Software Impacts 15 (2023) 100464

Contents lists available at ScienceDirect

Software Impacts

journal homepage: www.journals.elsevier.com/software-impacts

Original software publication

FluxPAW: A standalone software to calculate flux-based plant available water

Marina Luciana Abreu de Melo *, Quirijn de Jong van Lier

Soil Physics Laboratory, Center for Nuclear Energy in Agriculture, University of São Paulo, P.O. Box 96, Piracicaba, São Paulo, Brazil

ARTICLE INFO

Keywords:
Field capacity
Limiting point
Wilting point
Flux-criterion
Matric flux potential
Transpiration

ABSTRACT

Soil water contents at field capacity (FC), the limiting point (LP), and the wilting point (WP) delimit the fractions of soil water availability, the plant available water (PAW). FC is primarily a function of soil hydraulic properties, whereas LP and WP depend on soil, plant, and atmospheric conditions. The difference between FC and WP is called total available water, whereas FC minus LP is the readily available water. The flux-based method (FBM) predicts PAW from unsaturated soil water flow, rooting characteristics, and atmospheric water demand. This paper presents FluxPAW, a software to calculate PAW using the FBM algorithm.

Code metadata

Current code version	v3.0
Permanent link to code/repository used for this code version	https://github.com/SoftwareImpacts/SIMPAC-2022-291
Permanent link to reproducible capsule	https://codeocean.com/capsule/5187437/tree/v2
Legal code license	MIT license
Code versioning system used	git
Software code languages, tools and services used	Fortran-90
Compilation requirements, operating environments and dependencies	Fortran-90 compiler
If available, link to developer documentation/manual	https://github.com/marinalamelo/flux_based_PAW/blob/main/README.md
Support email for questions	marinaluciana94@gmail.com

1. Introduction

Plant available water (PAW) is a term used to refer to the fraction of soil water available to plants. To define PAW, three limiting values are commonly used. The upper limit of PAW, sometimes referred to as field capacity (FC), corresponds to a relatively low drainage rate, discounting the portion of water that quickly drains to deeper layers beyond the rooting depth at water contents higher than FC. A lower limit of PAW is the permanent wilting point (WP), corresponding to a condition in which the rate of water extraction by plant roots in the dry soil is too low for plant survival. The total available water (TAW) is defined by the difference between FC and WP. To refer to the readily available water (RAW), an intermediate condition is defined, the limiting point (LP), at which the plant transpiration turns from its potential sink-limited value into a lower source-limited rate, determined by soil hydraulic properties and root geometry. RAW is then defined as FC minus LP [1].

Recently, a method to quantify PAW based on flux-based approaches for FC and LP [2–4], and a novel flux-based approach for WP was proposed by Ref. [5], referred to as the FBM. The calculation of FC, LP, WP, TAW, and RAW according to the FBM is performed by an algorithm available as the standalone software FluxPAW. The current version of FluxPAW (v3.0) allows the quantification of PAW in monolayer Van Genuchten – Mualem type soils for different FC flux criteria, soil depths, root densities, and potential transpiration rates.

DOI of original article: https://doi.org/10.1016/j.geoderma.2022.116253.

The code (and data) in this article has been certified as Reproducible by Code Ocean: (https://codeocean.com/). More information on the Reproducibility Badge Initiative is available at https://www.elsevier.com/physical-sciences-and-engineering/computer-science/journals.

* Corresponding author.
E-mail address: melo.marina@usp.br (M.L.A. de Melo).

https://doi.org/10.1016/j.simpa.2023.100464
Received 7 December 2022; Received in revised form 21 December 2022; Accepted 31 December 2022

2665-9638/© 2023 The Author(s). Published by Elsevier B.V. This is an open access article under the CC BY license (http://creativecommons.org/licenses/by/4.0/).

