

HydrogeoSieveXL: an Excel-based tool to estimate hydraulic conductivity from grain-size analysis

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Abstract

For over a century, hydrogeologists have estimated hydraulic conductivity (K) from grain-size distribution curves. The benefits of the practice are simplicity, cost, and a means of identifying spatial variations in K . Many techniques have been developed over the years, but all suffer from similar shortcomings: no accounting of heterogeneity within samples (i.e., aquifer structure is lost), loss of grain packing characteristics, and failure to account for the effects of overburden pressure on K . In addition, K estimates can vary by an order of magnitude between the various methods, and it is not generally possible to identify the best method for a given sample. The drawbacks are serious, but the advantages have seen the use of grain-size distribution curves for K estimation continue, often using a single selected method to estimate K in a given project. In most cases, this restriction results from convenience. It is proposed here that extending the analysis to include several methods would be beneficial since it would provide a better indication of the range of K that might apply. To overcome the convenience limitation, an Excel-based spreadsheet program, HydrogeoSieveXL, is introduced here. HydrogeoSieveXL is a freely available program that calculates K from grain-size distribution curves using 15 different methods. HydrogeoSieveXL was found to calculate K values essentially identical to those reported in the literature, using the published grain-size distribution curves.

1. Introduction

Since the introduction of Darcy's Law, an enormous effort (by hydrogeological standards) has been directed at quantifying the hydraulic conductivity parameter, K . Since it was recognized early on that K was correlated with grain size – low in clays and high in gravels – it is not surprising that there were early efforts to estimate K from grain size analyses. It is also not surprising that these efforts enjoyed

some measure of success (Fuchs, 2010). At the same time, it must be conceded that after more than a century of trying, the goal of obtaining a value of K in the laboratory that is fully representative of K in an aquifer has yet to be achieved (Rosas *et al.*, 2014). The reasons for this include factors such as geologic heterogeneity (particularly as it affects aquifer structure, which is disrupted in the grain size analysis procedures), the nature of porosity, subtle effects related to grain shapes and packing (Dullien, 1991), and in some cases variations in porewater pressure (Barth *et al.*, 2001).

Despite the well-accepted limitations of K estimates from grain size analyses, there are no simpler or more economical measurement-based techniques for obtaining K estimates from aquifer samples. Where preliminary calculations are concerned, these measured values still represent an attractive starting point for hydrogeological investigations, or an inexpensive source of supporting data, particularly where sand and gravel deposits are of concern.

Among the earliest attempts to relate K to grain size, or grain size distribution, was work published by Hazen in 1892. Since that time, a large number of variations on the theme have been developed. Aguilar (2013) reviewed a subset of 20 of these different empirical relationships. The equations range from the very simple, such as the simplified Hazen formula given by Freeze and Cherry (1979) (first entry in Table 1), to the considerably more involved calculation offered by Kozeny and Carmen (eighth entry in Table 1). Unfortunately, the various approaches can produce estimates of K from the same sample that are an order of magnitude or more apart (Vuković and Soro, 1992). Although each equation comes with recommendations for the sediment types they apply to, many of the restrictions overlap so establishing a preference for one equation over another may be somewhat subjective. Rather than basing a K determination on any single equation, it may be prudent to estimate K from several methods and consider the range of

Table 1: Selected equations relating hydraulic conductivity, K in cm/s, with porosity and effective grain size in cm (taken from Devlin (2014)), modified and expanded from Vuković and Soro, 1992).

