Tittle: Ensemble modeling of the two-dimensional stochastic confined groundwater flow through the evolution of the hydraulic head's probability density function

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Abstract. Groundwater storage in aquifers has become a vital water source due to water scarcity in recent years. However, aquifer systems are full of uncertainties, which inevitably propagate throughout the modeling computations, mainly reducing the reliability of the model output. This study develops a novel two-dimensional stochastic confined groundwater flow model. The proposed model is developed by linking the stochastic governing partial differential equations by means of their one-to-one correspondence to the nonlocal Lagrangian-Eulerian extension to the Fokker-Planck equation (LEFPE). In the form of the LEFPE, the resulting deterministic governing equation describes the spatio-temporal evolution of the probability density function of the state variables in the confined groundwater flow process by one single numerical realization instead of requiring thousands of simulations in the Monte Carlo approach. Consequently, the ensemble groundwater flow process's mean and standard deviation behavior can be modeled under uncertainty in the transmissivity field and recharge and/or pumping conditions. In addition, an appropriate numerical method for LEFPE's solution is subsequently devised. Then, its solution is presented, discussed, and illustrated through a numerical example, which is compared against the results obtained by means of the Monte Carlo simulations. Results suggest that the proposed model appropriately characterizes the ensemble behavior in confined groundwater systems under uncertainty in the transmissivity field.

1 Introduction

Groundwater stored in aquifers has become a vital water source in the face of emerging droughts in many regions of the world. Moreover, this water scarcity is expected to aggravate due to both global population and economic growth. Therefore, the value of groundwater will increase as the water availability decreases in various regions of the world with the change in climate, making groundwater management a fundamental tool. Anderson and Woessner (2015) stated that Groundwater Models are a well-suited tool for predicting complex aquifer systems' behavior. Nevertheless, groundwater modeling is challenging since its predictive power predominantly depends on the input data representativity, commonly requiring large samples to estimate the hydraulic parameters.

Improving the representativity of the input data and, consequently, groundwater models' predictive power is complicated mainly for two reasons. First, there is always an incomplete understanding of the site conceptual model (Xia et al., 2019). Second, limited knowledge of the hydrogeological parameter values, typically due to the limited availability of suitable observations (Jim Yeh, 1992; Li et al., 2003). Beyond, these uncertainties inevitably propagate throughout the model calculations, mainly reducing the reliability of the model output.

Groundwater systems are highly heterogeneous in space, resulting in significant hydraulic parameter value variations. In particular, hydraulic conductivity is one of the most sensitive to spatial variation (Lu and Zhang, 2005). Moreover, this parameter is the primary parameter affecting the output accuracy of groundwater flow and contaminant transport models (Kitanidis, 1997; Bakshevskaya and Pozdnyakov, 2013; Zhu et al., 2016) since it controls both advective and dispersive transport (Neuman, 1990). Hydraulic conductivity depends on various factors, such as the size of pores, geological structure, and connectivity. Furthermore, it is not easy to estimate this parameter accurately with commonly used methods (Wu and Zeng, 2013). In addition, aquifer properties are scale-dependent and can vary over many orders of magnitude in typical aquifer systems (Dagan, 1986; Sudicky, 1986). Hence, subsurface heterogeneity's characterization must be incorporated into the modeling in order to accurately predict groundwater flow and contaminant transport in groundwater environments.

To date, the uncertainty quantification in groundwater modeling has been carried out mainly by two different techniques, (1) Monte Carlo simulations (Freeze, 1975; Tonkin and Doherty, 2009; Refsgaard et al., 2012) and (2) perturbation methods (Smith and Freeze, 1979; Connell, 1995; Li et al., 2003; Ma et al., 2009; Xia et al., 2019). The importance of quantifying the uncertainty inherent to any groundwater system relies on evaluating the risks coming from the heterogeneity and the lack of information on design and management (Renard, 2007). Furthermore, stochastic approaches align with a typical decision-making agency's expectation that predictions should be accompanied by uncertainty measures that allow risk assessment (Rajaram, 2016).

Monte Carlo (MC) simulations repeatedly solve the deterministic governing equations for a large number of equally likely realizations of the model parameters (e.g., hydraulic conductivity) to achieve multiple realizations. Then, the ensemble of solutions is further used to make statistical estimations. Furthermore, the MC approach is well known as the most robust approach for uncertainty evaluation and the benchmark to validate other methods (Scharffenberg and Kavvas, 2011). While the MC method may offer a robust approach for estimating uncertainty in groundwater flow and transport, it is computationally demanding, and therefore, its application is restricted (Connell, 1995).