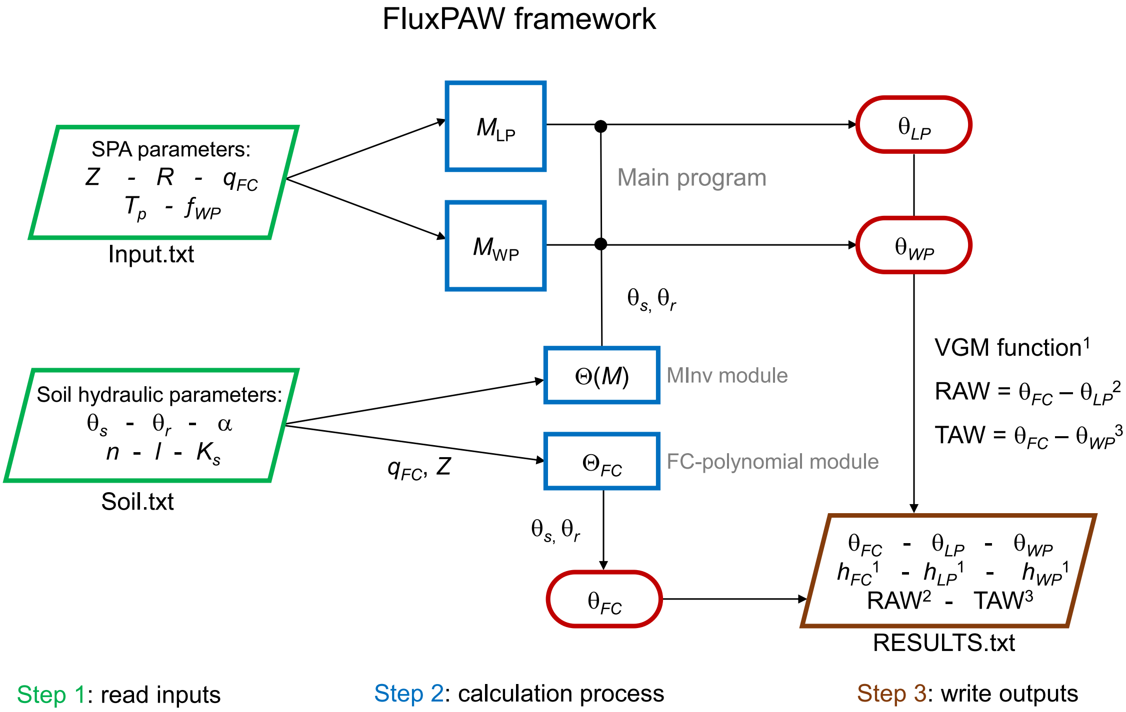

Fig. 1. Flowchart of the flux-based calculation of soil water content at field capacity (θ_{FC}), at the limiting point (θ_{LP}), and at the wilting point (θ_{WP}), their respective pressure heads (h_{FC}, h_{LP}, h_{WP}) calculated using eq. (3), readily available water (RAW), and total available water (TAW) according to the flux-based method to predict plant available water [5]. The soil hydraulic parameters refer to the Van Genuchten–Mualem (VGM) functions [6]. Effective saturation at FC (Θ_{FC}) is calculated using eq. (1). Matric flux potential at the LP (M_{LP}) and at the WP (M_{WP}) are calculated using eq. (2) and eq. (4).

2. Software design and functionality

The FBM algorithm is written as Fortran-90 routines (one main program and two modules), gathered, and compiled into a software executable in Windows (FluxPAW.exe) and available for download at https://github.com/marinalamelo/flux_based_PAW. Alternatively, the open-source code has been shared in The Code Ocean platform [7], in which the users can copy, execute and modify the adapted FBM algorithm on cloud.

The input parameters are provided in two input files (text file format, .txt) that should not be renamed or have their headers modified: "Input.txt" and "Soil.txt". These files should be placed in the same directory (folder) as the software or its source code. The file "Input.txt" includes the following Soil–Plant–Atmosphere (SPA) parameters: soil or rooting depth Z (cm); root length density R (cm cm^{-3}), FC flux criterion q_{FC} (mm d^{-1}), potential transpiration T_p (mm d^{-1}), and wilting factor (f_{WP}). The file "Soil.txt" includes soil identification, and the soil hydraulic parameters according to the Van Genuchten–Mualem (VGM) hydraulic functions [6]: residual soil water content θ_r, saturated soil water content θ_s, model fitting parameters α (cm^{-1}), n, and l, and the saturated hydraulic conductivity K_s (cm d^{-1}). After execution of the software by double left-clicking, an output file named "RESULTS.txt" is generated.

The number of soils or VGM parameter sets and the number of SPA parameter sets provided in the respective input files are unlimited. Each set of SPA parameters will be combined with all sets of VGM parameters. For example, if three sets of SPA parameters and five sets of VGM parameters are provided, the output file will contain three tables, each one with five lines of calculated values for the soil water content at field capacity θ_{FC}, limiting point θ_{LP}, and wilting point θ_{WP}, the pressure heads at field capacity h_{FC} (cm), limiting point h_{LP} (cm), and wilting point h_{WP} (cm), readily available water (RAW), and total available water (TAW).

