A New Automated Approach to Grain Size Analysis for Environmental Practitioners

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Background & Objectives

Introduction

- Estimation of hydraulic conductivity (K) from grain size distribution curves is well established with environmental practitioners as beneficial starting point for hydrogeological investigations.
- Developed automated procedure for Excel-based program, HydrogeoSieveXL™ (Figure 3), to streamline the calculation of K estimates in support of two-dimensional (2D) Stratigraphic Flux evaluations for multiple U.S. Air Force PFAS remedial investigations (RIs).
- Conventional approach requires up to 10 minutes per sample to manually format, import, and evaluate grain size results (Figures 3 and 4).
- The new tool extends analysis to include 16 methods to provide better indication of the statistically supported range of K that might apply.
- Primary objectives of new automation are to refine data ingestion, significantly reduce time required for data processing and evaluation and elimination of costs associated with labor.

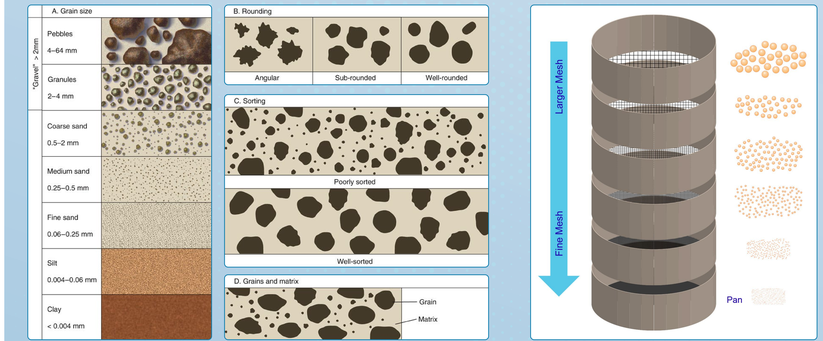


Figure 1 – Distribution of naturally-occurring grain sizes.

Figure 2 – Schematic depiction of grain separation using multiple sieve fractions to separate larger from smaller particles.

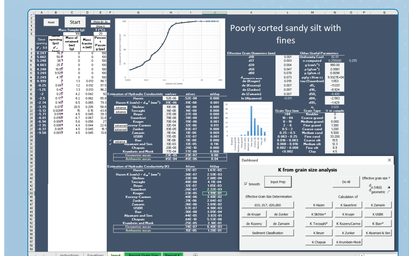


Figure 3

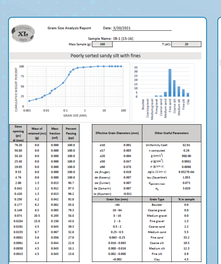
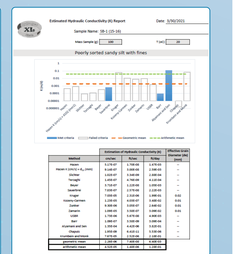


