A Multipoint Flux Approximation Method based on Harmonic Points to Simulate Highly Heterogeneous and Anisotropic Aquifers

Fernando R. L. Contreras[1], Darleson L. A. Oliveira[1], Paulo R. M. Lyra[2], Alessandro R. E. Antunes[1]Darlan K. E. Carvalho[2]

[1]*Nucleo de Tecnologia, Universidade Federal de Pernambuco*
Av. Marielle Franco, s/n - Km 59 - Nova Caruaru, 55014-900, Pernambuco/Caruaru, Brazil
fernando.raul@ufpe.br, darleson.oliveira@ufpe.br, alessandro.antunes@ufpe.br
[2]*Engenharia Mecânica, Universidade Federal de Pernambuco*
Av. Prof. Moraes Rego, 50670-901, Pernambuco/Recife, Brazil
paulo.lyra@ufpe.br, darlan.ecarvalho@ufpe.br

Abstract. Currently, groundwater has become an essential natural resource for human consumption, particularly in arid regions. It is well-known that aquifers have very complex geological characteristics due to the presence of zones of low permeability, vugs and fractures. The geological complexity and the presence of strongly coupled terms in the mathematical models make it difficult, if not impossible, to obtain an analytical solution, and solving this class of problem is a challenge for the hydraulic engineer. In this sense, computer simulators supported by numerical methods have become a fundamental tool for dealing with these mathematical models. Currently, in the context of numerical simulation of fluid flow in aquifers, several classical numerical methods are used in most commercial simulators such as FEFLOW, MODFLOW, and HydroGeoSphere. However, it is well known that these classical methods cannot deal with complex physical phenomena and can lead to inconsistent approximate solutions. In this sense, in the present work, the hydraulic head equation of the aquifer is solved for the first time using a cell-centered finite volume method, where the spatial and temporal terms are solved using the multipoint flux approximation method based on harmonic points (MPFA-H) and the backward Euler or Crank-Nicolson schemes, respectively. In this context, the MPFA-H method is characterized by being globally and locally conservative, piecewise-linear, and able to deal with highly heterogeneous and anisotropic porous media. Moreover, the harmonic points are calculated from physical and geometrical parameters, which allows a piecewise-linear solution and guarantees the positivity of the interpolation weights of the hydraulic head on the control surface of the computational mesh. The results show that the proposed method provides high accuracy and efficiency in groundwater simulation.

