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PKgui: A GUI software for Polubarinova-Kochina's solutions of steady unconfined groundwater flow

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ABSTRACT

A Python program and standalone executables with a graphical user interface (PKgui) have been developed to solve the classical semi-analytic solutions derived by Polubarinova-Kochina for a steady unconfined aquifer across a rectangular dam/aquifer. Although considered very useful in geotechnical and groundwater communities, these solutions have not been widely used in the literature due to their mathematical and computational complexities. Using nonlinear least squares optimization toolbox, this program solves a set of coupled nonlinear integral equations directly, efficiently, and accurately. Lastly, a theoretical limit to applicability of Polubarinova-Kochina's results and therefore the software outputs are also discussed.

Code metadata

Current code version	1.0.0
Permanent link to code/repository used for this code version	https://github.com/ElsevierSoftwareX/SOFTX-D-23-00635
Permanent link to Reproducible Capsule	https://zenodo.org/records/8034146
Legal Code License	MIT
Code versioning system used	git
Software code languages, tools, and services used	Python
Compilation requirements, operating environments & dependencies	Python version ≥ 3.5, Numpy ≥ 1.16, Scipy ≥ 1.5, PySimpleGUI ≥ 4.55.1 and Matplotlib ≥ 3.5.0.
If available Link to developer documentation/manual	https://github.com/mashadab/PKgui#readme
Support email for questions	mashadab@utexas.edu or mhesse@jsg.utexas.edu

Software metadata

Current software version	1.0.0
Permanent link to executables of this version	https://github.com/mashadab/PKgui/blob/main/Executables.zip
Permanent link to Reproducible Capsule	https://zenodo.org/records/8034146
Legal Software License	MIT
Computing platforms/Operating Systems	Windows, Mac
Installation requirements & dependencies	None. Download and run executable with administrator privileges (e.g., using `chmod 777 Pbk_Mac` on Mac).
If available, link to user manual — if formally published include a reference to the publication in the reference list	https://github.com/mashadab/PKgui#readme
Support email for questions	mashadab@utexas.edu or mhesse@jsg.utexas.edu

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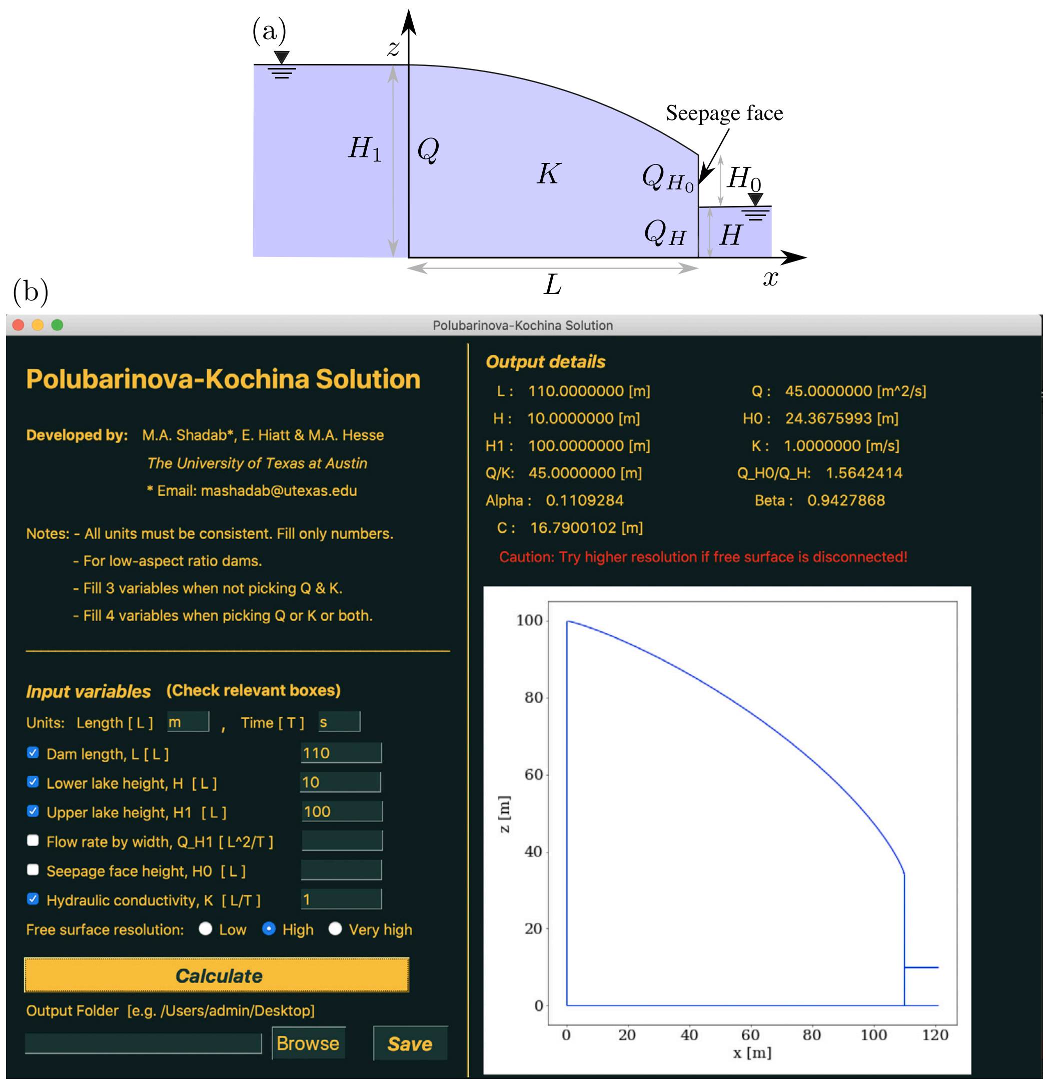