3. Calculation process

To calculate Θ_{FC}, the effective saturation at field capacity, the full FC-polynomial expression developed by Ref. [3] is applied using the VGM parameters α (m^{-1}), n and l, the saturated hydraulic conductivity K_s (m d^{-1}), the soil depth Z (m), and the FC flux criterion q_{FC} (mm d^{-1}) as predictors, according to

$$\Theta_{FC} = \mathrm{b_i} log_{10}\alpha + \mathrm{b_{i+1}} n^{-1} + \mathrm{b_{i+2}} l + \mathrm{b_{i+3}} log_{10} K_s + \mathrm{b_{i+4}} log_{10}\mathrm{Z} + \mathrm{b_{i+5}} log_{10} q_{FC} \cdots \tag{1}$$

where b_i is the ith coefficient of the FC-polynomial expression. Θ_{FC} is transformed into θ_{FC} according to

$$\theta_{FC} = \theta_r + \left(\theta_s - \theta_r\right) \Theta_{FC}$$

where θ_r and θ_s are the residual and saturated soil water content.

To find θ_{LP}, firstly the matric flux potential at the limiting point (M_{LP}, m^2 s^{-1}) is calculated using Z, R, and T_p as predictors [4]:

$$M_{LP} = \int_{h_{ref}}^{h_{LP}} K dh = \frac{1.69 T_p}{Z R} \tag{2}$$

Then, θ_{LP} is calculated using an inverse solution for the M expressions derived by Ref. [8], and h_{LP} is calculated from θ_{LP} using the VGM function according to

$$\left|h_{LP}\right| = \frac{\left[\left(\frac{\theta_{LP}-\theta_r}{\theta_s-\theta_r}\right)^{\frac{n}{1-n}} - 1\right]^{\frac{1}{n}}}{\alpha} \tag{3}$$

To calculate θ_{WP} and h_{WP}, an analogous procedure is applied. An additional parameter - f_{WP} - is required to calculate M_{WP}, the matric flux potential at the wilting point, according to

$$M_{WP} = \int_{h_{ref}}^{h_{WP}} K dh = \frac{1.69 T_p f_{WP}}{Z R} = M_{LP} f_{WP} \tag{4}$$

and, consequently, θ_{WP} and h_{WP}. Finally, RAW and TAW fractions are calculated straightforward by making RAW = θ_{FC} − θ_{LP}, and

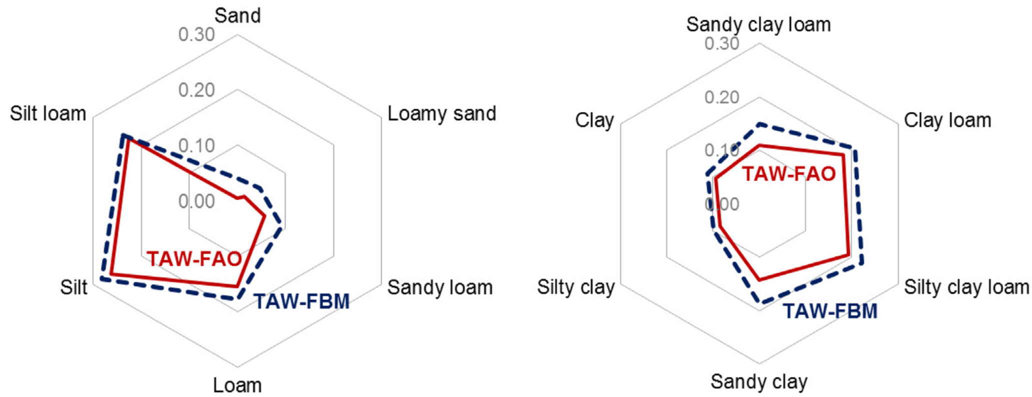

Fig. 2. Total available water (TAW) calculated according to the FAO method (FAO) and the flux-based method (FBM) using FluxPAW for 12 soil texture classes of the USA Soil Texture Classification. Fixed parameters: $h_{FC} = -1$ m, $h_{WP} = -150$ m (FAO); $Z = 100$ cm, $T_p = 4$ mm d^{-1}, $R = 1$ cm cm^{-3}, $q_{FC} = 1$ mm d^{-1} (FBM).

TAW = $\theta_{FC} - \theta_{WP}$. The flowchart in Fig. 1 shows the algorithm implementation. Further details of the theory underlying the FBM and FluxPAW are provided in Ref. [2–5,8].

