to the CCR clusters is via a Portable Batch System (PBS) resource manager and Maui scheduler, and programs are parallelized using the industry standard Message Passing Interface (MPI) specification (*6*). The utilized clusters consist of 32 1-GHz Intel Pentium III processors with 256-kB cache and 1-GB of 32-bit wide RAM, and 24 3.2-GHz Intel Pentium IV processors with 1-MB cache and 4-GB of 64-bit wide RAM. All processors run version 7.3 of the Red Hat Linux operating system. These parallel clusters were also utilized to perform an exhaustive search of the design space of all three problems, a process that established 'true' optimality for each of the considered problems.

S.7 Results Table S1 summarizes the optimal parameter settings and corresponding optimal performance for each algorithm and solute type.

[Table S1 goes about here]

Table S2 compares the tuning and main-effects confirmation runs against ANOVA-generated lower confidence limits on predicted performance.

[Table S2 goes about here]

Figure S5 compares the number of feasible designs having 4, 5, and 6 active layers, for each of the landfill liner design problems (distinguished by the type of organic solute).

[Figure S5 goes about here]

Literature Cited

(1) Bartelt-Hunt, S.L.; Smith, J.A.; Burns, S.E.; Rabideau, A.R. Evaluation of granular activated carbon, shale and two organoclays for use as sorptive amendments in clay

landfill liners. *J. Geotech. Geoenviron. Eng.* **2005**, doi: 10.1061/(ASCE)1090-0241(2005)131:7(848).

(2) Rabideau, A.J. MOUSER Version 1: Moderately User-friendly Reactive Transport Model; Department of Civil, Structural, and Environmental Engineering, University at Buffalo: Buffalo, NY, 2003. (available from www.groundwater.buffalo.edu)

(3) Rabideau, A.J.; Khandelwal, A. Boundary Conditions for Modeling Contaminant Transport in Vertical Barriers. *J. Environ. Eng.* **1998**, *124*, 1135-1141.

(4) Bartelt-Hunt, S.L.; Culver, T.B.; Smith, J.A.; Matott, L.S.; Rabideau, A.J. Optimal Design of a Compacted Soil Liner Containing Sorptive Amendments. *J. Environ. Eng.* **in press**.

(5) Matott, L.S. Ostrich: an Optimization Software Tool, Documentation and User's Guide, Version 1.6; Department of Civil, Structural, and Environmental Engineering, University at Buffalo: Buffalo, NY, 2005. (available from www.groundwater.buffalo.edu)

(6) Gropp, W; Lusk, W; Skjellum, A. *Using MPI: Portable Parallel Programming with the Message Passing Interface*, second edition; MIT Press: Cambridge, MA, 1999.

