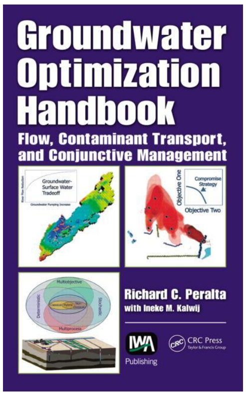

Groundwater Optimization Handbook
Flow, Contaminant Transport, and Conjunctive Management

Richard C. Peralta, Ineke M. Kalwij

Optimization with Uncertainty

Publication details
https://test.routledgehandbooks.com/doi/10.4324/9781439838068-8
Ineke M. Kalwij, Richard C. Peralta
Published online on: 26 Apr 2012

5

*Optimization with Uncertainty**

Ineke M. Kalwij and Richard C. Peralta

5.1 Introduction

Groundwater simulation models include values of physical and chemical parameters, assumed per field data, scientific literature, judgment, and calibration. Even so, uncertainties in subsurface lithology, stratigraphy, physical and chemical properties add to the complexity of system analysis and optimization. This text addresses parameter uncertainty, ignoring the uncertainty due to mathematically representing the physical system within a model.

Figure 5.1 illustrates possible outcomes of designing and implementing a contamination capture strategy. Figure 5.1a shows a contaminated plume approaching municipal wells. Required are a remediation well system and a pumping strategy that prevent the plume from reaching those wells. Figure 5.1b conceptualizes a well system designed via modeling to prevent the plume from entering a specified exclusion zone (a "forbidden zone" or area into which water that has concentration above maximum contaminant level [MCL] should not enter). The exclusion constraint is satisfied within the computer program. The concern is whether the constraint will be satisfied in the field.

Assume the well system is constructed and the pumping strategy is used. Figure 5.1c illustrates the situation in which the exclusion zone constraint is subsequently satisfied in the field. The plume does not enter into the exclusion zone, and the municipal well field is protected from contamination. Figure 5.1d illustrates a different outcome. The constraint is not satisfied in the field. The plume enters into the exclusion zone. Municipal wells become contaminated and cannot supply drinking water.

A likely cause of a Figure 5.1d outcome is the inherently uncertain knowledge of aquifer parameters and attendant assumptions. Uncertainties in subsurface heterogeneities, contaminant sources and extent, reaction pathways, and rates can profoundly affect physical system response to an implemented strategy. Simulation model uncertainty is viewed as the most significant

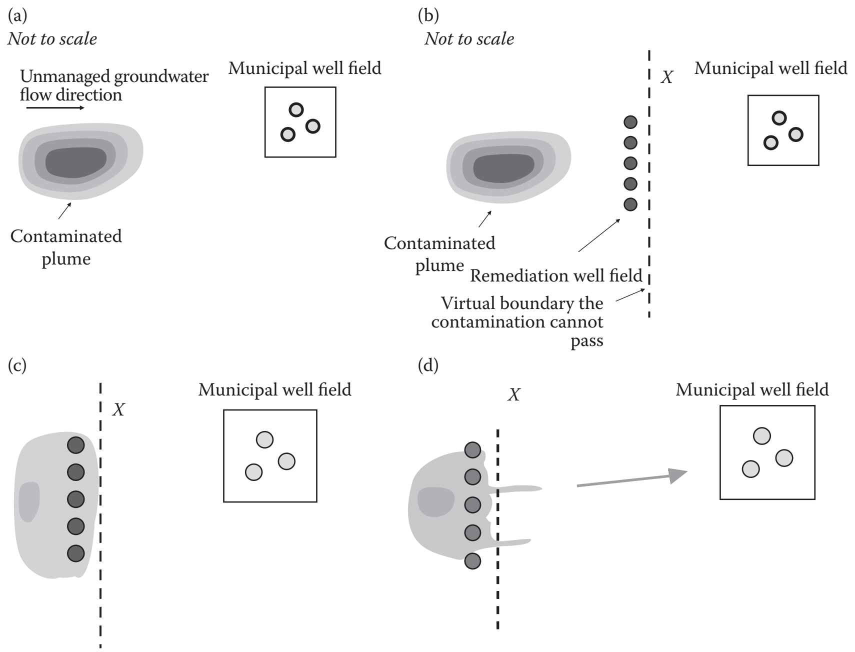

FIGURE 5.1
Plume migration uncertainty.

source of shortfall in deterministically designed strategies. A single deterministic simulation or optimization ignores, or does not directly consider, the modeler's uncertain knowledge of real system parameters.

After deterministic optimization, one usually considers uncertainty by performing sensitivity analysis on the computed optimal strategy. This involves using the optimal strategy in many different simulations. Each simulation addresses a different realization of the physical system, because each differs in assumed system input parameters. Each new realization can respond to the optimal strategy differently than the realization for which the optimal strategy was developed. Comparison and summary of these differences constitute a basic sensitivity analysis.

Sensitivity analysis identifies conditions under which implementing the optimal strategy in the field might not satisfy constraints that are satisfied in the original simulation model. Stated differently, it evaluates the effect of system uncertainty on the consequences of implementing a strategy developed while ignoring uncertainty.

The simplest and most commonly used way of creating alternative input values has no statistical significance. This statistical analysis method, sometimes termed robustness analysis, involves multiplying all values of one parameter type by a common factor (making a global change in those parameter values). A factor less than 1.0 reduces the magnitude of all such values by a common proportion. A factor greater than 1.0 increases the magnitudes proportionally. The robustness range of a strategy is the range of multiplication factors over which the strategy is expected to be successful in the field. For example, a strategy that satisfies constraints for hydraulic conductivity multiplication factors ranging from 0.85 to 1.6 has that conductivity robustness range. Aquifer hydraulic conductivity is the primary parameter affecting groundwater flow model simulation results.