Keywords: Groundwater, Hydraulic head, Finite volume method, MPFA-H

1 Introduction

Groundwater represents 97% of the planet's fresh and liquid water, which becomes aquifers or the largest reservoir of drinking water in the world. In recent decades, groundwater has become an important resource for consumption, especially in the semi-arid regions of Brazil. According to the National Water Agency (ANA), 52% of municipalities use groundwater for supply, 36% do exclusively and 16% partially. The private sector withdraws more than 17.5 billion m3 of water annually from aquifers through 2.5 million tube wells, 88% of which are clandestine. This extracted volume would be sufficient to supply the entire Brazilian population. This demand has led to excessive exploitation of groundwater. According to Hirata et al. [1], the over-exploitation of aquifers can cause: depletion of aquifers, deterioration of water quality, lowering of the water table of rivers and other water bodies, geotechnical problems, and problems of social equity and unfair competition between large and small consumers. On the other hand, groundwater pollution from landfills, mining activities, leaking wastewater collection networks, improper use of pesticides and fertilizers, and irrigation can lead to salinization problems or increase the leaching of pollutants into groundwater. These pollution processes can be fought from two angles: preventive treatments, which aim to avoid pollution and anticipate the problem, and curative treatments, which are applied when the water is already polluted. Due to the high economic cost of real-time contamination monitoring, the use of computational tools has become essential not only for groundwater contamination assessment and optimized groundwater management, but also for solving safety problems in resource exploration. For example, a flux model simulates hydraulic loading (and the elevation of the water table in aquifers) and groundwater flow rates within and outside the boundaries of the system under consideration. It can provide estimates of water balance and travel times along flow paths. A contaminant transport model simulates solute concentrations in groundwater. These models can simulate the migration of contaminants through the subsurface and system boundaries. In general, groundwater models can be used to calculate water fluxes and contaminant concentrations in the system, taking into account associated sources and discharges such as surface waters (rivers, lakes), pumping wells, and reservoirs adjacent to the aquifer. Currently, there are several numerical models developed for simulating the flow and transport of contaminants in groundwater, namely: FEFLOW (Trefry and Muffels [2]), HYDRUS (Simunek et al. [3]), MODFLOW (Langevin et al. [4]), and HydroGeoSphere (Brunner and Simmons [5]), which are based on conventional numerical methods such as the finite element method (FEM), the finite difference method (FDM) and the finite volume method (FVM). The FDM and the FEM are among the most commonly used numerical methods for groundwater simulation. However, the FDM is not flexible for geometries with irregular contours and may lose accuracy and robustness when hydraulic loading occurs near irregular contours of aquifers. FEM method is more suitable than FDM for representing irregular contours. However, the physical properties are not maintained at the local level, and it is difficult to apply it to arbitrary polygonal shapes. The FVM is the best algorithm because it can be easily adapted to irregular contours and preserves the physical properties both locally and globally. These commercial numerical models have acquisition and/or training costs that limit their use, especially for municipal entities responsible for the supply to small cities. In this context, we develop in this paper a fully cell-centered finite volume method (FVM) to solve the hydraulic head equation. The FVM is widely used to simulate highly complex multiphase flow problems in petroleum reservoirs. The hydraulic head equation is discretized by a non-conventional cell-centered multi-point flux approximation method with harmonic points (MPFA-H). This linear method is based on the classical nonlinear method Yuan and Sheng [6]. Using some basic ideas of nonlinear finite volume methods our proposed MPFA-H method first constructs the unilateral fluxes on each control surface independently and then obtains a unique flux expression by a convex combination of the unilateral fluxes. Unlike other classical MPFA methods, the fluxes on each control surface are explicitly expressed by a cell-centered unknown and by points on the control surface that do not necessarily belong to the same control surface shared by the adjacent cells. These interpolation points are calculated using the concept of harmonic points Agélas et al. [7].

2 Mathematical model

In this section we briefly describe the hydraulic head equation in confined aquifers. Without loss of generality, we assume that both the fluid and the rock are incompressible, that the flow is isothermal, that the effects of precipitation, infiltration, and evotranspiration are not considered, and that the gravitational term is neglect.

$$\mu_e \frac{\partial h}{\partial t} = -\nabla \cdot (\vec{v}) - f, \quad \vec{v} = -K\nabla h, \tag{1}$$

where h is the hydraulic head, $\vec{v}$ is the Darcy velocity, f is the source/sink term, K is the hydraulic conductivity tensor, $\mu_e = \mu_s M$ is the elastic release coefficient of the confined aquifer based on specific storativity μ_s and the thickness of aquifer M.

The equation (1), is completely defined by the boundary and initial conditions:

$$\begin{aligned} h(x,t) &= h_D, \quad on \quad \Gamma_D \times [0,t], \\ K\nabla h \cdot \vec{n} &= g_N, \quad on \quad \Gamma_N \times [0,t], \\ h(x,t) &= h_0, \quad on \quad \Omega \quad and \quad t=0, \end{aligned} \tag{2}$$

where the Dirichlet and Neumann boundaries are denoted by Γ_D and Γ_N, respectively. h_D is the well-known scalar function representing the hydraulic head defined on Γ_D. On the other hand, the flux $\bar{g}_N$ is predefined on Γ_N and $\vec{n}$ denotes the unit normal vector outward. In an initial time $t = 0$, the initial hydraulic head is denoted by h_0.

