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Stochastic Modelling of a Contaminated Aquifer

The Unconditional Approach

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A stochastic solute transport model is applied to a groundwater contamination case. The contamination is caused by leachate from an unprotected landfill situated in a highly-permeable unconfined aquifer.

The stochastic model combines the geostatistical techniques of semivariogram analysis and kriging with a numerical solute transport model. A Monte Carlo approach that utilizes the turning bands technique to genereate transmissivity fields is used. Here some preliminary results of the unconditional stochastic simulations are presented.

The contaminant plume is characterized by expected concentrations of chloride and standard deviations.

Introduction

In practical problems of ground water contamination the amount of hydrogeological and geochemical information available will always be limited. When doing contaminant model studies based on a given data set, it is important to estimate the uncertainties involved in the analyses. This can be achieved by defining the main parameters involved as statistical quantities, rather than as deterministically known properties. Thus the equations governing flow and transport through the porous geologic matrix become stochastic in nature. Their solutions, i.e. hydraulic head and contaminant concentrations, are characterized by expected values and deviations from these.

Another reason for formulating a solute transport problem in statistical terms is the complex nature of the dispersive mechanism of contaminant spreading. The classical formulation of the hydraulic dispersion in unconsolidated geologic materials defines the mechanism as the product of a dispersivity coefficient and a known flow velocity. Formulated in this way, it has become clear that dispersivity is a lump parameter related to the unknown velocity component of the total flow field. Thus

$$V_{\mathrm{TOTAL}} \equiv V_{\mathrm{UNKNOWN}} + V_{\mathrm{KNOWN}}$$

and, while neglecting chemical diffusion,

DISPERSION ≡ DISPERSIVITY × ADVECTION

TRANSPORT ≡ DISPERSION + ADVECTION

Advection is equal to the deterministically known part of the flow field, $V{-}0_{KNOWN}$. The unknown flow component lumps contributions from both material and non-material properties of the aquifer.

The main material properties that contribute to dispersion are undetermined variations in the hydraulic conductivity and effective porosity. As non-material contributions transient flow phenomena can be mentioned. Such transients can be caused a.o. by seasonal variations in surface recharge. As far as the induced transient flow is not described deterministically, it contributes to the dispersive spreading of the contaminant.

A major parameter that influences the solute concentration pattern is the spatial distribution of the hydraulic conductivity. By treating this property as a stochastic quantity it is possible to separate the conductivity contribution to the dispersion from the other contributions. The calculated contaminant plume can then be characterized by expected values and statistical deviations. The latter can be viewed as uncertainties related to variations in the hydraulic conductivity. In this paper a stochastic modelling approach that combines geostatistical techniques and numerical modelling is used. The aproach is applied to a contaminated groundwater system.

The Stochastic Approach

Characterizing the transmissivity distribution in an aquifer as a random field requires knowledge of expected values and expected variations. Further, a spatial autocorrelation structure and a probability distribution have to be specified. Possibly, different statistical properties have to be assigned to different subareas or directions. Stationarity, i.e. statistical homogeneity, is accepted as a working hypothesis. Deriving the above properties from a given data set requires the assumption of ergodicity, i.e. the properties derived from the one member available are an acceptable approximation of the ensemble properties. It is worth recognising that the single realisation available, i.e. the aquifer, is only sampled in a limited number of data points. More information about the stochastic theory can be found in, a.o.

Journel and Huijbregts (1978), Neuman (1982).

A Study by Freeze (1975) indicates that the hydraulic conductivity is approximately lognormal distributed. The lognormal probability distribution has been used in the analyses presented here. Geostatistics offers techniques to estimate the other stochastic properties from a data set. The techniques that have been used are semivariogram estimation and kriging. Both are applied to transmissivity and hydraulic head.