Source	N	$\phi(n)$	d_e	Applicable Conditions
Hazen simplified (Freeze and Cherry, 1979)	$10 \frac{\mu}{\rho g}$	1	d_{10}	uniformly graded sand, $n = 0.375$ $T = 10^\circ\text{C}$
Hazen (1892) ^a	6×10^{-4}	$[1 + 10(n - 0.26)]$	d_{10}	$0.01 \text{ cm} < d_{10} < 0.3 \text{ cm}$ $U < 5$
Slichter (1898) ^a	1×10^{-2}	$n^{3.287}$	d_{10}	$0.01 \text{ cm} < d_{10} < 0.5 \text{ cm}$
Terzaghi (1925) ^a	10.7×10^{-3} smooth grains 6.1×10^{-3} coarse grains	$\left(\frac{n - 0.13}{\sqrt[3]{1 - n}}\right)^2$	d_{10}	sandy soil, coarse sand
Beyer (1964) ^a	$5.2 \times 10^{-4} \log \frac{500}{U}$	1	d_{10}	$0.006 \text{ cm} < d_{10} < 0.06 \text{ cm}$ $1 < U < 20$
Sauerbrei (1932) ^a (Vuković and Soro, 1992)	$(3.75 \times 10^{-5}) \times \tau$ $\tau \cong 1.093 \times 10^{-4} T^2$ $+ 2.102 \times 10^{-2} T$ $+ 0.5889$	$\frac{n^3}{(1 - n)^2}$	d_{17}	sand and sandy clay $d_{10} < 0.05 \text{ cm}$
Krüger (1919) ^a	4.35×10^{-4}	$\frac{n}{(1 - n)^2}$	$\frac{1}{\sum_{i=1}^m \frac{\Delta w_i}{d_i}}$	medium sand $U > 5$ $T = 0^\circ\text{C}$
Kozeny-Carmen (1953) ^a	8.3×10^{-3}	$\frac{n^3}{(1 - n)^2}$	d_{10} or 1 $\frac{3 \Delta w_1}{2 d_1} + \sum_{i=2}^m \Delta g_i \frac{d_i^g + d_i^d}{2 d_i^g d_i^d}$ $d_1 = \frac{1}{\frac{1}{2} \left(\frac{1}{d_i^g} + \frac{1}{d_i^d} \right)}$	Coarse sand
Zunker (1930) ^a	0.7×10^{-3} for nonuniform, clayey, angular grains 1.2×10^{-3} for nonuniform 1.4×10^{-3} for uniform, coarse grains 2.4×10^{-3} for uniform sand, well rounded grains	$\frac{n}{(1 - n)}$	$\frac{1}{\sum_{i=1}^m \Delta g_i \frac{d_i^g - d_i^d}{d_i^g d_i^d \ln \left(\frac{d_i^g}{d_i^d} \right)}}$	no fractions finer than $d = 0.0025 \text{ mm}$
Zamarin (1928) ^a	8.65×10^{-3}	$\frac{n^3}{(1 - n)^2} C_n$ $C_n = (1.275 - 1.5n)^2$	$\frac{1}{\sum_{i=1}^m \Delta g_i \frac{\ln \left(\frac{d_i^g}{d_i^d} \right)}{d_i^g - d_i^d}}$	Large grained sands with no fractions having $d < 0.00025 \text{ mm}$

Source	N	$\phi(n)$	d_e	Applicable Conditions
USBR (United States Bureau of Reclamation) (Bialas, 1966) ^a	$(4.8 \times 10^{-4})(10^{0.3})$	1.0	$d_{20}^{1.15}$	Medium grained sands with $U < 5$; derived for $T = 15$ °C
Barr (2001)	$\frac{1}{(36)5C_s^2}$ $C_s^2 = 1$ for spherical grains $C_s^2 = 1.35$ for angular grains	$\frac{n^3}{(1-n)^2}$	d_{10}	unspecified
Alyamani and Sen (1993)	1300	1.0	$[I_o + 0.025(d_{50} - d_{10})]$	unspecified
Chapuis (2004)	$\frac{\mu}{\rho g}$	$10^{1.291\xi - 0.6435}$ $\xi = \frac{n}{1-n}$	$d_{10} \left(\frac{10^{(0.5504 - 0.2937\xi)}}{2} \right)$	$0.3 < n < 0.7$ $0.10 < d_{10} < 2.0$ mm $2 < U < 12$ $d_{10}/d_5 < 1.4$
Krumbein and Monk (1942)	7.501×10^{-6}	$e^{(-1.31 \times \sigma_\phi)}$ $\sigma_\phi = \frac{d_{84\phi} - d_{16\phi}}{4}$ $\frac{d_{95\phi} - d_{5\phi}}{6.6}$	$2 \left(\frac{d_{16\phi} + d_{50\phi} + d_{84\phi}}{3} \right)$	natural sands with lognormal grain size distribution