3 Numerical formulation using a finite volume method

The equation (1) can be expressed in integrated form on a generic cell $L \in \Omega$, as:

$$\mu_e \int_L \frac{\partial h}{\partial t} dx = -\int_L \nabla \cdot \vec{v} dx - \int_L f dx. \tag{3}$$

The divergence theorem is applied in the equation (3), so we have:

$$\mu_e \int_L \frac{\partial h}{\partial t} dx = -\sum_{e \in \partial L} \int_e \vec{v} \cdot \vec{n}_e ds - \int_L f dx, \tag{4}$$

and using the mean-value theorem and Euler's Backward method implicitly in the time discretization of the transient term, we have that:

$$h_L^{n+1} = h_L^n - \frac{\Delta t}{\mu_e |L|} \left\{ \sum_{e \in \partial L} \vec{v}_e \cdot \vec{N}_e \right\}^{n+1} - \frac{\Delta t}{\mu_e} \bar{f}. \tag{5}$$

Here, Δt denotes the step time, and the average sink/source is denoted by $\bar{f} = \frac{1}{|L|} \int_L f dx$, and the flow rate $\vec{v}_e \cdot \vec{N}_e$ is approximated by:

$$\vec{v}_e \cdot \vec{N}_e = \|e\| \left(\varpi_{L,e} h_L - \varpi_{R,e} h_R + \sum_{\gamma=i,j} a_{R,\gamma(e)} h_{R,\gamma(e)} - a_{L,\gamma(e)} h_{L,\gamma(e)} \right), \tag{6}$$

where $\varpi_{r,e} = w_{r,e} \left(\zeta_{r,i(e)} + \zeta_{r,j(e)} \right)$, $a_{r,i(e)} = w_{r,e} \zeta_{r,i(e)}$ and $a_{r,j(e)} = w_{r,e} \zeta_{r,j(e)}$, with $r = L, R$. The auxiliary variables $h_{r,\gamma(e)}$ localized in the harmonic points are calculated by:

$$h_{r,\gamma(e)} = w_{r,\gamma(e)} h_r + w_{s,\gamma(e)} h_s \text{ and } r = L \text{ or } R, \;\; \gamma = i, j \tag{7}$$

where the h_s is the hydraulic head centered in cell $s = P$ or Q if $\gamma = j$, in otherwise $s = L$ or R with $r \neq s$.

The weights $w_{r,\gamma(e)}$ in equation (7), are calculated by following equation:

$$w_{L,e} = \frac{d_{R,e} \kappa_{L,e}}{d_{L,e} \kappa_{R,e} + d_{R,e} \kappa_{L,e}} \text{ and } w_{R,e} = 1 - w_{L,e}. \tag{8}$$

where $d_{r,e}$ denotes distance of the barycenter of cell r to edge e (see figure 1) and $\kappa_{r,e} = \vec{n}_e^\top K_r \vec{n}_e$, $r = L, R$.

$$\zeta_{r,i(e)} = \frac{\|K_r \vec{n}_e\| \sin(\theta_{r,j(e)})}{\left\| x_r x_{r,i(e)} \right\| \sin(\theta_{r,i(e)} + \theta_{r,j(e)})} \text{ and } \zeta_{r,j(e)} = \frac{\|K_r \vec{n}_e\| \sin(\theta_{r,i(e)})}{\left\| x_r x_{r,i(e)} \right\| \sin(\theta_{r,i(e)} + \theta_{r,j(e)})} \tag{9}$$

In the equation (9), the coefficients exist when the angles formed by segments $x_r x_{r,i(e)}$ (resp. $x_r x_{r,j(e)}$) and the co-normal $K_r \vec{n}_e$, satisfies the following conditions $\theta_{r,i(e)}, \theta_{r,j(e)} < \pi$ and $\theta_{r,i(e)} + \theta_{r,j(e)} < \pi$. It is important to note that the coefficients $\zeta_{r,i(e)}$ and $\zeta_{r,j(e)}$ are non-negatives, this property is essential in our methods to assure the consistent flux approximation.