Semivariogram Analysis

In order to estimate the spatial autocorrelation structure of a random field, e.g. transmissivities, a semivariogram analysis can be applied. The semivariogram describes the spatial structure in a random field and is directly related to the autocovariance by

$$\gamma(h) \equiv C(o) - C(h) \tag{1}$$

$\gamma(h)$ is the semivariogram, $C(o)$ is the field variance and $C(h)$ is the covariance. They are functions of the distance or lag, h, between the measurement points. $\gamma(h)$ is given by

$$\gamma(h) = \frac{1}{2}\,\mathrm{var}[Z(x+h) - Z(x)] \tag{2}$$

where Z is the field value at the location vectors x and $x + h$. For practical purposes a sample semivariogram, γ_s, is calculated from the data, thus

$$\gamma_s(h) = \frac{1}{2N}\sum_{i=1}^{N} [Z(x_i+h_j) - Z(x_i)]^2 , \quad j = 1 , \quad M \tag{3}$$

with N the number of data pairs with lag h_j and M the number of lags considered. The data pairs are grouped in lag intervals. Then a theoretical semivariogram or autocovariance function is fitted to the sample. The interested reader is referred to a.o. Delhomme (1978) and Delhomme (1979).

Kriging

Kriging is an interpolation technique that provides both expected values and standard deviations. The interpolation is based on the semivariogram and is expressed by

$$Z_j^{kr} \equiv \sum_{i=1}^{n} \lambda_{ij} Z_i , \qquad j = 1 , \quad NE \tag{4}$$

where Z_j^{kr} is the interpolated value based on n measured values Z_i, and NE is the number of discrete grid points considered. The essence of kriging is to find the weighting coefficients λ_{ij} in an optimal way. This is done by solving the so-called kriging system

$$[\lambda] \equiv [C]^{-1} \times [b] \tag{5}$$

and

$$\sum_{i=1}^{n} \lambda_{ij} = 1 \tag{6}$$

where $[C]$ and $[b]$ contain terms directly derived from the covariance or semivariogram. If the field variance exists and is finite, then the semivariogram approaches a constant value, called the sill, after a certain lag, called the range. This is usually the case when dealing with transmissivities. When applying kriging to hydraulic head one usually has to resort to generalised covariance functions. More information can be found in a.o. Kafritsas and Bras (1981) and Virdee and Kottegoda (1984).

Stochastic Solute Transport

Once the stochastic process has been determined, different members all belonging to the same ensemble can be generated by various methods. In this study the turning bands technique has been used because of its advantageous computing cost to accuracy rate. For more information about the turning bands see Mantoglou and Wilson (1982). Thus a large number of transmissivity realisations, belonging to the same stochastic ensemble, is generated and each of them is treated as a single deterministic field. A numerical solute transport model is then applied to calculate contaminant plumes corresponding to each transmissivity field. Here a modified form of the solute transport model developed by Konikow and Bredehoeft (1978) has been used. This model employs a block-centered finite difference solution to solve the flow equation and approximates transport by a method of characteristics solution. Unconditional simulations are obtained by calculating the mean and standard deviation of concentration in every grid point of the plume.

Case Study

The above described stochastic modelling techniques have been applied to a case of groundwater contamination in Zealand, Denmark. Fig. 1 shows the location and main features of the study area.

The landfill started operating in 1959 in an old gravel pit, and the last recorded disposals are from 1982. Both municipal and toxic industrial wastes have been disposed. The site is unprotected, i.e. there is no liner placed at the bottom. The waste thickness ranges from 5-10 meters, and the bottom is in immediate contact with the water table.

The contaminated aquifer is unconfined and consists of highly-permeable glacial sand and gravel. Fig. 2 displays a simplified cross-sectional view.

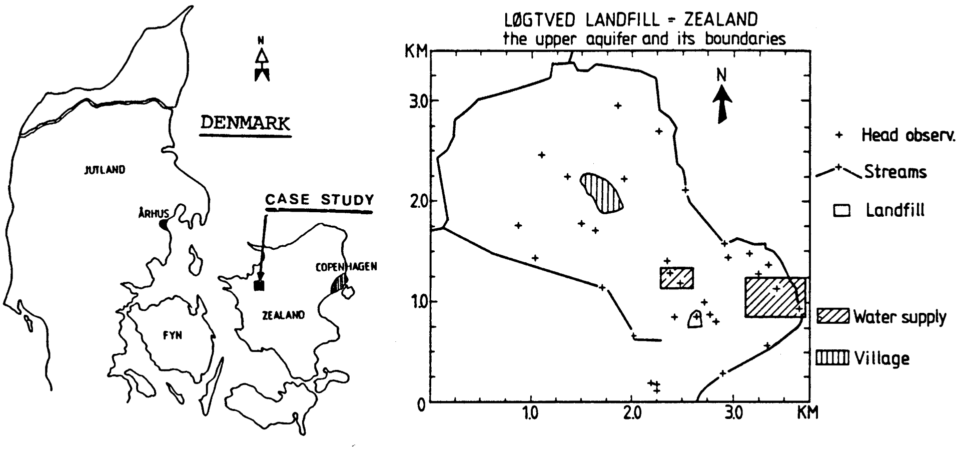

Fig. 1. The main features of the contaminated aquifer.