The above-described process of sensitivity analysis, and robustness range determination is common where useful statistical information on system parameters is lacking. If the estimated strategy robustness is unsatisfactory, one can modify the strategy to try to improve its robustness. Without using S-O modeling, this involves iterative trial and error simulation modeling.

The rest of this chapter discusses tools for determining (Section 5.3.1), and enhancing the likelihood (Sections 5.3.2–5.3.5), that a strategy satisfies constraints (is feasible) in the field. Most of those tools employ statistical information, but not all.

5.2 Addressing Uncertainty

By using safety factors within deterministic optimization problem constraints, one can compensate somewhat for parameter uncertainty. For the Figure 5.1 problem, including a constraint to exclude (0.5 × MCL) contaminated water instead of merely MCL contaminated water, might cause the optimal strategy to pump enough to actually satisfy the exclusion constraint in the field. Determining the safety factor value is accomplished via trial and error or experience.

Presented in subsequent sections are alternative ways to develop strategies that may improve the likelihood of constraint satisfaction in the field. Largely because these methods can employ probabilistic information, they are more computationally intense than the safety factor approach. Fortunately, they are generally automated.

Postoptimization uncertainty analysis predicts a strategy's statistical reliability of satisfying optimization problem constraints in the field (Section 5.3.1). One determines reliability via an interative process akin to that of Section 5.1 (uncertainty analysis is similar to sensitivity analysis, but has more statistical rigor).

Section 5.3.2 shows automated uncertainty analysis with particle tracking to design practically optimal strategies without using formal optimization theory. Section 5.3.3 shows a formal stochastic optimization approach, the multiple realization approach that employs deterministic constraints for numerous realizations simultaneously. Section 5.3.4 shows another formal optimization approach. That chance-constrained optimization approach utilizes constraint(s) based upon probability distribution function(s), also termed stochastic constraints or chance-constraints. The Section 5.4 robustness optimization approach can improve either strategy are robustness or reliability, depending on whether adequate statistical data are available. It couples goal-programming optimization with model parameter sensitivity analysis.

Figure 4.1 illustrates how stochastic and robustness optimization techniques relate to other optimization techniques (deterministic, multiobjective, multimodel) and optimizer types (classical and nonclassical optimization types). For example, both deterministic and stochastic optimization methods can use a genetic algorithm optimizer to solve a mixed integer nonlinear problem. However, a stochastic method will differ from a purely deterministic approach by addressing the stochastic nature of one or more parameters.

In conclusion, if data are available to develop multiple statistically meaningful realizations, one would prefer using stochastic methods and optimization. However, the computation time involved in stochastic optimization is generally much greater than for deterministic optimization.

5.3 Stochastic Modeling Tools

5.3.1 Uncertainty Analysis

Uncertainty analysis is usually performed on an existing pumping strategy (nonoptimal or optimal), to determine the likelihood that the strategy will be successful, or unsuccessful, in the field, after it is implemented.

When possible, it is desirable to quantify uncertainty in terms of reliability. Reliability evaluation involves simulating the responses of different system realizations to the same set of decision variables or stimuli. Each different physical system realization is developed by changing one or more physical system assumptions stochastically based on a probability density function (PDF) or on other statistically derived information.

The Monte Carlo method usually uses random number generation and single or multivariate lognormal (Figure 5.2) or Gaussian PDFs. Evaluating the simulation results determines the proportion or percent yielding satisfactory system responses.

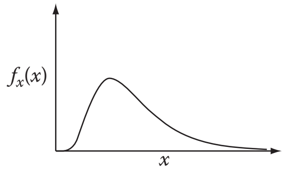

FIGURE 5.2
A lognormal probability density function.

Figure 5.3 illustrates six representative heterogeneous hydraulic conductivity fields for a hypothetical problem. These fields were generated for Layer 1 of a groundwater system consisting of two layers, eight rows, and six columns. For each model cell, a hydraulic conductivity value was stochastically developed by a random field generator (RFG). The RFG employed the geometric mean of the hydraulic conductivity, variance of the natural log of conductivity, and the correlation length and decay. RFG examples are the turning bands method, matrix inversion method, and fast Fourier transform method, to name a few.

Figure 5.4 summarizes a Monte Carlo procedure evaluating the reliability of an optimal pumping strategy (postoptimization analysis), assuming uncertain hydraulic conductivity. Each pass through the Monte Carlo

Realization 1

28.24	56.74	18.27	82.33	23.09	92.52
99.4	117.8	41.82	34.04	29.99	25.06
45.64	40.57	14.82	31.14	35.33	151.9
36.77	70.74	105.9	64.13	17.53	56.49
33.07	30.85	101.1	50.03	90.38	76
36.66	12.48	8.64	50.27	75.62	38.9
122.4	51.46	129.8	31.8	63.68	33.34
48.57	31.95	61.65	23.14	28.33	20.15

Realization 2

54.79	67.78	40.51	36.25	71.12	42.44
55.92	18.11	43.51	14.09	56.76	40.09
23.92	65.89	18.1	16.08	30.79	65.19
63.55	73.7	33.5	30.46	37.67	36.79
57.51	77.44	74.37	45.27	49.3	56.05
104.8	72.16	18.82	45.52	98.27	68.19
49.41	20.77	52.79	42.33	72.3	39.58
83.82	45.67	51.21	22.87	41.72	40.24

Realization 3

75.13	30.21	61.86	32.29	32.35	31.9
19.41	92.21	57.27	17.65	60.76	45.96
86.11	11.51	44.65	53.77	68.54	57.85
25.36	67.64	163.4	92.55	120	99.96
27.18	56.16	13.74	130.1	22.08	61.49
30.42	24.35	23.25	14.01	84.81	95.43
21.06	59.52	50.88	27.39	22.23	30.5
31.3	81.1	61.28	79.77	67.56	16.21