Fig. 1. A cross-sectional view of an unconfined groundwater flow through a rectangular dam/aquifer: (a) A schematic highlighting the variables considered in the solution by Polubarinova-Kochina [1]. (b) A snapshot of PKgui software in action. The supplementary video S1 contains the tutorial for downloading and using PKgui software either in Python or as a standalone executable.

1. Motivation and significance

Groundwater has been intensively studied for centuries [1–4], and an understanding of groundwater hydrology is necessary to deliver clean water for agricultural use and human consumption as well as mitigating its effects on civil engineering projects such as dams [5–7]. For these reasons, many useful approximations have been developed to investigate groundwater flow, however each approximation leans on various underlying assumptions that reduce the complexity of the associated physics [4,8,9]. These assumptions are key to allowing sophisticated software to remain computationally tractable while making accurate predictions ranging from aquifer recharge rates to contaminant mitigation [10,11].

The simplifying assumptions in some models may disregard a grou ndwater process of interest. For example, seepage faces are land surfaces where groundwater debouches directly from an aquifer into atmospheric conditions [12]. Seepage face dynamics cannot be captured using typical Boussinesq-type methods and must be treated with either more complex mathematics or non-physical numeric treatment of the approximation being implemented [13–18]. There is, however, one semi-analytic solution to the seepage face boundary without capillary fringe effects that was introduced by Polubarinova-Kochina in 1962 [1]. However, this solution is seldom used either directly or to validate numeric models. This lack of usage is attributed to the complexity of the mathematical equations and their numerical implementation [19–21].

In this study, we develop a user-friendly GUI software, referred to as PKgui [22], to evaluate Polubarinova-Kochina's seepage formulas to study steady unconfined groundwater flow across rectangular dam/aquifer. The results of PKgui software are validated and compared with the literature (see Supplementary Information file linked in Appendix A). In addition to the applications towards scientific studies concerning groundwater flow and engineering designing of dams, the results of PKgui software can serve a fundamental test for such groundwater models, as suggested in [23]. We also discuss in detail the critical limit beyond which the Polubarinova-Kochina solutions may not be applicable.

2. Software description

PKgui software considers the steady unconfined aquifer with a vertical seepage face. For a given set of inputs aquifer/dam parameters the software can provide other crucial parameters as well as phreatic surface height (water table elevation). The outputs shown in the software can be saved in a designated folder in CSV format for further analysis. The algorithm is very fast and provides accurate results which can eliminate the need to run expensive high-fidelity simulations. The software executables can be run without installation after downloading on Mac and Windows operating systems (OS). The open-source Python GUI program can be run on any OS with required dependencies installed. Below we summarize the different aspects and components of PKgui software.