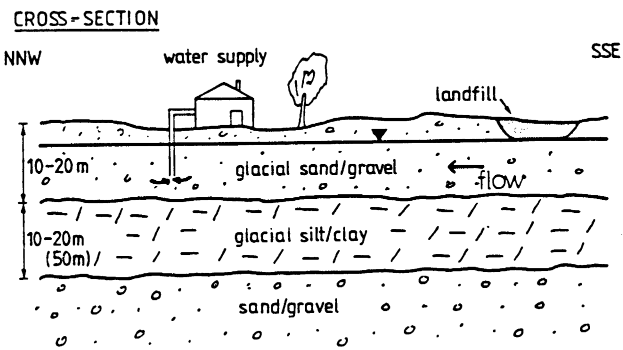

Fig. 2. Cross-section through the aquifer.

A clay layer of substantial thickness separates the upper from the lower aquifer. No contamination has been observed in the lower aquifer. Thus this study is limited to the upper one. The streams in Fig. 1 are assumed to be in direct hydraulic contact with the upper flow region and are treated as the flow boundaries.

Geostatistical Analyses of Hydraulic Head and Transmissivities

A large number of hydraulic head observations were made during a two-day field campaign in April 1985 (see TERRAQUA 1985). High precision levelling instrumentation was used. These data were kriged, and Fig. 3 shows the kriged hydraulic head map and standard deviations. Universal kriging of order 1 and a neighbourhood size of 12 data points was used. Standard deviations increase with the distance from the data points. In the autumn of 1985 slug tests were performed to determine transmissivities. The contaminated subarea of about 1.5×1.5 km^2 was covered with 11 slug tests, giving a data density of 4.9 measurements/km^2. The

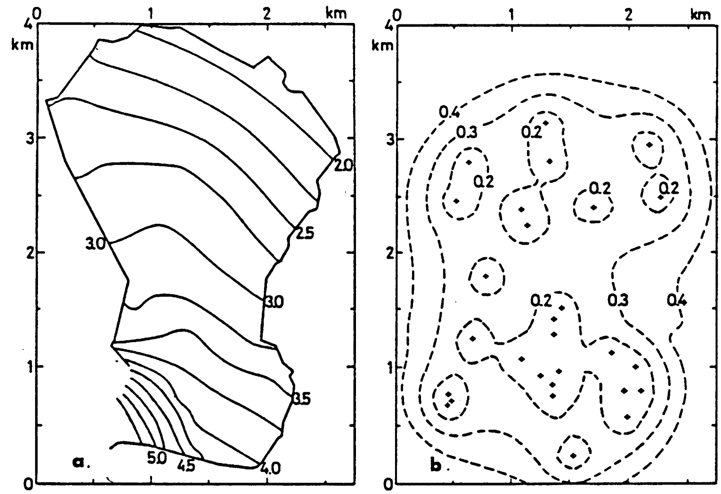

Fig. 3. a) Universal kriging of hydraulic head: number of data = 28, order = 1, neighbourhood = 12 points, generalized covariance = − 0.1733|h| (interval 0.25 m)
b. Kriging standard deviations (interval 0.10 m).

mean transmissivity was estimated as 5.4×10^{-3} m^2/s. The slug test results were compared with short pumping tests, and good agreement was found in most cases. Fig. 4 shows a semivariogram analysis of the logtransmissivity values. An exponential model was fitted to the sample semivariogram. The correlation length is 0.3 km and the range is 0.9 km.

Deterministic Simulations

In order to determine some of the model parameters a number of deterministic simulations were done. The solute transport model developed by Konikow and Bredeshoeft (1978) was used.