Realization 4

72.34	33.8	41.45	34.98	30.65	43.73
138.2	32.36	45.52	183.5	53.33	45.53
30.56	16.39	27.7	27.89	84.04	35.35
39.99	57.13	33.85	46.96	26.11	35.8
214.8	45.67	18.47	31.39	68.54	26.6
28.46	55.45	40.26	34.17	29.38	23.97
21.67	87.34	46.34	31.86	25.58	54.37
78.2	26.11	22.14	41.82	32.38	46.47

Realization 5

80.31	14.62	42.64	28.54	23.69	37.63
19.53	158.9	48.13	20.46	50.12	38.51
20.62	34.78	51.54	32.12	65.06	61.1
13.59	94.66	60.84	58.89	23.88	6.51
32.45	53.05	143.3	51.32	21.05	80.66
175.9	14.28	29.18	20.49	48.67	31.57
17.11	66.34	32.55	91.03	50.54	71.97
29.14	44.24	69.36	122.2	55.99	25.46

Realization 6

18.86	126.1	71.96	132.7	135.9	78.62
30.08	73.77	38.85	104.3	75.86	16.59
36.84	45.4	11.96	28.36	52.32	19.41
83.71	19.13	77.85	22.97	83.94	18.3
42.8	31.13	82.34	58.61	58.98	50.48
42.74	51.6	43.79	130.9	34.41	60.52
24.53	85.7	14.15	37.18	26.4	129.3
23.58	62.51	97.97	45.81	40.1	53.67

FIGURE 5.3
Randomly generated heterogeneous hydraulic conductivity fields.

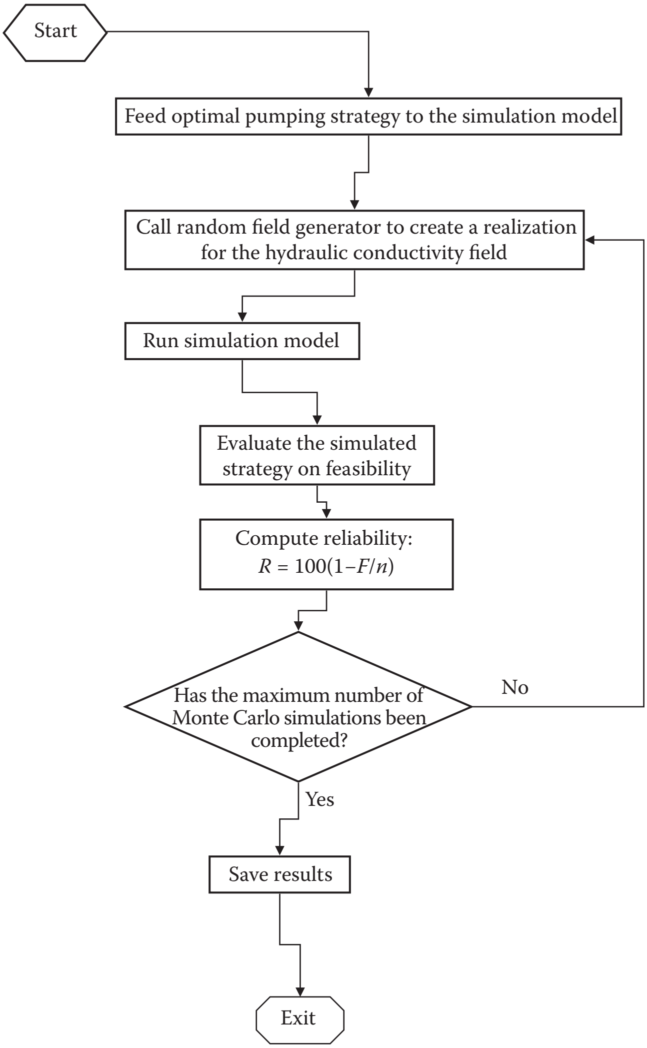

FIGURE 5.4
Monte Carlo simulations flowchart.

process generates a new hydraulic conductivity field (realization). Simulating the strategy in each pass can yield a different simulation output (system response). Each simulation output is evaluated to determine whether all optimization problem constraints are satisfied. If not, the strategy is considered a failure for that realization. Strategy reliability is based on the proportion of failures or successes (Equation 5.1).

$$R = \left(1 - \frac{F}{N}\right) * 100 = \left(\frac{S}{N}\right) * 100 \quad (5.1)$$

where R is the reliability in percentage (%), F is the total number of failures or infeasible strategies out of N Monte Carlo simulations, and S is the total number of successes or feasible strategies out of N Monte Carlo simulations.

Often, reliability is expressed as a proportion or probability value (i.e., sans multiplication by 100 in Equation 5.1). It is a function of the probability of failure or the probability of success, P{F} and P{S}, respectively.

In other words, a strategy's reliability is the percentage of statistically valid physical system realizations that it satisfies. If there are 300 failures in 1000 Monte Carlo simulations, the estimated pumping strategy reliability is 70%. In other words, the chance that the mathematically optimal pumping strategy will be feasible in the field is 70%.

The desired reliability is situation-dependent. Most deterministic strategy designs based upon a least-squares calibrated model are considered to have 50% reliability. Because reliability is not included within the objective function (OF) of a deterministic model, modifying a strategy to increase its reliability usually harms the OF value (OFV). Obtaining significantly greater reliability often causes significant OFV impact. To illustrate, assume the objective is to minimize pumping. Assume the OFV for the original 50% reliability strategy is 1300 m^3/d. To obtain a 75% reliability one might have to increase pumping to 1800 m^3/d. A 90% reliability strategy might require 2100 m^3/d.