The harmonic points are calculated by the following equation:

$$x_e = \frac{d_{L,e} \kappa_{R,e} x_R + d_{R,e} \kappa_{L,e} x_L + d_{L,e} d_{R,e} (K_L - K_R)}{d_{L,e} \kappa_{R,e} + d_{R,e} \kappa_{L,e}}. \tag{10}$$

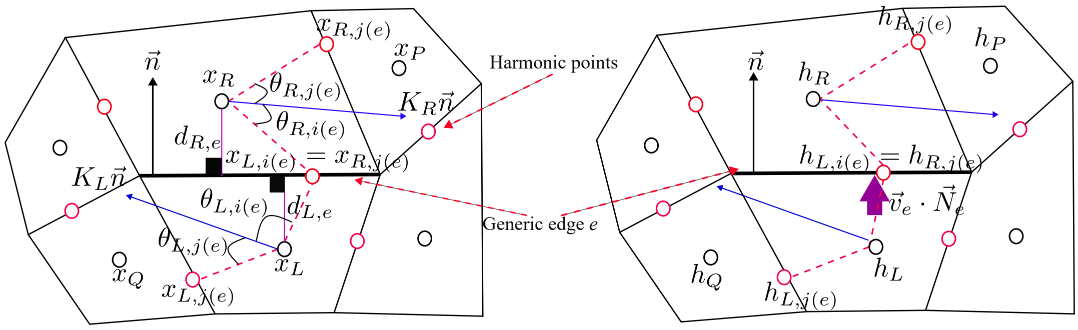

Figure 1. Physical-geometric parameters and the auxiliary variables.

3.1 Treatment of boundary fluxes

The harmonic point in the boundary edge coincides with the middle point, and the flow rate over boundaries Γ_D is defined by:

$$\vec{v}_e \cdot \vec{N}_e = \|e\| \, \varpi_{L,e} h_L - \|e\| \sum_{\gamma=i,j} \zeta_{L,\gamma(e)} h_{D_{L,\gamma(e)}}, \tag{11}$$

where $\varpi_{L,e} = \zeta_{r,i(e)} + \zeta_{r,j(e)}$, the middle point hydraulic head h_D are prescribed on Γ_D. On the other hand, the flow rate on the boundary Γ_N is prescribed and denoted by $\vec{v}_e \cdot \vec{N}_e = ||e||\bar{g}_N$.

4 Numerical experiments

4.1 The hydraulic head field in an isotropic homogeneous confined aquifer

This problem was adapted from Qian et al. [8] to verify the accuracy of our scheme and compare it with the Vertex Centered Finite Volume (VCFV) method proposed by Qian et al. [8]. The physical properties and the computational domain are given in table 1 and figure 2, respectively. The step time and simulation time are given by $\Delta t = 0.01$ and $t_f = 20$ days, respectively. In general, our proposed scheme is suitable for arbitrary polygonal

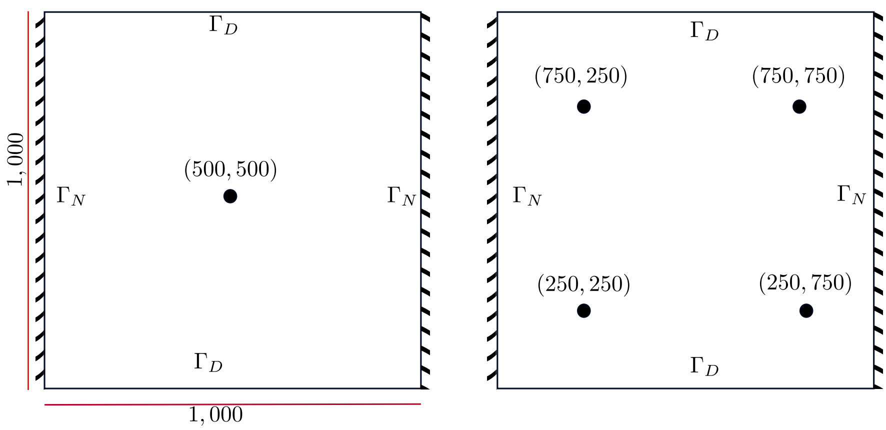

Figure 2. Domain for case I (left) and Case II (right).

Table 1. Initial and boundary conditions

	K	Γ_D	Γ_N	M	μ_e	h_0	t_f
Case I and II	$k_{xx} = k_{yy} = 33.33$	$h_D = 100$	$g_N = 0$	3	0.001	100	20

meshes. The reference solution was obtained using the commercial simulator MODFLOW Langevin et al. [4].