The saturated thickness was taken constant at 10.0 m over the whole aquifer. This value is representative for the largest part of the aquifer and is especially well documented in the contaminated subarea. The effective porosity was taken at 20%

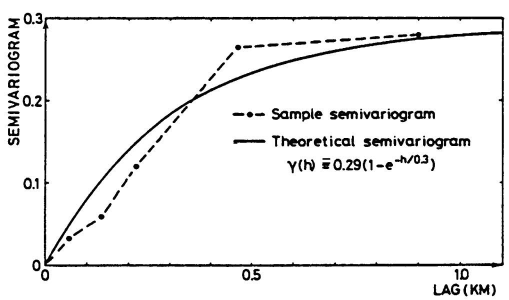

Fig. 4.
Sample semivariogram and theoretical model for logtransmissivities, base e (h = lag).

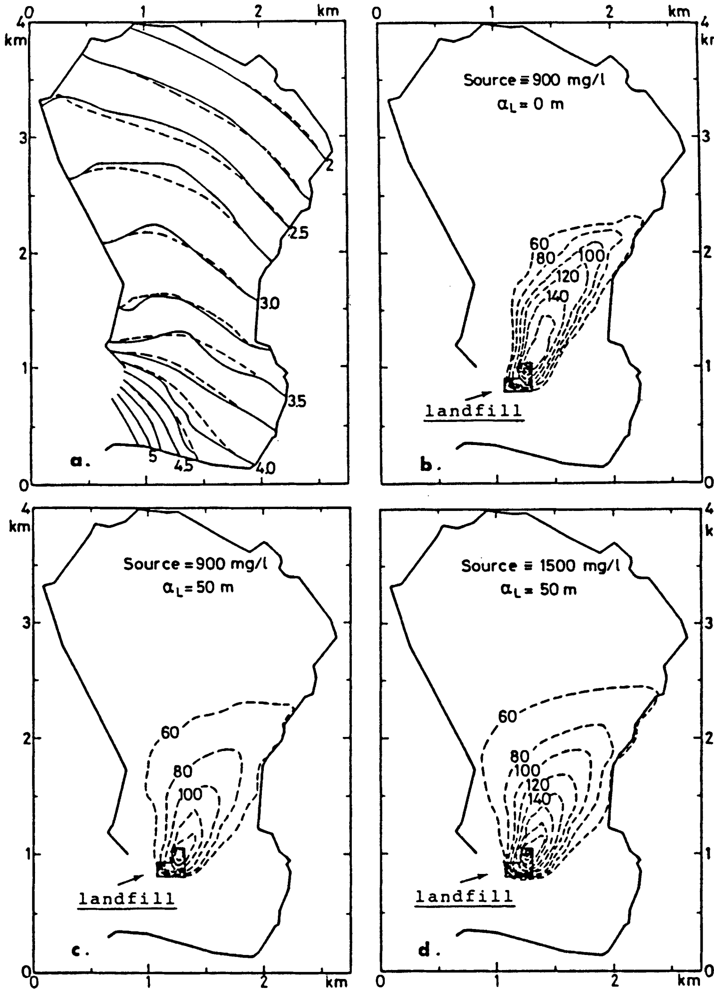

Fig. 5 a) Deterministic model calibration: kriged and calculated (broken line) hydraulic heads (interval 0.25 m).
b) c) d) Calculated contaminant plumes of chloride with different values of source concentration and dispersivity (interval 20 mg/l, background 50 mg/l).

and, based on meteorological data, the surface recharge is estimated to be 140 mm/year. The streams are treated as constant head boundaries.

The flow model is put in steady-state mode, since only one snap-shot picture of the hydraulic head was available. Calibration of the model was done by adjusting the transmissivity field. In the contaminated subarea kriged values of the measured transmissivities were used.

Fig. 5 shows the calculated and kriged head and three deterministic transport

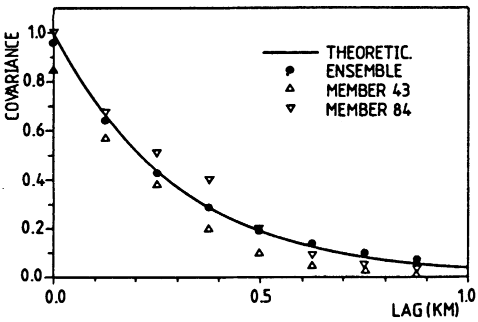

Fig. 6. The simulated autocovariance structure of logtransmissivity, normalized.