5.3.2 Stochastic Risk-Based Particle Tracking Optimization

This optimization approach is implemented within a powerful commercial groundwater modeling package. It uses the brute force algorithm, parameter estimation optimization, and Monte Carlo modeling coupled with economic-risk analysis. For a remediation problem, the brute force algorithm systematically explores the best remediation well locations with respect to maximum particle removal within a specific time. The approach is initialized by simulating pumping rates for each well individually, followed by ranking the wells according to particle removal performance. Optimization proceeds with the well that ranks highest (i.e., captures the greatest number of mass weighted particles) by systematically incrementing the pumping rate until all particles are captured within a specified particle tracking travel time and subject to other constraints. If a single well cannot capture all particles without exceeding the specified constraints, further optimization using additional well(s) considers only particles not already captured. The approach systematically adds wells until a time or another mass capture percentage is achieved within the specified capture time or another stopping criterion is reached (e.g., maximum allowable number of wells is used).

Monte Carlo simulations are used to determine the probability of design and capture failure of an optimized remedial design (well configuration). Design failure occurs if one or more pumping wells go dry. Capture failure occurs if contaminant particles escape capture.

Parameter statistical input distributions for the Monte Carlo model are determined a priori by parameter estimation modeling. The determined probability of failure P{*F*} is input to an economic-risk analysis model. The P{*F*} impacts the cost-of-failure component of the total cost. This stochastic risk-based particle tracking optimization approach aided the successful design of a Kansas City plant interceptor system. A strategy that considered P{*F*} would be ultimately more cost-effective than not considering P{*F*}. The most economical system yielded a 65% P{*F*}. A more robust strategy would cost more to implement. This practical optimization approach quantifies the cost probability of failure and economic risk analysis, aiding in developing and negotiating a system design that is satisfactory to all involved stakeholders.

5.3.3 Multiple Realization Optimization

Each distinct representation of the physical system and boundary conditions is termed a realization or reality. Deterministic optimization models represent only one realization during optimization. The underlying assumption of multiple realization optimization is that reliability will be greater for a strategy developed to simultaneously satisfy the constraints of multiple realizations, than for a strategy created to satisfy the constraints of only one realization. A multiple realization stochastic model addresses uncertainty by simultaneously representing more than one possible reality of the physical system or boundary conditions within the optimization problem. For groundwater, it could include flow and transport equations for more than one realization during optimization. Applications of multiple realization approaches for solving groundwater management problems are numerous. In traditional multiple realization optimization, one cannot preselect the reliability to be achieved, until one has performed uncertainty analysis on at least some strategies.

Assume M^{real} sets of groundwater flow model input parameters of equal statistical validity (all having equivalent calibration statistics and being hydrogeologically reasonable). Conceptually, a multiple realization stochastic S-O model would arrange the constraints for each realization, one after the other. Figure 5.5 illustrates this concept for a constraint limiting the maximum concentration, $cmax_{\hat{o},k}$, existing in a particular region at a particular time. The S-O model includes M^{real} constraints (with M^{real} being the number of realizations). In other words, an S-O model solves the problem using the M^{real} realizations simultaneously, each embedded as a constraints in a model. Section 12.5 illustrates using the multiple realization approach with classical optimization to solve a hydraulic containment problem.

Figure 5.6 shows the multiple realization heuristic optimization process for solving a groundwater management problem. Assume uncertainty in

$[cmax_{\hat{o},k}] < cmax^{U}_{\hat{o},k}$ for Realization 1
$[cmax_{\hat{o},k}] < cmax^{U}_{\hat{o},k}$ for Realization 2
$[cmax_{\hat{o},k}] < cmax^{U}_{\hat{o},k}$ for Realization 3
…
$[cmax_{\hat{o},k}] < cmax^{U}_{\hat{o},k}$ for Realization M^{real}

FIGURE 5.5
Multiple realizations.

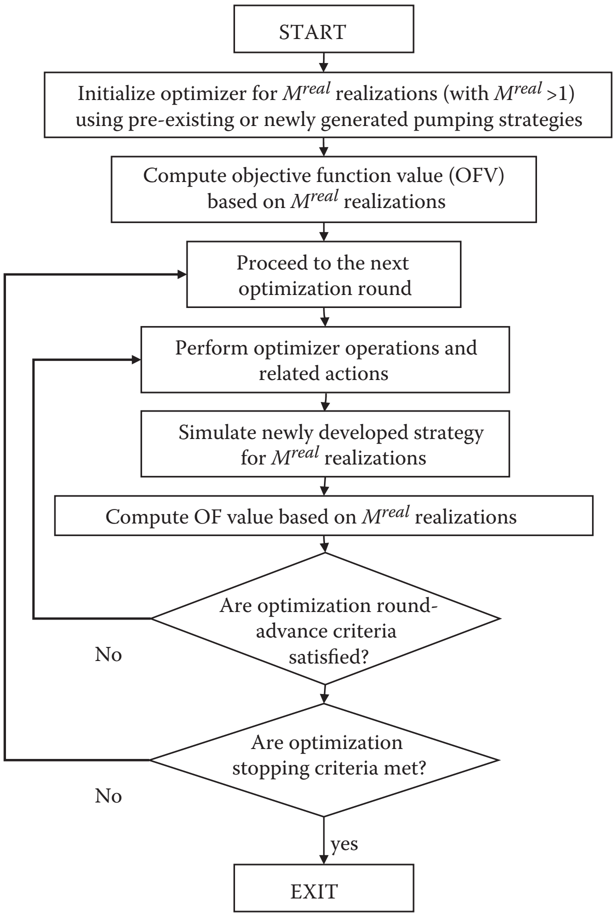

FIGURE 5.6
Multiple realization heuristic optimization flowchart. (Modified from Kalwij, I. M. and Peralta, R. C., *Ground Water*, 44(4), 574–582, 2006.)

hydraulic conductivity. Implementing heuristic optimization using M^{real} realizations means that each pumping strategy is applied M^{real} times, once per realization. The result is M^{real} different simulated system responses.