Alternatively, the regular perturbation method incorporates variability into the model using a different approach. This method decomposes the state variables into a mean plus a perturbation. By design, the regular perturbation has a zero mean and a variance equal to the original variable variance. Even though the regular perturbation method could offer significant savings in computation over MC methods (Townley and Wilson, 1985; Yeh, 1992), its accuracy is directly related to the magnitude of the process variance (Connell, 1995). Therefore, solutions by the regular perturbation approach may be poor approximations for highly heterogeneous ($coefficient\ of\ variation\ of \log hydraulic\ conductivity > 1$) aquifers (Zhang, 1999; Gotovac et al., 2009). Moreover, regular perturbation approaches result in a closure problem, where the equation for a specific moment requires information about higher moments' behavior (Keese, 2003). Hence, one can close the system of equations only by employing some ad-hoc assumptions.

Even though stochastic groundwater modeling has developed considerably in the last fifty years, the developed modeling techniques are not standard tools in practice. Why the practice has not adopted stochastic analysis is of substantial debate (Gelhar, 1986; Dagan, 2002; Renard, 2007; Rubin et al., 2018). The gap between theory and practice in stochastic modeling of groundwater systems is attributed to diverse factors, such as (1) economic constraints and lack of regulations (Rubin et al., 2018), (2) the need to construct statistical models of field heterogeneity from limited data (Dagan, 2002), and (3) the assumptions and simplifications adopted in most theoretical analyses (Renard, 2007). However, all authors agree that (4) the excessive computational requirement of available stochastic numerical methods is one of the primary factors limiting these techniques' application.

In view of the above discussion, to avoid the drawbacks of Monte Carlo simulations and regular perturbation methods, this study proposes a novel methodology to solve the expected system behavior in a single simulation. This proposed methodology upscales the governing stochastic differential equations from a point-scale (at which they are valid) to a field scale. Thus, the conservation equations describing the groundwater flow in confined aquifers are consistent with the scale of the grid areas over which they describe the hydrologic process. Furthermore, through this general framework, not only the mean and the variance of the targeted state random variable/function can be estimated, but also the probability density function (PDF) of the process, which evolves in space and time.

Ensemble averaging has been a popular approach in hydrology to upscale both linear (Gelhar and Axness, 1983; Rubin and Dagan, 1989; Wood and Kavvas, 1999) and nonlinear (Mantoglou and Gelhar, 1987; Tayfur and Kavvas, 1994; Dogrul et al., 1998) hydrologic processes. To upscale the stochastic governing equations of groundwater flow, they are averaged to become deterministic. Thus, statistical descriptions represent the values of the stochastic parameters. However, most studies performing the ensemble averaging technique used the regular perturbation method, which only works for small fluctuations in the dependent variables (Kavvas, 2003).

To upscale the point-scale conservation equations to the scale of computational grid areas, a general ensemble average conservation equation was developed to determine hydrologic processes' probabilistic and mean behavior (Kavvas ,2003). To carry out this task, the one-to-one correspondence between any governing equation under uncertainty (that represents a hydrologic process) and a mixed Eulerian-Lagrangian extension to the Fokker-Planck equation (LEFPE) (to the second order) was shown (Kavvas, 2003). The resulting "master key" equation allows for dealing with uncertainties in the parameters and the forcing terms in their corresponding point-scale governing equations. Thus, by employing this approach, it is possible to estimate the probability density function's time-space evolution for any nonlinear or linear hydrologic process.

Within this framework, the modeling methodology by the LEFPE has been successfully applied to various hydrologic processes. Kim et al. (2005) used the methodology to model the one-dimensional root-water uptake under uncertainty in the saturated hydraulic conductivity. Cayar and Kavvas (2009) modeled the effect of uncertainty in the hydraulic conductivity for the one-dimensional horizontal unconfined groundwater flow. They transformed the governing PDE into an ordinary differential equation using the Boltzmann transformation and Lie Group theory. Ercan and Kavvas (2012) used this methodology to explore variability in the channel properties and lateral flow conditions to upscale the kinematic open-channel flow governing equation. Tu et al. (2019, 2020) applied the methodology for describing the ensemble behavior for the 1D and 2D solute transport in open channel flow under uncertain flow and solute loading conditions. Even though this stochastic framework was initially developed to tackle uncertainties for hydrologic processes, it has also been used in the geomechanics field. Jeremić et al. (2007) and Sett et al. (2007) used the "master key" equation for the 1-D elastic-plastic constitutive rate equations to quantify the uncertainty in material parameters. Later, Karapiperis et al. (2016) applied this stochastic upscaling framework together with stochastic Galerkin techniques to solve 1-D elastoplastic boundary value problems with non-Gaussian parametric uncertainty.