2.1. Mathematical framework and computation strategy

The software relies on the theory and numerical implementation presented in this section. Fig. 1*a* shows the schematic of this problem and highlights the parameters and variables. The variables under consideration are the length of the homogeneous porous aquifer [L], L, and the heights [L] of the lower lake (also referred to as tailwater), H, upper lake, H_1 and seepage face, H_0. The hydraulic conductivity of the porous medium [L/T] is denoted by K. The flow rates per unit width (in the third dimension) [L^2/T] are Q_{H_0} across the seepage face, Q_H across the boundary adjacent to the lower lake and Q (or Q_{H_1}) being the total flow incoming from the left boundary. Lastly, x and z are the coordinates in horizontal and vertical directions respectively. The semi-analytical solution by Polubarinova–Kochina [1] can be written as a set of nonlinear integral equations as

$$L = C \int_0^{\pi/2} \frac{\mathcal{K}(\alpha + (\beta - \alpha)\sin^2\varphi)}{(1 - \alpha - (\beta - \alpha)\sin^2\varphi)^{1/2}} \mathrm{d}\varphi, \tag{1}$$

$$H = C\sqrt{\alpha} \int_0^{\pi/2} \frac{\mathcal{K}(\alpha \sin^2\varphi)\sin\varphi}{((1 - \alpha\sin^2\varphi)(\beta - \alpha\sin^2\varphi))^{1/2}} \mathrm{d}\varphi, \tag{2}$$

$$H_0 = C \int_0^{\pi/2} \frac{\mathcal{K}(\cos^2\varphi)\sin\varphi\cos\varphi}{((1 - \alpha_1\sin^2\varphi) - (1 - \beta_1\sin^2\varphi))^{1/2}} \mathrm{d}\varphi, \tag{3}$$

$$H_1 = H + H_0 + C \int_0^{\pi/2} \frac{\mathcal{K}(\cos^2\varphi)\sin\varphi}{((1 - \alpha\sin^2\varphi) - (1 - \beta\sin^2\varphi))^{1/2}} \mathrm{d}\varphi, \tag{4}$$

$$Q_H = KC\sqrt{\alpha} \int_0^{\pi/2} \frac{\mathcal{K}(1 - \alpha\sin^2\varphi)\sin\varphi}{((1 - \alpha\sin^2\varphi)(\beta - \alpha\sin^2\varphi))^{1/2}} \mathrm{d}\varphi, \tag{5}$$

$$Q_{H_0} = KC \int_0^{\pi/2} \frac{\mathcal{K}(\sin^2\varphi)\sin\varphi\cos\varphi}{((1 - \alpha_1\sin^2\varphi) - (1 - \beta_1\sin^2\varphi))^{1/2}} \mathrm{d}\varphi \quad \text{and} \tag{6}$$

$$Q = Q_H + Q_{H_0}. \tag{7}$$

where $\alpha, \beta, C \in \mathbb{R}$ are the unknown model parameters with $0 \le \alpha < \beta < 1$, $\alpha_1 = 1 - \alpha$ and $\beta_1 = 1 - \beta$. The function $\mathcal{K}(\cdot)$ is the elliptic integral of the first kind defined as

$$\mathcal{K}(k) = \int_0^{\pi/2} \frac{\mathrm{d}\varphi}{(1 - k\sin^2\varphi)^{1/2}}. \tag{8}$$

The formula for the phreatic surface (water table) as a curve in the $x - z$ plane is parametrized in terms of Ψ where x is the location and z is the corresponding phreatic surface height. These formulae are

$$x(\Psi) = L - C \int_0^{\Psi} \frac{\mathcal{K}(\sin^2\varphi)\sin\varphi}{((1 - \alpha\sin^2\varphi)(1 - \beta\sin^2\varphi))^{1/2}} \mathrm{d}\varphi \quad \& \tag{9}$$

$$z(\Psi) = H + H_0 + C \int_0^{\Psi} \frac{\mathcal{K}(\cos^2\varphi)\sin\varphi}{((1 - \alpha\sin^2\varphi)(1 - \beta\sin^2\varphi))^{1/2}} \mathrm{d}\varphi. \tag{10}$$