^a indicates formulas were taken from Vuković and Soro, (1992)

N = constant dependent on characteristics of the porous medium

$\phi(n)$ = function of porosity

T = water temp. (°C)

g = 980 cm s⁻²

$\rho = 3.1 \times 10^{-8} T^3 - 7.0 \times 10^{-6} T^2 + 4.19 \times 10^{-5} T + 0.99985$

$\mu = -7.0 \times 10^{-8} T^3 + 1.002 \times 10^{-5} T^2 - 5.7 \times 10^{-4} T + 0.0178$

$\tau = 1.093 \times 10^{-4} T^2 + 2.102 \times 10^{-2} T + 0.5889$

n = porosity as fraction of aquifer volume

d_i^s = the maximum grain diameter in fraction i

d_i^d = the minimum grain diameter in fraction i

d_{10} = grain size (cm) corresponding to 10% by weight passing through the sieves

d_{20} = grain size (cm) corresponding to 20% by weight passing through the sieves

d_{50} = grain size (cm) corresponding to 50% by weight passing through the sieves

d_{60} = grain size (cm) corresponding to 60% by weight passing through the sieves

$U = d_{60}/d_{10}$

Δg_i = the fraction of mass that passes between sieves i and $i+1$ where i is the smaller sieve

Δw_i = fraction of total weight of sample with fraction identifier ' i '

d_i = mean grain diameter of the fraction i

m = the total number of fractions

$d_{i\phi}$ = mean grain diameter of the fraction i in phi units ($\phi = \log_2(d_e/d_o)$, d_e in mm, $d_o = 1$ mm)

I_o = x-intercept (grain size) of a percent grain-retention curve plotted on arithmetic axes and focussing on data below 50% retained

values they produce. The goal of this work was to create a tool that would compute K estimates from several selected relationships that users could compare and evaluate.

The development of a software tool that estimates K from grain size analyses is not new. Aguilar (2013) developed a Microsoft Visual Basic® code that computes K using 20 different estimation methods. Kasenow (2002) reviewed the subject in a 97 page book that included a software package to evaluate K using 6 different methods. Vuković and Soro (1992) developed a Fortran program to compute K using 10 different grain size analysis methods. However, the earlier software tools are either currently out of date, i.e., will not execute in the most common operating systems currently in use, or require some form of purchase to acquire. In contrast, the software described here, HydrogeoSieveXL, is readily available from the Devlin (2015) website, is free of charge, and runs in the Excel environment, to which most hydrogeologists have familiarity and ready access. It is also available as electronic supplementary material (ESM) with this article. The Vuković and Soro (1992) report was used as the basis for this work. HydrogeoSieveXL includes all 10 of the methods they considered plus 5 additional methods representing more recent research or alternative approaches (see Table 1).

2. Theory

In accordance with Vuković and Soro (1992), the general form of the relationship between K and grain size, which can be rationalized from the Darcy-Weissbach equation, is expressed as

$$K = \frac{\rho g}{\mu} N \phi(n) d_e^2 \quad (1)$$

where, ρ is the temperature-dependent water density (g mL^{-1}), g is the gravitational constant (cm s^{-2}), μ is the temperature-dependent dynamic viscosity of water ($\text{g cm}^{-1}\text{s}^{-1}$), N is a case-specific constant regarded as a ‘shape factor’, $\phi(n)$ is a function of porosity, and d_e is an effective grain size or function of the grain size distribution. The values of N , $\phi(n)$, and d_e have been defined in various ways, and these are summarized in Table 1. Note the similarity of this equation to the simpler representation given by Freeze and Cherry (1979),

$$K = k \frac{\rho g}{\mu} \quad (2)$$

where k is defined as the intrinsic permeability (cm^2). The equivalency of these two equations requires that k is dependent on the shape factor and porosity, both characteristics of the porous medium. The density and viscosity terms are representative of the fluid (water).