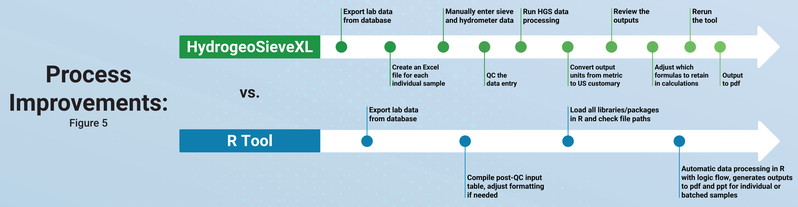
Figure 4



Design Approach

R Software™ Tool

- Digital workflow developed to integrate laboratory electronic data deliverables (EDDs) of grain size analysis results with automated data quality review, formatting, analyses, and reporting (Figure 5).
- Tool integrates same logic built into conventional HydrogeoSieveXL™ tool through scripts created in R software™.
- Processing steps:
  - Calculates effective grain size diameter for selected fundamental method and provides soil classification and weight percentages (in standard sieve and hydrometer ranges) to assess percent passing.
  - Calculates K estimates for each of the 16 methods and tests if fundamental criteria are met.
  - Calculates an innovative extrapolation to the zero for fine-grained fraction using monotone piecewise cubic interpolation (when needed).
  - Reports final K estimates along with arithmetic and geometric means with automated recommendation as an expression of central tendency.
  - Generates 1-page summary of grain size evaluation for each sample and master summary table of all outputs as a batch export.
- Process improvements – automation and batch processing eliminate manual data entry with refined method selection, resulting in significant reduction in time and costs.
- Representative central tendency value – computer algorithm to derive representative mean K value relying on Shapiro-Wilk normality test (Shapiro and Wilk, 1965) (n≥4) or coefficient of variation.
- Tool benefits include process automation, batch processing, customized inputs and outputs (Figure 7), in addition to the following:
  - New 1-page "At-A-Glance" summary.
  - Smoothing cubic-spline interpolation between points permits extrapolation to zero for finer materials.
  - Preferred US customary units of feet/second and feet/day.
- Current tool limitations:
  - Biased low estimates of K for mostly poorly-sorted samples with high gravel content.



α	Sorting Descriptor	Primary Component	d10 Value Specs	d10 Hazen	d10 Hazen K	d10 Schlichter	d10 Terzaghi	d10 Beyer	d10 Barr	d17 Sauerbrei	d17 Kruger	d17 Kozeny-Carmen	d17 Zunker	d17 Zamarin	d17 USBR	d17 Alyamani and Sen	d17 Chapuis	d17 Krumbein and Monk	d17 Shepherd	# of Methods Used
α, < 0.80	well sorted	clay	--						✓	✓										2
α, < 0.80	well sorted	silt	--					?	✓	✓										3
α, < 0.80	well sorted	fine sand	--			✓		✓	✓	✓			✓			✓	✓	✓	✓	8
α, < 0.80	well sorted	medium sand	--	✓		✓		✓	✓	✓	✓		✓		✓	✓	✓	✓	✓	11
α, < 0.80	well sorted	coarse sand	--	✓		✓	✓	✓	✓			✓	✓	✓		✓	✓	✓	✓	10
α, < 0.80	well sorted	gravel	--				?						?				?		?	3
0.80 < α, < 1	moderately sorted	clay	--						✓	✓										2
0.80 < α, < 1	moderately sorted	silt	--						✓	✓										2
0.80 < α, < 1	moderately sorted	fine sand	--					✓	✓	✓							✓	✓	✓	5
0.80 < α, < 1	moderately sorted	medium sand	--					✓	✓	✓							✓	✓	✓	5
0.80 < α, < 1	moderately sorted	coarse sand	--				✓	✓	✓					✓						5
0.80 < α, < 1	moderately sorted	gravel	--					?						?			?		?	3
α, > 1	poorly sorted	clay	--						✓	✓										2
α, > 1	poorly sorted	silt	--						✓	✓										2
α, > 1	poorly sorted	fine sand	--					✓	✓	✓									?	3
α, > 1	poorly sorted	medium sand	< 0.016					✓	✓	✓									?	3
α, > 1	poorly sorted	medium sand	> 0.016				✓	✓	✓	✓							✓		?	5
α, > 1	poorly sorted	coarse sand	< 0.016					✓	✓	✓									?	3
α, > 1	poorly sorted	coarse sand	> 0.016				✓		✓								✓		?	3
α, > 1	poorly sorted	gravel	< 0.016						?	?										2
α, > 1	poorly sorted	gravel	> 0.016						?								?		?	2
	Effect of trace fines	high bias	--	general low bias		low bias	--	low bias @ > 10%	--	--	significant high bias				general low bias	high or low bias	high bias	--	--	
	Effect of trace coarse sand/gravel	--	--	general low bias		low bias	--	low bias	--	--					general low bias	high or low bias	--	--	high bias	

Key: ✓ Method is applicable for this selection ? Method may be applicable for this selection, needs individual review

Figure 6 – Logic script and method comparison.