Now we describe the numerical strategy used in PKgui software to solve the semi-analytic model. First, the input variables are non-dimensionalized using a characteristic variable chosen from the inputs provided. Next, a set of three equations corresponding to the given input variables is selected from Eqs. (1)–(7). The chosen equations are then solved simultaneously for α, β and C using the nonlinear least squares optimization toolbox in python. The rest of the variables are evaluated from other equations by plugging in the estimated values of these unknowns and then redimensionalizing. Note that the number of required input variables changes from three to four depending on whether Q and/or K are specified. A list of all valid combinations of input parameters is provided in Table 1. Finally, the free surface heights, $z(\Psi)$, at horizontal locations, $x(\Psi)$, are evaluated from Eqs. (9) and (10) for the different values of Ψ corresponding to $0 \le x \le L$ depending on the requested resolution. For example the in Fig. 1*b*, providing the values of L, H and H_1 as inputs will prompt a simultaneous solution of Eqs. (1), (2) and (4) for α, β and C. The remaining variables, namely H_0, Q_H, Q_{H_0} and Q can be calculated from Eqs. (3) and (5)–(7) respectively. The free surface height z is evaluated for horizontal location x from Eqs. (9) and (10), depending on the requested resolution.

2.2. Software architecture

The architecture of the software is very simple and straightforward, as shown Fig. 1*b*. The portion left of the vertical bar represents the input section, whereas the right side represents the output.

2.3. Software functionalities

2.3.1. Estimating multiple dam/aquifer parameters

PKgui software allows for the selection of a set of three or four problem variables while studying a groundwater problem or designing a dam. The rest of the physical parameters are calculated as

Table 1
A summary of self-consistent sets of input variables for PKgui software.

S.No.	L [L]	H [L]	H_1 [L]	Q (or Q_{H_1}) [L^2/T]	H_0 [L]	K [L/T]
1	✓	✓	✓			
2		✓	✓	✓		
3	✓		✓	✓		
4	✓	✓		✓		
5	✓	✓	✓		✓	
6		✓	✓	✓	✓	
7	✓		✓	✓	✓	
8	✓	✓		✓	✓	
9	✓	✓	✓			✓
10		✓	✓	✓		✓
11	✓		✓	✓		✓
12	✓	✓		✓		✓
13	✓	✓			✓	✓
14	✓		✓		✓	✓
15		✓	✓		✓	✓
16		✓		✓	✓	✓
17			✓	✓	✓	✓
18	✓			✓	✓	✓

a result, which makes it very useful to choose independently depending on the choice of physical observations in field or laboratory experiments [24]. Variables include different lengths, flow rates, and hydraulic conductivity of the aquifer.

2.3.2. Calculation of free surface elevation

The software also outputs the resulting groundwater table elevation at each horizontal location. This resolution can be changed from low to very high in the software by using the radio button. For a low aspect ratio, low resolution leads to faster computation and provides a continuous water table profile. However, relatively high aspect ratio dams/aquifers will require higher free surface resolution for the full profile, which will take a longer time for computation.

2.3.3. Storing the output data

PKgui software shows both the output variables as well as the image of the free surface profile to provide the user more information and accessibility. The software creates a new folder corresponding to a unique test problem in the directory selected by user. Inside the folder, several new output files are created. The input and output variables are stored in file 'details.csv' in CSV format. The free surface profile (x vs z) values are stored with the filename 'free-surface-profiles_XandZ.csv' in CSV format for further analysis. High and low resolution images are stored with the filename 'free-surface-profile' in both high resolution PDF and low resolution PNG formats.

2.3.4. Range of applicability

Polubarinova-Kochina [1] results are not valid for a very high aspect ratio aquifer with $L < H_1$ that has not been studied in detail in the literature. In fact, the original source [1] only presents results for geometries with lower aspect ratio using infinite series approximations and graphical interpolations, except for some limiting cases amenable to simple analytic solutions. Here we find that Polubarinova-Kochina's solutions for free surface height become nonphysical for large aspect ratios when vertical flow effects are negligible compared to the horizontal flow effects [25]. To understand the range of applicability of Polubarinova-Kochina [1] solutions, the equations of the governing model [1,17] are scaled in [26], resulting in a dimensionless parameter

$$\Pi = \frac{2Q}{KL} = \left(\frac{H_1}{L}\right)^2 - \left(\frac{H}{L}\right)^2, \quad (11)$$