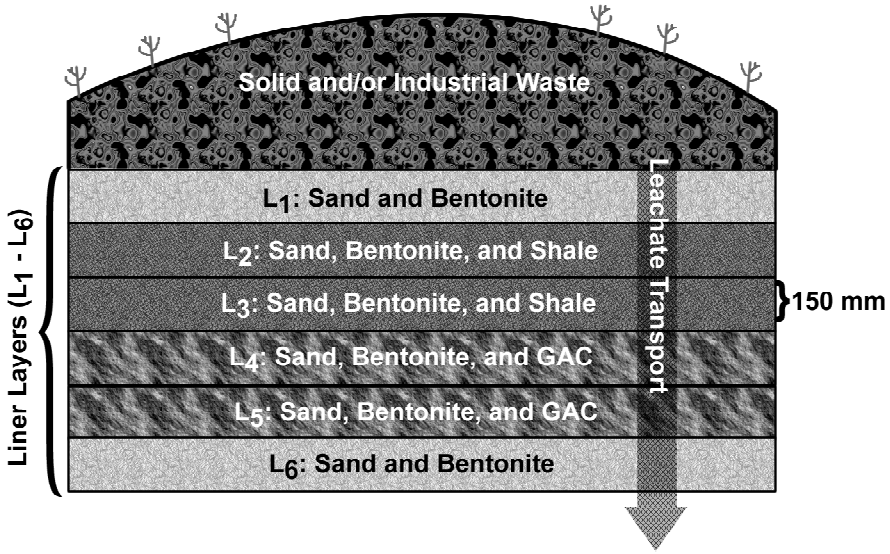

Figure S1: Example multi-layered sorptive landfill liner design

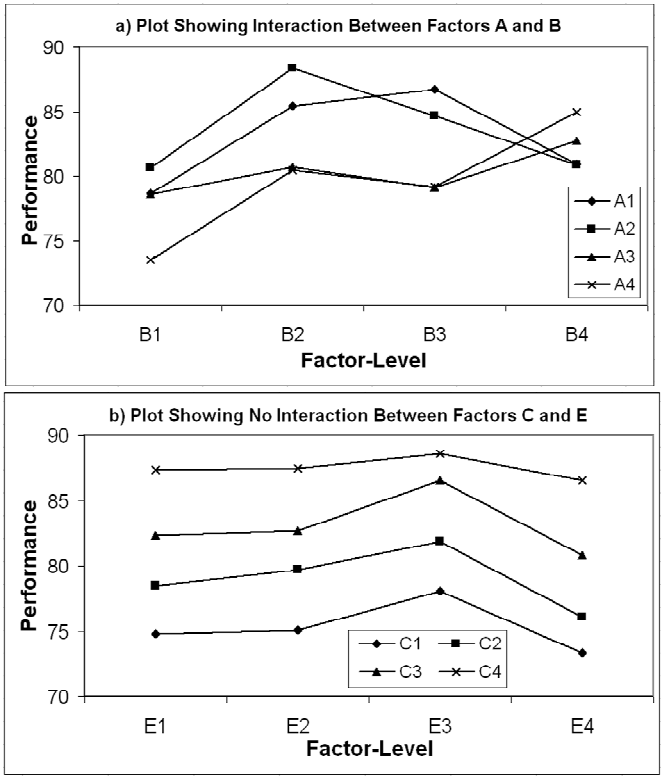

Figure S2: Illustrative factor interaction plots, (a) plot showing interaction between Factors A and B, (b) plot showing no interaction between Factors C and E

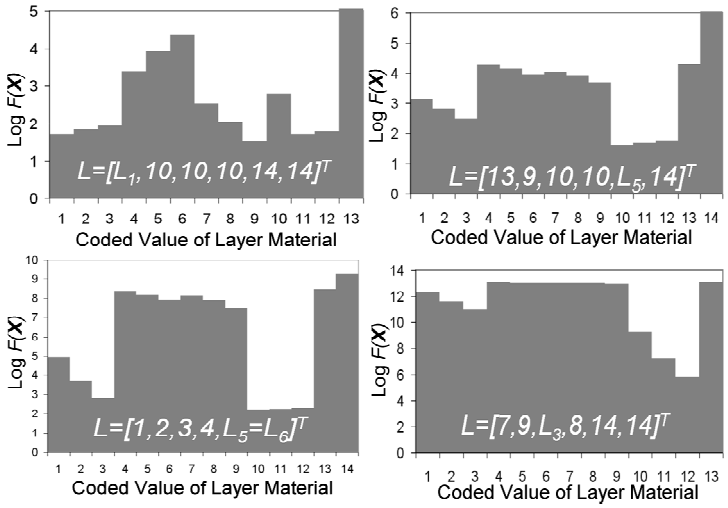

Figure S3: One dimensional slices of the design space highlighting the non-linear and discrete-valued nature of the sorptive barrier problem, as formulated in this study.

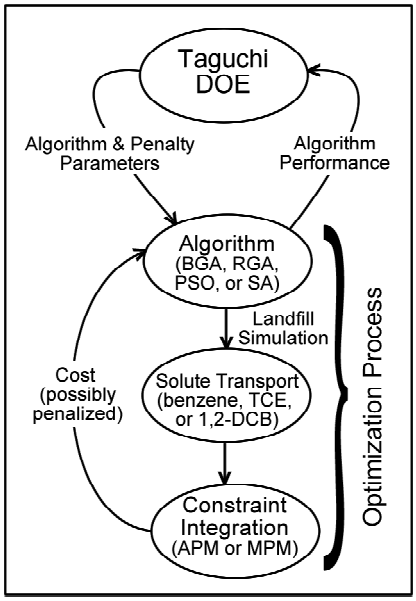

Figure S4: Overview of the Experimental Setup
(DOE = design of experiments, BGA = binary-coded genetic algorithm, RGA = real-coded genetic algorithm, PSO = particle swarm optimization, SA = simulated annealing, TCE = trichloroethylene, DCB = dichlorobenzene, APM = additive penalty method, MPM = multiplicative penalty method)