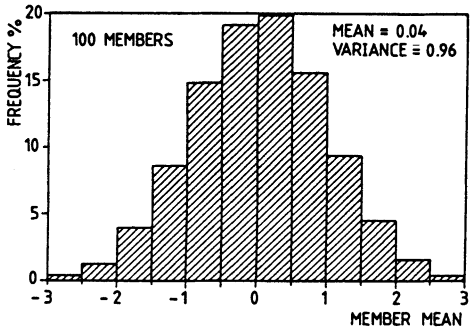

Fig. 7. The normalized sample ensemble histogram of logtransmissivity.

models: Two with source concentrations of chloride equal to 900 mg/l at the landfill. Transverse dispersivity is 0.3 × α_L in all models. Based on the available observations, it has not been possible to distinguish unambiguously between the different calculated plumes.

Stochastic Simulation

Based on the semivariogram analysis of transmissivities, a sample ensemble consisting of 100 members was generated using the turning bands technique. Fig. 6 shows the covariance of the sample ensemble. Also shown in the figure are the covariances of the members 43 and 84. These members were picked at random. The normalized global histogram is shown in Fig. 7. The simulated mean was 0.04, and the variance was 0.96. These are very close to the theoretical values 0.0 and 1.0, respectively. The transmissivity members were used as deterministic input to a solute transport model and the outcome is shown in Figs. 8 and 9. As expected the standard deviations of the hydraulic head are small near the flow boundary and become increasingly larger towards the center of the flow domain. In Fig. 9 the plumes of the members 43 and 84 are shown. As can be seen, the plume patterns are considerably different. Furthermore, the contamination levels are distinctly different for the two cases. Maximum concentrations of around 120 mg/l are reached for member 43, whereas member 84 shows levels of more than 180 mg/l. It must be remembered that the same source concentration was applied and that the differences are solely due to different conductivity distributions. Also shown are the mean concentration plume and the standard deviations. The ensemble plume is very like the deterministic plume shown in Fig. 5.

The longitudinal dispersivity was set equal to 2.0 m in all stochastic runs to take small-scale dispersion into account. Comparing the mean plume in Fig. 9c with the deterministic plume with source concentration 900 mg/l and dispersitivy 50 m, Fig. 5c, shows that large-scale dispersion has been simulated completely in a statistical sense.

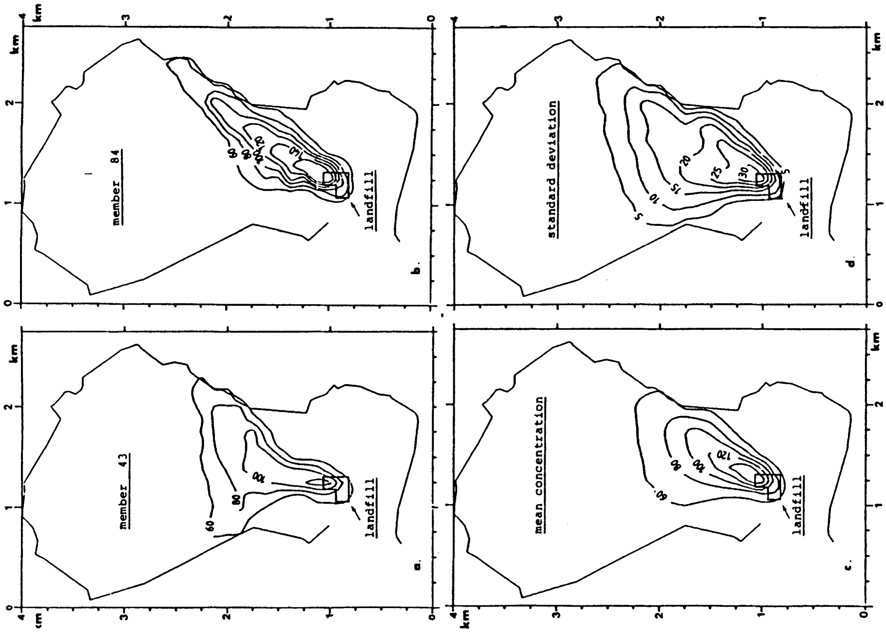

Fig. 9. Stochastic simulations of the chloride-contaminant plume [mg/l, interval 20 mg/l]
a) b) members 43 and 84, respectively.
c) mean concentrations of 100 members.
d) concentration standard deviations (interval 5 mg/l).