During optimization, the OFV is penalized (worsened) if one or more realizations yields an infeasible strategy. Optimizer operations (such as GA crossover and mutation) produce new strategies from old strategies. The optimization terminates per stopping criteria. The optimizer will try to create an optimal strategy based on M^{real}-realization optimization that is feasible for each of those M^{real} realizations. The strategy might not be feasible for a different newly developed conductivity field (i.e., one not used during the optimization).

Generally, the greater the number of simultaneous realizations included during optimization, the more reliable the optimal strategy. However, there is a trade-off between targeted and the reliability and computational time. At some point, the gain in reliability due to increased number of realizations is outweighed by the increased computational time or cost.

A multiple realization stochastic optimization problem is much larger than the original deterministic optimization problem. The computational load of including constraint sets for all additional realizations often limits how many realizations are utilized. For one California site, optimizing a pump-and-treat system design by increasing the number of realizations beyond 10 would not significantly increase strategy reliability, but would significantly increase optimization problem complexity and computational time.

The multiple realization technique provides a more realistic stochastic strategy than a chance-constrained approach (discussed next). However, the multiple realization approach requires larger optimization problems.

5.3.4 Chance-Constrained Optimization

The chance-constrained optimizer is another approach for reducing the probability that a constraint that is satisfied within a computer model will not be satisfied in the field. This approach allows the user to specify, before optimization, the desired reliability. Equation 5.2 applies to continuous variables such as concentration and head. For example, it can assure. An example of applying Equation 5.2 is that there is a greater than at least R^L probability that concentration $cmax_{\hat{o},k}$ does not is less than the upper bound $cmax^U_{\hat{o},k}$, (for example, at least 80% probability that $cmax_{\hat{o},k}$ does not exceed a 5 ppb upper limit). Following Chien et al (2002):

$$P[\Psi_i \le \Psi_i^U] = R \ge R^L \quad (5.2)$$

$$R = (1 - P\{F\}) \quad (5.3)$$

where $P[\Psi_i < \Psi_i^U]$ is the probability that $\Psi_i < \Psi_i^U$ (i.e the reliability R that the constraint is satisfied), are state variable value and the upper bound on variable, respectively, and $P\{F\}$ is the probability of failure (infeasibility). When R equals R^L within the model, the constraint has the specified R^L reliability of being satisfied in the field.

Reformulating Equation 5.2 as a deterministic equivalent, yields the chance constraint Equation 5.4.

$$E[\Psi_i] + V_{scd}^{-1}(R)\sigma[\Psi_i] < \Psi_i^U \tag{5.4}$$

where $E[\Psi_i]$ is the expected value for Ψ_i, $V_{scd}^{-1}(R)$ is the value of the inverse of the standard-normal cumulative distribution function (cdf) when R is the reliability, and $\sigma[\Psi_i]$ is the standard deviation of Ψ_i. The inverse cdf is also termed the quantile function. It is the cdf value pertaining to reliability R.

For example, a chance-constraint formulation for the $cmax_{\hat{o},k}$ employed in Figure 5.1 is

$$E[cmax_{\hat{o},k}] + V_{scd}^{-1}(R)\sigma[cmax_{\hat{o},k}] < cmax_{\hat{o},k}^U \tag{5.5}$$

Clearly, chance constraint optimization allows developing a remediation strategy designed to meet the decision maker's reliability preference. Multiple realization optimization does not have this preoptimization specification capability. However, the consensus is that chance-constrained optimization is overly restrictive or conservative in results.

As does multiple realization optimization, chance constrained optimization relies on the ability to quantify random processes and establish a PDF. Determining a reasonable PDF requires a significant amount of field data, which is often not available due to cost for most real-world problems. For this reason most groundwater S-O model projects perform postoptimization sensitivity analysis and do not perform stochastic optimization. The next section presents an innovative optimization approach that incorporates elements of sensitivity analysis in S-O modeling.

5.4 Robustness Optimization

The robustness optimization approach was designed for situations in which (a) one wants to increase the likelihood that the strategy will be successful in the field without harming the primary OF value, but (b) one might or might not have sufficient information to develop a PDF or multiple statistically equivalent realizations.

The implemented patented robustness enhancing optimizer (REO) couples S-O modeling with model parameter sensitivity analysis to guide multiple realization optimization. During processing, REO automatically filters out possible management strategies that will not yield a robust result.

Assuming a single uncertain parameter, the robustness range of a pumping strategy is the range of global multipliers applied to that parameter for which the strategy is feasible. For a multiplier (and its resulting realization), a strategy is considered feasible if the results of simulating the strategy satisfy all optimization problem constraints. Here realizations are identified using numbered subscripts. Realizations R_1 and R_2 should not be confused with reliability R.

Maximizing a robustness range requires pumping strategy modifications. Figure 5.7 shows the REO process for one parameter and two realizations. (One of the two realizations, for example R1, can be the realization for which a deterministic strategy is successful.) The model initializes with the identification of the parameter(s) for which the robustness range is to be maximized. Then the user provides or the model generates strategies (sets of decision and state variable values). REO evaluates these initial strategies based on feasibility and OF value. The strategy with the best primary OF value (e.g., cost) is identified.