3. Implementation of the code

The majority of the calculations in HydrogeoSieveXL are performed in the Visual Basic® environment within Excel®. The tool is suitable for use with Excel 2010 and 2013. Other versions of Excel® have not been tested. The computation

of grain size characteristics, such as d_{10} , and K are initiated by clicking on labelled buttons in forms, and the code is contained in modules attached to those buttons. The primary user form in the program is the ‘Dashboard’, which is launched by clicking on the ‘Start’ button in the Input worksheet (Fig. 1).

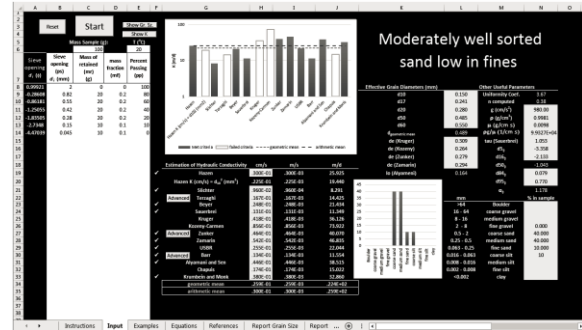


Figure 1: Screen capture of the HydrogeoSieveXL Input screen.

4. The HydrogeoSieveXL workbook

The HydrogeoSieveXL workbook comprises 7 worksheets: 1) a user manual that describes the details of the operation and functionality of the tool, 2) the HydrogeoSieveXL input worksheet where all the computational work is initiated, 3) a worksheet with sample data from selected literature sources, and where user-specific data sets can be stored for future reference, 4) a copy of Table 1, above, for reference, 5) a reference list with citations to contributing literature, 6) a sheet that summarizes the grain size data in a format suitable for pdf report generation and 7) a sheet that summarizes the K estimation calculations in a format suitable for pdf report generation. In general, work with HydrogeoSieveXL will be concentrated on the Input worksheet (Fig. 1).

Data can be entered into HydrogeoSieveXL in several ways. In all cases the sieve openings (in mm) are entered beginning at cell B8 and proceeding down the sheet. Next the user can choose to enter the remaining data as mass retained per sieve (in grams), mass fraction per sieve, or percent fraction per sieve. HydrogeoSieveXL will calculate and complete the remaining columns. To begin the data processing, the user clicks on the ‘‘Start’’ button under column C (Fig. 1). This action brings up the ‘‘Dashboard’’ userform (Fig. 2). The input data table is completed by clicking on the ‘‘Input Prep’’ button on the Dashboard. This must be done before any further calculations are initiated or an error results. To interpolate between data points, for the purposes of estimating characteristic grain sizes, such as d_{10} , either linear interpolation can be used or a smoothed curve can be generated using the Akima spline (adapted from the Fortran code of Moreau). The spline is activated by default, but can be disabled when the ‘smooth’ checkbox is deselected (see Fig. 2).

Upon completion of this step, a grain size distribution curve is produced in the upper central portion of the sheet (Fig. 1). Next, the user can select the ‘‘Do All’’ button on the

Dashboard to launch the entire suite of functions in the sheet. If the user wishes to execute only selected functions, the

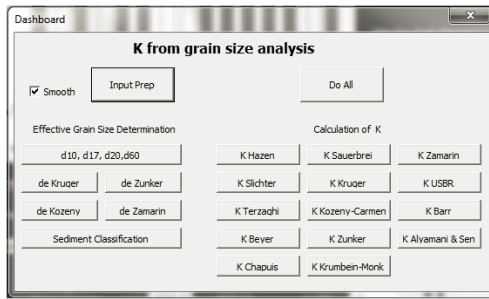


Figure 2: Screen capture of the Dashboard userform

Dashboard features buttons for each module in the workbook. The functions can be initiated or updated one at a time with these buttons. Details of the program functions are given in the user manual in the workbook.