Benefits of Our New Tool: R Software

Automation
- Removes the manual entry of data and having to create each file

Batch Processing
- Utilizing digital improvements to streamline data processing and increase efficiency, reduction in processing time translates to cost savings
- Built-in logic script to review method selection and reduce anomalies/bias

Customized Inputs
- Can modify the code to process any input file design, promotes increased flexibility

Customized Outputs
- Allows for project-specific K-estimate selection methodology
- Extrapolation to zero passing using natural cubic-spline interpolation
- Customized graphics and design to meet client needs

Figure 7

Results

Summary

- New automation eliminates traditional manual data entry, has capability to analyze unlimited number of grain size results as batch exports, incorporates strengthened statistical review, generates report-ready exhibits (Figures 8 and 9), and greatly reduces data processing time required with conventional method from hours to minutes.
- Addresses pervasive issue of costly data analysis, while providing an improved solution through automated refinement, which includes auto-formatted data, method selection, statistical strength, interpolation of finer sieve fractions, improved lithologic descriptions, and reduction in human error.
- Automated tool processes grain size results in <7 seconds per sample, resulting in 100% reduction in data entry, 100% reduction in time spent formatting report-ready figures and tables, 98.8% reduction in data processing and a 600% improvement to productivity (irrespective of project scale).
  - Advantages of automated tool:
    - Improved data digestion automation and bulk processing.
    - Interpolation for an expanded understanding of finer grained fractions.
    - Improved statistical rationale.
    - Faster reporting and time to delivery, saving time and cost.
    - Facilitated scalability, potential for global application.

Figure 8

Figure 9

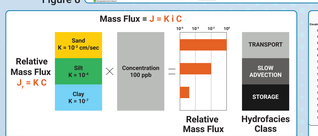


Figure 10 – Simplified equation for Stratigraphic Flux (aka. relative mass flux).

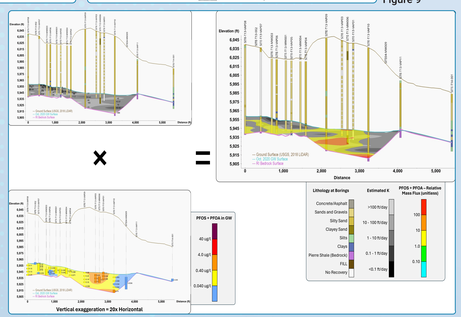


Figure 11 – 2D Stratigraphic Flux evaluations conducted during PFAS Remedial Investigations (RIs) at U.S. Air Force installations.

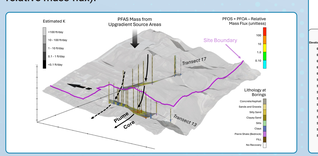


Figure 12 – 3D depiction of interpretated core plume migration pathways based on Stratigraphic Flux evaluations.

References

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HydrogeoSieve v.2.2: Devlin, J.F. 2016. Reply to "Comment on "HydrogeoSieveXL: an Excel-based tool to estimate hydraulic conductivity from grain-size analysis": report published in Hydrogeology Journal (2015) 23: 837-844 by J.F. Devlin", Hydrogeology Journal, DOI 10.1007/s10040-016-1510-z.
(Note the current version is v2.3.10 released March 26, 2024.)

R software: R Core Team (2024). R: A Language and Environment for Statistical Computing. R Foundation for Statistical Computing, Vienna, Austria. <https://www.R-project.org/>.

Packages used by R software tool: Librarian, readr, readxl, dplyr, doBy, lubridate, DescTools, devtools, flextable, ggplot2, officer, openxlsx, splines, scales, EnvStats, grid, viridis, gridtext, stringr, and docxtractr. (https://cran.r-project.org/web/packages/available_packages_by_name.html)

Shapiro, S.S. and M.B. Wilk. 1965. An analysis of variance test for normality (complete samples). Biometrika, 52, 591-611.

Figure 1 – https://www.geologyin.com/2015/11/study-reveals-how-climate-influences.html

Figure 2 – Sieve Analysis - Particle Technology Labs (particletechlabs.com)

Acknowledgements

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