At least one initial strategy must be feasible for at least one realization before a robustness range can be determined. As mentioned above, each realization is created deterministically by globally multiplying the parameter's calibrated spatially distributed values by an assumed factor smaller than or larger than one (respectively representing global proportional reductions or increases in array values). Within its innermost loop, REO does this to make new realizations. Hence, the realizations represented by R_1 and R_2 change during optimization.

REO can employ as few as two realizations, one at each end of a changing robustness range, although it can employ more for multiple parameters. REO assumes that if a strategy is feasible for realizations at both ends of a robustness range, it is feasible for all realizations within the range. Realizations R_1 and R_2 result from using parameter multipliers ≤1 and ≥1, respectively.

Figure 5.7 shows that, after robustness evaluation, the heuristic optimization conditions the pumping rates to give a greater robustness range. Conditioning employs goal programming and modifies the pumping rates to cause previously tight critical constraints to become as loose as possible. The fact that this expands the robustness range is manifest in the next REO loop, when REO again evaluates the robustness range of the best pumping strategy.

After completing an optimization round, the feasibility of developed strategies is determined. If at least one strategy is feasible for at least one of the two realizations, robustness evaluation occurs. REO proceeds to the next optimization round and repeats the process until no further robustness range increases are possible.

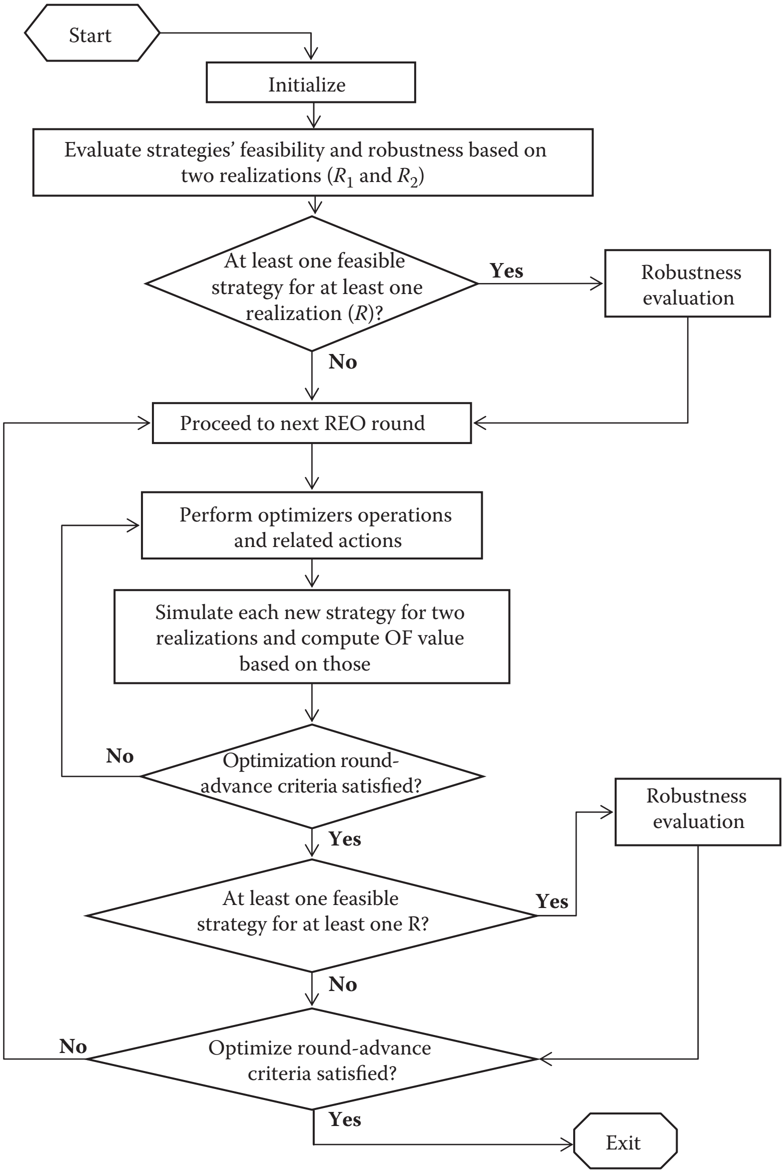

FIGURE 5.7
REO™ flowchart. (Modified from Kalwij, I. M., and Peralta, R. C., *Ground Water* 44(4), 547–582, 2006.)

The REO output is an optimal strategy that is robust for a robustness range established during optimization. The robustness of the strategy depends on the strategy configuration (i.e., selected well locations) and the degree of uncertainty of the evaluated parameter.

An advantage of REO is that it requires it less field data if PDF-generated realizations are not used. It can use them, but it does not have to. REO-developed strategies might not achieve as high a mathematical reliability as strategies developed using many realizations based on real aquifer parameter PDFs. REO also maintains the primary OF value to the extent possible, while conditioning the pumping strategy to improve robustness. An REO application is presented in Section 15.4.

Bibliography

Ahlfeld, D. P., J. M. Mulvey and G. F. Pinder. 1988. Contaminated groundwater remediation design using simulation, optimization and sensitivity theory. 2. Analysis. *Water Resources Research* 24(3):442–452.

Aly, A. H. and R. C. Peralta. 1999. Optimal design of aquifer cleanup systems under uncertainty using a neural network and a genetic algorithm. *Water Resources Research* 35(8):2523–2532.

Askew, A. J., W. W.-G. Yeh and W. A. Hall. 1971. Use of Monte Carlo techniques in the design and operation of a multi-purpose reservoir system. *Water Resources Research* 7(4):819–826.

Brigham, E. O. 1988. *Fast Fourier Transform and Its Application*. Prentice-Hall Signal Processing Series. Upper Saddle River, NJ: Prentice Hall, Inc.

Cantiller, R. R. A. and R. C. Peralta. 1989. Computational aspects of chance-constrained sustained groundwater yield management. *Transactions of the ASAE* 32(3): 939–944.