Case I: Single pumping wells in a confined aquifer

In the first case, we have calculated the distribution of the field of hydraulic head in the domain influenced by a pumping well is located in $(500, 500)$ (see figure 2 left), the flow rate in this well is $f = 10^4\ m^3d^{-1}$.

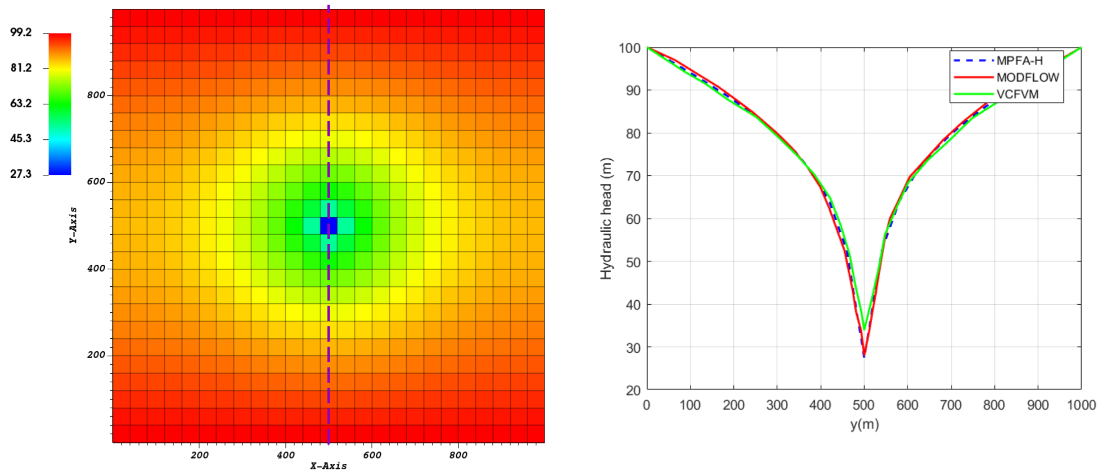

Figure 3. The hydraulic head field obtained by MPFA-H scheme (left) and profile in $(x = 500)$ (right).

In this case, the hydraulic field obtained by the proposed method is shown in figure 3 left. In this figure, it can be seen that the values of the hydraulic field are bounded by the Dirichlet boundary condition, as expected. The profile obtained with the MPFA-H scheme is very similar to the MODFLOW result, see figure 3 right. Moreover, the profile obtained with the VCFV scheme is slightly less accurate than the results obtained with the MPFA-H scheme.

Case II: Multiple pumping wells in a confined aquifer

The flow rate in each pumping well is 2500 m^3d^{-1} and the localization of wells is shown in figure 2 right.