When fully executed, HydrogeoSieveXL presents the completed data table, a grain size distribution curve, an extensive list of grain size characteristics from which effective grain diameters are calculated, a histogram of grain size distribution presented in terms of conventional grain size classes (clay, sand, gravel, etc.), and 15 estimates of K calculated from the formulas in Table 1. Each method is tested against the ‘applicable conditions’ specified in Table 1, and those that pass are indicated with check marks in column F and solid bars in the K summary bar chart. Quantitative criteria were used wherever possible. Where only qualitative criteria were available, (e.g., Kozeny-Carmen only specified ‘coarse sand’), d_{50} values were used to verify the sediment sample was in the range specified. Geometric and arithmetic means of the estimated K values are also calculated. A graphic illustrating the variation in K estimations can be displayed by clicking on the “Show K ” button, located next to the “Start” button on the Input screen (Fig. 3).

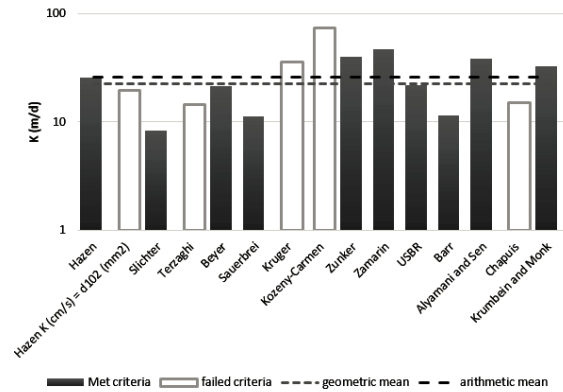


Figure 3: Screen capture of the HydrogeoSieveXL calculated K summary graphic.

5. Comparison with published K estimates

The validity of the calculations in HydrogeoSieveXL was verified by comparing calculated estimates of K with estimates calculated by Vuković and Soro (1992) and Odong (2013) (Fig. 4). Not all methods executed in HydrogeoSieveXL are represented in the comparisons shown below, but similar care was taken to ensure the calculations were completed correctly in all cases. The comparisons show that HydrogeoSieveXL is computing K estimates that are consistent with the earlier literature reports, and that this conclusion applies across a range of sediments. The slight differences in estimated K values visible in Fig. 4 are attributable to differences in the estimated values of characteristic grain size diameters, such as d_{10} , and d_{60} , possibly related to round-off errors, and are of no practical significance.

Conclusions

Grain size sieve analyses offer a convenient and economical means of acquiring preliminary estimates of hydraulic conductivity for sand and gravel deposits. Many techniques for extracting these estimates have been developed over the past century, and reliance on any single technique is probably unwise in many, if not most, cases. HydrogeoSieveXL is an Excel®-based tool for calculating K from grain size distributions curves using 14 different methods. The tool is available for free downloading from the Devlin (2015) website, and includes a user manual in the workbook. The HydrogeoSieveXL calculations compare well against previously published work.