Chan, N. 1993. Robustness of the multiple realization method for stochastic hydraulic aquifer management. *Water Resources Research* 29(9):3159–3167.

Chan, N. 1994. Partial infeasibility method for chance constrained aquifer management. *Journal of Water Resources Planning and Management—ASCE* 120(1):70–89.

Charnes, A. and W. W. Cooper. 1963. Deterministic equivalents for optimizing and satisfying under chance constraints. *Operations Research* 11(1):18–39.

Chien, C. C., M. A. Medina, Jr., G. F. Pinder, D. R. Reible, B. E. Sleep and C. Zheng. 2002. *Environmental Modeling and Management. Theory, Practice, and Future Directions*. Wilmington, DE: Today Media.

Copty, N. K. and A. N. Findikakis. 2000. Quantitative estimates of the uncertainty in the evaluation of groundwater remediation schemes. *Ground Water* 38(1):29–37.

Datta, B. and S. D. Dhiman. 1996. Chance-constrained optimal monitoring network design for pollutants in ground water. *Journal of Water Resource Planning and Management—ASCE* 122(3):180–188.

Davis, M. W. 1987. Production of conditional simulation via the LU triangular decomposition of the co-variance matrix. *Mathematical Geology* 19(2):91–98.

Delhomme, P. 1979. Spatial variability and uncertainty in groundwater flow parameters: A geostatistical approach. *Water Resources Research* 15(2):269–280.

ESI. 1998. Guide to using Stochastic MODFLOW for Monte Carlo Simulation. Environmental Simulations, Inc. Virginia.

Fenton, G. A. 1990. Simulation and Analysis of Random Fields. PhD dissertation, Princeton University.

Freeze, R. 1975. A stochastical conceptual analysis of one-dimensional groundwater flow in nonuniform homogeneous media. *Water Resources Research* 11(5):725–741.

Freeze, R. A. and S. M. Gorelick. 1999. Convergence of stochastic optimization and decision analysis in engineering design of aquifer remediation. *Ground Water* 37(6):934–954.

Freeze, R. A., J. Massmann, L. Smith, T. Sperling and B. James. 1990. Hydrogeological decision analysis: 1. a framework. *Ground Water* 28(5):738–766.

Gelhar, L. 1986. Stochastic subsurface hydrology from theory to applications. *Water Resources Research* 22(9S):135S–145S.

Gorelick, S. M. 1987. Sensitivity analysis of optimal groundwater contaminant capture curves: Spatial variability and robust solutions. In *Proceedings of the National Water Well Association Conference, Solving Ground Water Problems with Models*, Dublin, OH, 133-146. NWWA.

Gorelick, S. M. 1990. Large scale nonlinear deterministic and stochastic optimization: Formulations involving simulation of subsurface contamination. *Mathematical Programming* 48(1–3):19–39.

Harter, T. 1994. Unconditional and conditional simulation of flow and transport in heterogeneous, variably saturated porous media, PhD dissertation, University of Arizona.

He, L., G. H. Huang, and H. W. Lu. 2008. A simulation-based fuzzy chance-constrained programming model for optimal groundwater remediation under uncertainty. *Advances in Water Resources* 31(12):1622–1635.

Hilton, A., B. Chan and T. B. Culver. 2005. Groundwater remediation design under uncertainty using genetic algorithms. *Journal of Water Resources Planning and Management—ASCE* 131(1):25–34.

Isaaks, E. H. and R. M. Srivastava. 1989. *An Introduction to Applied Geostatistics*. Oxford University Press.

Jensen, K. and A. Mantoglou. 1992. Application of stochastic unsaturated flow theory, numerical simulations, and comparisons to field observations. *Water Resources Research* 28(1):269–284.

Kalwij, I. M. and R. C. Peralta. 2006. Simulation/optimization modeling for robust pumping strategy design. *Ground Water* 44(4):547–582.

Kourakos, G. and A. Mantoglou. 2008. Remediation of heterogeneous aquifers based on multiobjective optimization and adaptive determination of critical realizations. *Water Resources Research* 44, W12408, doi:10.1029/2008WR007108.

Laase, A. D., N. Merrick and J. O. Rumbaugh III. 2006. Applied comparison of gradient, particle-tracking and transport optimization schemes. In *Proceedings of the Fifth International Conference on Remediation of Chlorinated and Recalcitrant Compounds*, Monterey, CA, May 22–25, 2006.

Laase, A. and J. Rumbaugh III. 1999. Application of economic-risk analysis for design and optimization of the Kansas City plant interceptor system. In *Calibration and Reliability in Groundwater Modelling* (Proceedings of the ModelCARE 99 Conference, Zurich). *IAHS* 265:41–46.

Lee, S. L. and P. K. Kitanidis. 1991. Optimal estimation and scheduling in aquifer remediation with incomplete information. *Water Resources Research* 27(9):2203–2217.

Mantoglou, A. and G. Kourakos. 2007. Optimal groundwater remediation under uncertainty using multi-objective optimization. *Water Resources Management* 21(5):835–847.

Mantoglou, A. and J. L. Wilson. 1992. The turning bands method for simulation of random fields using line generation by a spectral method. *Water Resources Research* 18(5):1379–1394.

Meyer, P. D., A. J. Valocchi and J. W. Eheart. 1994. Monitoring network design to provide initial detection of groundwater contamination. *Water Resources Research* 30(6):1897–1906.

Minsker, B. S. and C. A. Shoemaker. 1998. Quantifying the effects of uncertainty on optimal groundwater bioremediation policies. *Water Resources Research* 34(12): 3615–3625.