4. Impact overview

The FluxPAW software allows straightforward calculation of flux-based plant available water (PAW). It does not make use of any traditional pressure head value to define field capacity and the wilting point, nor does it apply empirical parameters to calculate the limiting point [5]. Programming skills are not required, filling in the input files is easy and calculation process is fast.

Regarding the potential applications for decision-making in agricultural systems, the prediction of flux-based PAW can improve irrigation management strategies, avoid productivity losses due to water stress and even allow the saving of irrigation water due to a proper and process-based definition of the limits and ranges of PAW. The flux-based method proposed by Ref. [5] and implemented in FluxPAW is a promising approach to quantify water availability mediated by unsaturated soil water flow, rooting characteristics, and atmospheric water demand, serving an important role in vadose zone research.

5. Limitations

FluxPAW requires at least 11 environmental parameters to run. Some of them, such as soil hydraulic properties and root length density, are not always available. As exemplified by Ref. [5], the soil hydraulic parameters can be predicted from pedotransfer functions but this may add additional uncertainty to the predictions. Indeed, it is implicit that the application of a more robust method to predict PAW will also demand a better prospection of the environment. Hence, it is a subjective and cost-benefit matter of whether it is worth it for the common user to change his routine predictions in order to refine the crop water use assessment and management.

Concerning theory limitations, the calculation of PAW using FluxPAW is only applicable to single-layered homogeneous soil profiles regarding the soil hydraulic properties and the root density distribution. Besides, since free drainage conditions are assumed at the bottom of the soil profile for FC prediction, the influence of groundwater levels and capillary rise on FC is neglected. The ability of plants to use water between saturation and FC [9] is also neglected since FC is assumed as the upper limit of PAW. Despite these limitations, the proposed flux-based method is an advance in the process-based prediction of PAW, which may help overcome some limitations of traditional calculations of PAW [5].

6. Future improvements and applications

Improvements in the structure of FluxPAW towards the development of a user-friendly interface with an automatic graph generator will be addressed in the future to improve the user's experience. Further development of the theory behind FluxPAW will focus on better addressing the FC flux criterion, the definition of the bottom boundary condition for shallow groundwater tables, the discretization of the soil profile into layers with different soil hydraulic properties, as well as a comprehensive evaluation of the residual transpiration associated with the wilting point. A link to user-defined pedotransfer functions may also be included.

FluxPAW predictions can be compared with those of the traditional FAO method [10]. Here, both methods were applied to a generic crop, for several soils. The soils were represented by average hydraulic parameters estimated by Ref. [11] for the 12 texture classes of the USDA Soil Texture Classification. For the FAO method, the water content at FC and the WP was associated with pressure heads of −1 m and −150 m, respectively. The water content at the LP was calculated using the depletion fraction $p = 0.5$. For the flux-based method (FBM) implemented in FluxPAW, the soil depth, the potential transpiration, the root length density, the FC flux criterion, and the wilting factor were set at 100 cm, 4 mm d^{-1}, 1 cm cm^{-3}, 1 mm d^{-1} and 10^{-2}, respectively. In this scenario, TAW values were relatively similar between the methods for all texture classes, with a root mean square deviation (RMSD) equal to 0.03 (Fig. 2), while RAW values were considerably higher for the FBM (RMSD = 0.1), except for sand and loamy sand classes (Fig. 3). The inclusion of rooting characteristics to calculate RAW instead of using a fixed fraction of TAW was the main driving factor for the differences between the methods.

There are a number of other applications of the software within our ideas for future research. Ongoing research projects will use the software to predict PAW using experimental data of soil water content related to plant water status, and transpiration or water uptake rates in different environmental conditions. Other studies are encouraged to intensively test the accuracy of flux-based PAW predictions in numerous observed scenarios focusing on a consistent validation of the method [5].

Dynamic predictions of PAW could be made by coupling FluxPAW to a model that simulates soil water dynamics, such as SWAP [12] or Hydrus [13]. The predictions of flux-based PAW using FluxPAW can also be compared with several methods to predict PAW for different soil textures, plant, and atmospheric conditions in order to verify its effectiveness and robustness as a tool in environmental studies.

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.