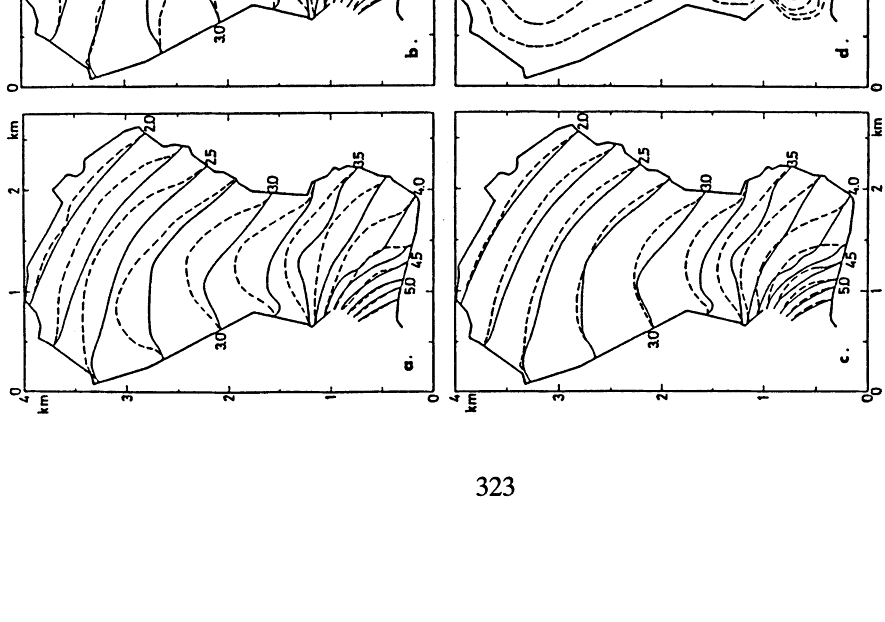

Fig. 8. Stochastic simulations of hydraulic head; full line is kriged and broken line is simulated head.
a) b) members 43 and 84 (interval 0.25 m).
c) mean head of 100 members (interval 0.25 m).
d) head standard deviations (interval 0.02 m).

Discussion

The stochastic approach of solute transport modelling used in this study makes it possible to characterize a contaminant plume by expected or mean values and standard deviations. The latter can be interpreted as uncertainties related to unknown spatial variations in the transmissivity distribution. The spatial distribution of transmissivity affects both the plume pattern and the concentration levels.

Further, the stochastic formulation provides a way to express solute dispersion as a function of the statistical properties of the transmissivity field, rather than defining it as a lump parameter.

The contamination case presented here is proposed for a pilot research project. More data will be collected and conditioning of the stochastic models will be done.

References

Delhomme, J. P. (1978) Kriging in hydrosciences, *Adv. Water Resour. Vol. 5 (1),* pp. 251-266.

Delhomme, J. P. (1979) Spatial variabily and uncertainty in groundwater flow parameters: a geostatistical approach, *Wat. Resour. Res., Vol. 15 (2),* pp. 269-280.

Freeze, R. A. (1975) A stochastic- conceptual analysis of one-dimensional groundwater flow in non-uniform homogeneous media, *Wat. Resour. Res., Vol. 11 (5),* pp. 725-741.

Journel, A.G., and Huijbregts, Ch. J. (1978) *Mining geostatistics,* Academic Press, New York, pp. 600.

Kafritsas, J., and Bras, R. L. (1981) The practice of kriging, MIT report No. 263, pp. 107.

Konikow, L. F., and Bredehoeft, J. D. (1978) Computer model of two-dimensional solute transport and dispersion in ground water, USGS, Book 7, Chapter C2, Washington, pp. 90.

Neuman, Sh. P. (1982) Statistical characterization of aquifer heterogeneities: an overview. In: *Recent trends in hydrology,* ed. Narasimhan, T. N., Boulder, Co., pp. 81-102.

Mantoglou, A., and Wilson, J. L. (1982) The turning bands method for simulation of random fields using line generation by a spectral method, *Wat. Resour. Res., Vol. 18 (5),* pp. 1379-1394.

Terraqua Aps (1985) Undersøgelse af forurening fra Løgtved losseplads, Statusrapport + bilag (in Danish).

Virdee, T.S., and Kottegoda, N. T. (1984) A brief review of kriging and its application to optimal interpolation and observation well selection, *J. Hydr. Sc., Vol. 29 (4),* pp. 367-387.

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