Morgan, D. R., J. W. Eheart and A. J. Valocchi. 1993. Aquifer remediation design under uncertainty using a new chance constrained programming technique. *Water Resources Research* 29(3):551–561.

Mylopoulos, Y. A., N. Theodosiou and N. A. Mylopoulos. 1999. A stochastic optimization approach in the design of an aquifer remediation under hydrogeologic uncertainty. *Water Resources Management* 13(5):335–351.

Peck, A., S. Gorelick, G. de Marsily, S. Foster and V. Kovalevsky. 1988. *Consequences of Spatial Variability in Aquifer Properties and Data Limitations for Groundwater Modeling Practice*. Washington, DC: IAHS 175.

Pradeep, M. and C. A. Shoemaker. 2004. Time varying optimization for monitoring multiple contaminants under uncertain hydrogeology. *Bioremediation Journal* 8(3–4):129–146.

Ranjithan, S., J. W. Eheart and J. H. Garrett, Jr. 1993. Neural network-based screening for ground water reclamation under uncertainty. *Water Resources Resarch* 29(3):563–574.

Reichard, E. G. 1995. Groundwater–surface water management with stochastic surface water supplies: A simulation optimization approach. *Water Resources Research* 31(11):2485–2865.

Ricciardi, K., L. George, F. Pinder et al. 2007. Efficient groundwater remediation system design subject to uncertainty using robust optimization. *Journal of Water Resources Planning and Management—ASCE* 133(3):253–263.

Ritzel, B. J., J. W. Eheart and S. Ranjithan. 1994. Using genetic algorithms to solve a multiple objective ground water pollution containment problem. *Water Resources Research* 30(5):1589–1603.

Ruskauff, G. 1994. A methodology for performing Monte Carlo analysis with MODFLOW and MODPATH. In *Proceedings of the 1994 Groundwater Modelling Conference.* J. W. Wamer and P. K. M. van der Heijde (eds.). Fort Collins, CO, pp. 183–192.

Sawyer, C. S. and Y. F. Lin. 1998. Mixed-integer chance-constrained models for groundwater remediation. *Journal of Water Resources Planning and Management—ASCE* 124(5):285–294.

Siegfried, T. and W. Kinzelbach. 2006. A multiobjective discrete stochastic optimization approach to shared aquifer management: Methodology and application. *Water Resources Research* 42, W02402, doi:10.1029/2005WR004321.

Singh, A. and B. Minsker. 2003. Modeling and characterization of uncertainty for optimization of ground water remediation at the Umatilla Chemical Depot. In *Proceedings of the World Water and Environmental Resources Congress 2003 and Related Symposia*. P. Bizier and P. A. DeBarry (eds.), pp. 1–9. ASCE.

Singh, A. and B. Minsker. 2004. Uncertainty based multi-objective optimization of groundwater remediation at the Umatilla Chemical Depot. In *Proceedings of the ASCE/EWRI World Environmental and Water Resources Congress*, Salt Lake City, UT.

Smalley, J. B., B. S. Minsker and D. E. Goldberg. 2000. Risk based in situ bioremediation design using a noisy genetic algorithm. *Water Resources Research* 36(10): 3043–3052.

Springer, M. D. 1979. *The Algebra of Random Variables*. New York: John Wiley & Sons.

Tiedeman, C. and S. M. Gorelick. 1993. Analysis of uncertainty in optimal groundwater contaminant capture design. *Water Resources Research* 29(7):2139–2153.

Tung, Y. 1986. Groundwater management chance-constrained model. *Journal of Water Resources and Planning Management—ASCE* 112(1):1–19.

Wagner, B. J. 1995. Recent advances in simulation–optimization groundwater management modeling. *Reviews of Geophysics* 33(S1):1021–1028.

Wagner, B. J. 1995. Sampling design methods for groundwater modeling under uncertainty. *Water Resources Research* 31(10):2581–2591.

Wagner, B. J. 1999. Evaluating data worth for ground-water management under uncertainty. *Journal of Water Resources Planning and Management—ASCE* 125(5): 281–288.

Wagner, B. J., and S. M. Gorelick. 1987. Optimal groundwater quality management under parameter uncertainty. *Water Resources Research* 23(7):1162–1174.

Wagner, B. J. and S. M. Gorelick. 1989. Reliable aquifer remediation in the presence of spatially variable hydraulic conductivity: from data to design. *Water Resources Research* 25(10):2211–2225.

Wagner, J. M., U. Shamir and H. R. Nemati. 1992. Groundwater quality management under uncertainty: stochastic programming approaches and the value of information. *Water Resources Research* 28(5):1233–1246.

Ward, R. L. and R. C. Peralta. 1990. EXEIS, expert screening and optimal extraction/injection pumping systems for short-term plume immobilization. AFESC Project Completion Report, ESL-TR-89-57.

Watkins, D. W. and D. C. McKinney. 1995. Robust optimization for groundwater quality management under uncertainty. In *Proceedings of the 22nd Annual Conference,* Cambridge, Massachusetts, M. F. Domenica (ed.), ASCE, pp. 879–882.

Watkins, D. W. and D. C. McKinney. 1997. Finding robust solutions to water resources problems. *Journal of Water Resources Planning and Management—ASCE* 123(1):49–58.

Wong, H. and W. W.-G. Yeh. 2002. Uncertainty analysis in contaminated aquifer management. *Journal of Water Resources Planning and Management—ASCE* 128(1):33–45.

Yeh, W. W.-G. 1986. Review of parameter estimation procedures in groundwater hydrology: The inverse problem. *Water Resources Research* 22(2):95–108.

Yeh, W. W.-G., Y. S. Yoon and K. S. Lee. 1983. Aquifer parameter identification with kriging and optimum parameterization. *Water Resources Research* 19(1):225–233.