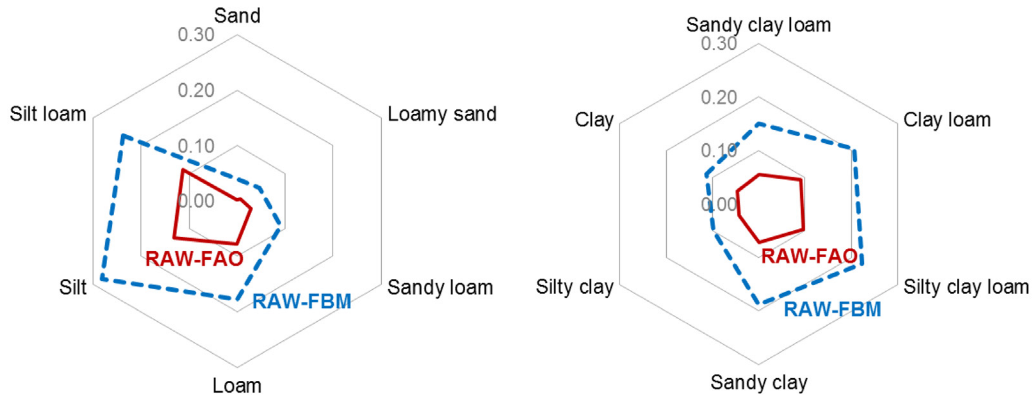

Fig. 3. Readily available water (RAW) calculated according to the FAO method (FAO) and the flux-based method (FBM) using FluxPAW for 12 soil texture classes of the USA Soil Texture Classification. Fixed parameters: h_{FC} = −1 m, h_{WP} = −150 m, p = 0.5 (FAO); Z = 100 cm, T_p = 4 mm d^{-1}, R = 1 cm cm^{-3}, q_{FC} = 1 mm d^{-1}, f_{WP} = 0.01 (FBM).

Acknowledgments

The authors acknowledge MSc. Leonardo Inforsato and Dr. Everton Alves Rodrigues Pinheiro for research background that led to software development. The authors also acknowledge the National Council for Scientific and Technological Development (CNPq, Brazil), grant number 141197/2020-0, and the São Paulo Research Foundation (FAPESP, SP, Brazil), grant numbers 2022/00853-2, and 2020/07294-3 for supporting the research.

References

[1] Q. de Jong van Lier, S.D. Logsdon, E.A.R. Pinheiro, P.I. Gubiani, Encyclopedia of Soils in the Environment, 2022, http://dx.doi.org/10.1016/B978-0-12-822974-3.00043-4.

[2] Q. de Jong Van Lier, K. Metselaar, J.C. Van Dam, Vadose Zone J. 5 (2006) 1264–1277, http://dx.doi.org/10.2136/vzj2006.0056.

[3] L. Inforsato, Q. de Jong van Lier, Geoderma 404 (2021) 115308, http://dx.doi.org/10.1016/j.geoderma.2021.115308.

[4] E.A.R. Pinheiro, Q. de Jong van Lier, K. Metselaar, Vadose Zone J. 17 (2018) 1–10, http://dx.doi.org/10.2136/vzj2016.09.0083.

[5] M.L.A. de Melo, L. Inforsato, E.A.R. Pinheiro, Q. de Jong van Lier, Geoderma 429 (2023) 116253, http://dx.doi.org/10.1016/j.geoderma.2022.116253.

[6] M.T. Van Genuchten, Soil Sci. Am. J. 44 (1980) 892–898, http://dx.doi.org/10.2136/sssaj1980.03615995004400050002x.

[7] M.L.A. de Melo, Q. de Jong van Lier, Code Ocean [Source Code], 2022, http://dx.doi.org/10.24433/CO.6533097.v2.

[8] Q. de Jong van Lier, D. Dourado Neto, K. Metselaar, Water Resour. Res. 45 (2009) http://dx.doi.org/10.1029/2008WR006938.

[9] Q. de Jong van Lier, Agricult. Water Manag. 193 (2017) 214–220, http://dx.doi.org/10.1016/j.agwat.2017.08.017.

[10] R.G. Allen, L.S. Pereira, D. Raes, M. Smith, Rome: Food and Agriculture Organization of the United Nations, Vol. 56, 1998, e156, http://www.fao.org/docrep/x0490e/x0490e00.htm.

[11] R.F. Carsel, R.S. Parrish, Water Resour. Res. 24 (1988) 755–769, http://dx.doi.org/10.1029/WR024i005p00755.

[12] J.G. Kroes, J.C. van Dam, R.P. Bartholomeus, P. Groenendijk, M. Heinen, R.F.A. Hendriks, H.M. Mulder, I. Supit, P.E.V. van Walsum, 2017, http://dx.doi.org/10.18174/416321.

[13] J. Šimunek, M.T. Van Genuchten, M. Šejna, Trans. ASABE 55 (2012) 1263–1274, http://dx.doi.org/10.13031/2013.42239.