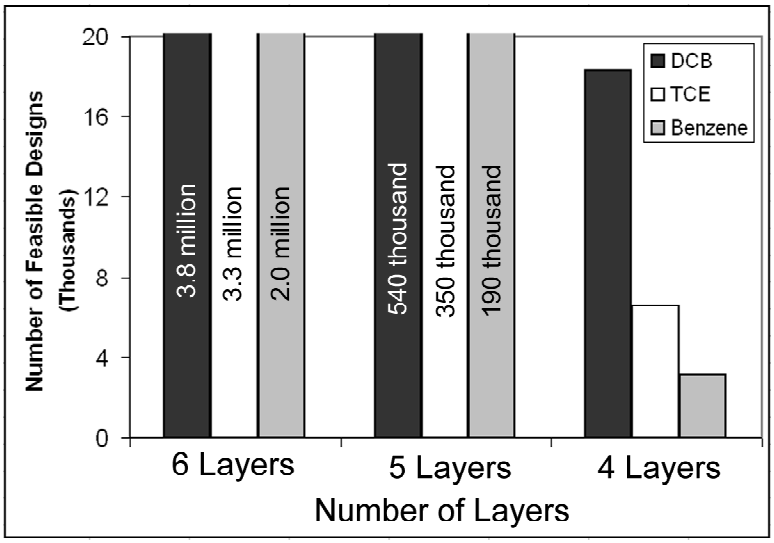

Figure S5: Feasible solutions as a function of the number of active layers

Table S1: Summary of tuned parameter settings

Binary-Coded Genetic Algorithm									
Solute	Penalty Method	Penalty Weight	Pop. Size	Number of Generations	Number of Elites	Mutation Rate	Perform-ance	System Cost ($/m2)	MOUSER Runs
Benzene	MPM	$1/ug	100	100	3	15%	95.00	$34.27	10,100
1,2-DCB	APM	$1/ug	50	20	3	15%	99.38	$16.66	1,050
TCE	APM	$1/ug	50	50	3	15%	98.55	$8.66	2,550
Real-Coded Genetic Algorithm									
Solute	Penalty Method	Penalty Weight	Population Size	Number of Generations	Number of Elites	Mutation Rate	Perform-ance	System Cost	MOUSER Runs
Benzene	MPM	$1/ug	50	50	3	15%	89.68	$41.86	2,550
1,2-DCB	MPM	$1/ug	100	50	3	15%	97.37	$16.66	5,100
TCE	MPM	$1/ug	50	50	3	15%	87.16	$16.26	2,550
Particle Swarm Optimization									
Solute	Penalty Method	Penalty Weight	Swarm Size	Number of Generations	Inertia Weight	Cognitive Weight	Social Weight	Perform-ance	System Cost	MOUSER Runs
Benzene	APM	$1/ug	100	100	2	4	1	90.55	$38.00	10,100
1,2-DCB	MPM	$1/ug	50	20	2	1	4	99.48	$16.66	1,050
TCE	APM	$1/ug	100	50	2	4	4	97.39	$8.66	5,100
Simulated Annealing									
Solute	Penalty Method	Penalty Weight	Equilibration Steps	Temperature Reductions	Melting Trials	Cooling Rate		Perform-ance	System Cost	MOUSER Runs
Benzene	MPM	$10/ug	50	100	20	20%		88.27	$41.98	5,120
1,2-DCB	APM	$10/ug	50	100	20	20%		97.36	$16.66	5,120
TCE	APM	$1/ug	20	100	50	50%		87.36	$16.26	2,150

Table S2: Comparison of tuning results against lower confidence limit on predicted performance. Y_{main} and Y_{inter} are the confirmation performances of the main-effects and interaction tuning procedures, respectively, and Y_{LCL} is the lower confidence limit of the tuned performance.

Leachate Composition	Algorithm	Penalty Method	Y_{main}	Y_{inter}	Y_{LCL}	$Y_{main} > Y_{LCL}$?	$Y_{inter} > Y_{LCL}$?
Benzene	BGA	APM	90.00	95.00	92.95	no	yes
		MPM	90.00	95.00	90.19	no	yes
	PSO	APM	90.00	90.55	73.53	yes	yes
		MPM	86.09	90.09	82.70	yes	yes
	RGA	APM	81.02	88.73	84.49	no	yes
		MPM	80.77	89.68	83.38	no	yes
	SA	APM	88.42	88.88	93.68	no	no
		MPM	83.99	88.27	81.61	yes	yes
1,2-DCB	BGA	APM	98.66	99.38	83.16	yes	yes
		MPM	97.45	99.18	92.08	yes	yes
	PSO	APM	97.48	98.95	87.73	yes	yes
		MPM	98.68	99.48	89.36	yes	yes
	RGA	APM	94.84	97.27	91.38	yes	yes
		MPM	94.84	97.37	90.95	yes	yes
	SA	APM	97.05	97.36	95.34	yes	yes
		MPM	89.94	97.20	91.53	no	yes
TCE	BGA	APM	97.83	98.55	95.96	yes	yes
		MPM	87.80	99.10	100.68	no	no
	PSO	APM	94.95	97.39	92.12	yes	yes
		MPM	94.65	97.30	83.77	yes	yes
	RGA	APM	85.72	87.16	84.08	yes	yes
		MPM	85.71	87.16	87.01	no	yes
	SA	APM	83.41	87.36	82.75	yes	yes
		MPM	83.37	87.72	82.06	yes	yes
					Total	16	22
					Within	67%	92%