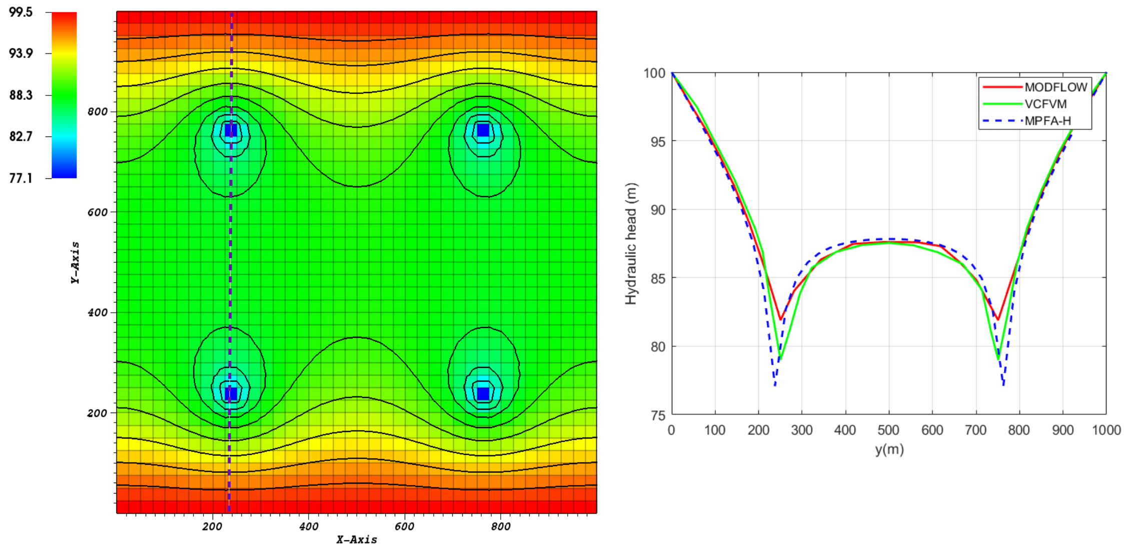

Figure 4. The hydraulic head field obtained by MPFA-H scheme (left) and profile in $(x = 250)$ (right).

In a similar way as in case I, the hydraulic field obtained with the proposed scheme is shown in figure 4 left. The hydraulic profile is obtained in $x = 250m$, in this case we see that our MPFA-H method is less accurate than the CVFV scheme, for more details see figure 4 right. This anomaly is still a reason for research in our group.

5 Conclusions

In this article, we have proposed a Multipoint Flux Approximation Finite Volume Method based on the Harmonic Point (MPFA-H) to solve the hydraulic head equation. In general, we can see in the tests, that our method is able to deal with homogeneous isotropic confined aquifers. This ability is evident in the numerical solution of cases I and II, where the MPFA-H scheme together with the backward Euler method obtains a hydraulic head profile similar to that of the commercial simulator MODFLOW. These preliminary results show that our proposed scheme has great potential for application in groundwater simulation.

Acknowledgements. The authors would like to thank the following Brazilian research agencies: Fundação do Amparo a Ciência e Tecnologia de Pernemabuco (FACEPE) e Consejo Nacional de Desarrollo Científico y Tecnológico (CNPq).

Authorship statement. The authors hereby confirm that they are the sole liable persons responsible for the authorship of this work, and that all material that has been herein included as part of the present paper is either the property (and authorship) of the authors, or has the permission of the owners to be included here.

References

[1] R. Hirata, A. V. Suhogusoff, S. S. Marcellini, P. C. Villar, and L. Marcellini. As águas subterrâneas e sua importância ambiental e socioeconômica para o brasil, 2019.

[2] M. G. Trefry and C. Muffels. Feflow: A finite-element ground water flow and transport modeling tool. *Groundwater*, vol. 45, n. 5, pp. 525–528, 2007.

[3] J. Simunek, M. T. Van Genuchten, and M. Sejna. The hydrus software package for simulating two-and three-dimensional movement of water, heat, and multiple solutes in variably-saturated media. *Technical manual, version*, vol. 1, pp. 241, 2006.

[4] C. D. Langevin, A. M. Provost, S. Panday, and J. D. Hughes. Documentation for the modflow 6 groundwater transport model. Technical report, US Geological Survey, 2022.

[5] P. Brunner and C. T. Simmons. Hydrogeosphere: a fully integrated, physically based hydrological model. *Groundwater*, vol. 50, n. 2, pp. 170–176, 2012.

[6] G. Yuan and Z. Sheng. Monotone finite volume schemes for diffusion equations on polygonal meshes. *Journal of computational physics*, vol. 227, n. 12, pp. 6288–6312, 2008.

[7] L. Agélas, R. Eymard, and R. Herbin. A nine-point finite volume scheme for the simulation of diffusion in heterogeneous media. *Comptes Rendus. Mathématique*, vol. 347, n. 11-12, pp. 673–676, 2009.

[8] Y. Qian, Y. Zhu, X. Zhang, J. Wu, M. Ye, W. Mao, J. Wu, J. Huang, and J. Yang. A local grid-refined numerical groundwater model based on the vertex-centred finite-volume method. *Advances in Water Resources*, vol. 173, pp. 104392, 2023.