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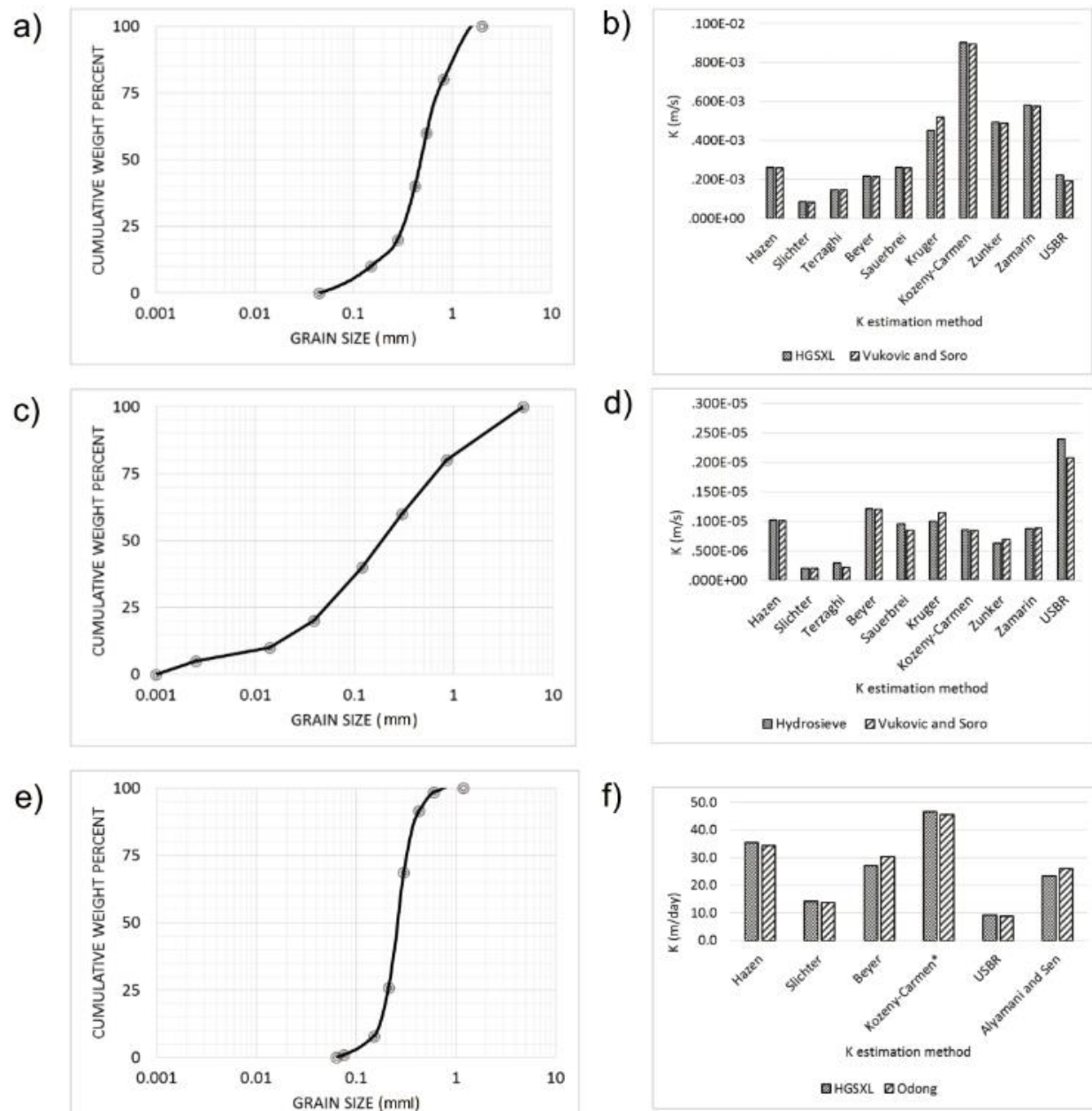


Figure 4: Comparison of HydrogeoSieveXL estimated K values and those calculated by others for three different sediments. a) the grain-size distribution curve of a moderately well sorted sand, b) comparison of K estimates from various methods and comparison of HydrogeoSieveXL calculations vs. calculations reported by Vuković and Soro (1992). c) the grain-size distribution curve of a poorly sorted sand with fines, d) comparison of K estimates from various methods and comparison of HydrogeoSieveXL calculations vs. calculations reported by Vuković and Soro (1992). e) the grain-size distribution curve of a well sorted sand, f) comparison of K estimates from various methods and comparison of HydrogeoSieveXL calculations vs. calculations reported by Odong (2013). Note: to match the Kozeny-Carmen K calculated by Odong, the d_e was set to d_{10} .

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