that compares the relative importance of vertical and horizontal flow across the aquifer [26]. Semi-analytical solutions for the free surface height deteriorate below a critical value of $\Pi = 0.1$ and therefore this value is set as the lowest threshold value for PKgui software. This limit is corroborated by the original results [1,27] where the value of Π for the cases with the highest aspect ratio considered lie close to this critical value. For example, Polubarinova-Kochina [1] results in Supplementary Figure S1*c* end at the red dot which corresponds to $\Pi = 0.175 \pm 0.071$. In [26], we found the same critical Π value for a recently proposed model [17] using a physics-informed machine learning approach. The Dupuit–Forchheimer discharge formula [12] should work well below this critical value of Π for such steady-state flows, because the vertical flow effects as well as the seepage face height become negligible.

3. Illustrative examples

3.1. Instructions to use PKgui software

1. Fill in the *units* of length and time or leave it blank.
2. Check the relevant boxes to select the input variables and enter the values with consistent units and dimensions given in brackets. See Table 1 for all self-consistent sets of input variables for PKgui software.
3. Select resolution of the free surface using the radio button.
4. Click *Calculate* to evaluate.
5. Click *Browse* to select a location of the output folder.
6. Click *Save* for saving the output files.

3.2. An example problem

For the problem shown in Fig. 1*b*, the parameters selected are units of meters for distance and seconds for time, length of the dam/aquifer $L = 110$ m, lower lake height $H = 10$ m, upper lake height $H_1 = 100$ m and hydraulic conductivity $K = 1$ m/s. Although hydraulic conductivity K is not needed to perform the calculations, either K or the flow rate is required to estimate the corresponding flow variables. The supplementary video gives a short tutorial on the working of this software, starting from downloading the Python program or standalone executable to running this example problem.

3.3. More examples including code verification and model validation (see supplementary information linked in Appendix A)

An array of tests is performed for validation against data available in the literature [1,19], limiting cases amenable to simple analytic results [1] and high-fidelity two-dimensional groundwater flow simulations [23]. The supplementary information contains these validation examples along with the corresponding discussions. In general, PKgui software shows excellent validation with literature. Furthermore, the results of the two-phase groundwater flow simulations show an excellent comparison with the software results (Supplementary Figure S2).

4. Impact

Our developed software, PKgui, brings multiple benefits to several fields in science and engineering. In science, it can help to understand and predict the flow of groundwater and contaminants. It helps eliminate the need for charts [21] and approximations that use infinite series as well as graphical interpolation [1] that may not be accurate. Moreover, it may help avoid the usage of highly expensive, high-fidelity groundwater flow simulations. PKgui software results can be used directly in hydrological and environmental sciences. In the groundwater modeling community, it offers a simple, yet challenging benchmark problem for high-fidelity groundwater flow simulators, as suggested in [23]. The field currently lacks such benchmark problems that impede the rapid advancement of mathematical and computational groundwater modeling [28]. Several laboratory [24] and field studies require this software to be able to compare against laboratory and field data. PKgui software outputs can also be used in the geotechnical engineering community for dam construction and planning. Finally, PKgui software can be integrated with advanced machine learning algorithms, as discussed in [25], to account for the capillary effects associated with various types of soils.

5. Conclusions

In this work, we present a simple GUI-based software called PKgui to evaluate semi-analytical solutions for an unconfined aquifer with a vertical seepage face provided by Polubarinova-Kochina [1]. The software takes a diverse set of input dam/aquifer parameters and numerically solves the system of non-linear integral equations directly, efficiently, and accurately. The output variables as well as water table location are shown instantly for accessibility and can be stored at a designated location in CSV format. The solutions work well for relatively low aspect ratio aquifers. PKgui software results are useful for comparison with the literature data and high-fidelity groundwater flow simulations, thus eliminating the need for the latter. This user-friendly software impacts fields including hydrology, environmental science, geotechnical engineering, and flow modeling. The software identifies and utilizes a theoretical limit for the applicability of Polubarinova-Kochina's semi-analytical solutions, particularly for high aspect ratio aquifers (with $\Pi \lesssim 0.1$), where vertical flow effects and seepage face height are negligible.

Declaration of competing interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

Data availability

I have shared the zenodo repository of the code.

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Appendix A. Supplementary data

Supplementary material related to this article can be found online at https://doi.org/10.1016/j.softx.2023.101573.

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