In this paper, motivated by the probabilistic responses of aquifers to the influence of spatial uncertainties in aquifer characteristics, a stochastic model for confined aquifer flow is proposed, where both a formulation and a numerical solution scheme are discussed. Thus, the uncertainties in the transmissivity field and source/sink term in the governing equation are accounted for. This general framework is carried out using the above-discussed methodology (Kavvas, 2003), where the ensemble average governing equation is obtained, determining the probabilistic behavior of the dynamical system. The

resulting expression, in the form of a deterministic partial differential equation, simulates in one single solution the complete ensemble behavior of groundwater flow due to the spatio-temporal variability of the hydraulic conductivity in terms of the time-space evolving pdf of the hydraulic head in confined aquifers. Furthermore, the derived LEFPE corresponding to the confined groundwater flow process is described by employing an illustrative example. The methodology developed in this study can be extended to three dimensions and allows for incorporating randomness in the boundary conditions.

2 Confined groundwater flow equations

This section describes the governing equation which controls the subsurface flow in confined aquifers, including the assumptions used for its derivation. Later on, employing the method of characteristics, the governing PDE is recast into a system of ordinary differential equations (ODE). This ODE system will be crucial in the next section to develop a solution for its ensemble behavior in order to upscale the governing groundwater flow equation from the point-scale to the field scale.

2.1 Point-scale governing equation

Hydraulic groundwater flow theory in a fully saturated geologic porous media is based on the mass balance principle combined with Darcy's equation. It is then assumed that the grains' volume does not change, so the porosity must change in the elastic range instead. Additionally, considering the aquifer is slightly compressible and neglecting the horizontal stresses, the groundwater flow partial differential equation (PDE) can be represented as follows (Bear and Verruijt, 1987)

$$\frac{\partial}{\partial x_i}\left(K_i\,(x,t)\frac{\partial h(x,t)}{\partial x_i}\right)+Q(x,t)=S_s(x,t)\frac{\partial h(x,t)}{\partial t} \tag{1}$$

subject to boundary conditions on $\Gamma=\Gamma_N\cup\Gamma_D$, which are defined by

$$h(x)=h_D(x)\ on\ \Gamma_D\ , \tag{2}$$

$$\left(K_i(x,t)\frac{\partial h(x,t)}{\partial x_i}\right)\cdot n=q_N(x)\ \ on\ \Gamma_N\ , \tag{3}$$

where $x=\{x,y,z\}$ is the position vector [L], t is time [T], h is the hydraulic head [L], K_i is the hydraulic conductivity tensor [LT^{-1}], S_s is the specific storage [L^{-1}], Q is a sink or source term [L^3T^{-1}], $h_D(x)$ is the prescribed head at the boundary Γ_D, $q_N(x)$ is the flux at the boundary Γ_N, and n is a unit vector normal to Γ_N.

Then, it is possible to model the three-dimensional aquifer's flow as a horizontal two-dimensional flow by neglecting vertical fluxes and averaging properties over the aquifer thickness. These simplifications are called the Dupuit-Forchheimer

approximation. Under this assumption, the equation for two-dimensional horizontal flow in a confined aquifer can be expressed as (Bear and Verruijt, 1987)

$$\frac{\partial}{\partial \underline{x}_i}\left(T_i(\underline{x},t)\frac{\partial h(\underline{x},t)}{\partial \underline{x}_i}\right) + Q(\underline{x},t) = S(\underline{x},t)\frac{\partial h(\underline{x},t)}{\partial t} \tag{4}$$

where $\underline{x} = \{x, y\}$ is the two-dimensional position vector [L], $S(\underline{x},t) = S_s(x,t)\cdot b(x)$ is the storativity [1], $b(x)$ is the confined aquifer thickness [L], and T is the transmissivity [L^2T^{-1}], which is defined by

$$T_i(\underline{x},t) = \int_0^{b(\underline{x})} K_i(x,t)dz \tag{5}$$

2.2 Characteristic form of the confined groundwater flow equation

By expanding the spatial derivates, equation (4) can be expressed as

$$\underbrace{\frac{\partial T_i(\underline{x},t)}{\partial \underline{x}_i}\frac{\partial h(\underline{x},t)}{\partial \underline{x}_i}}_{\text{Convective terms}} + \underbrace{T_i(\underline{x},t)\frac{\partial^2 h(\underline{x},t)}{\partial \underline{x}_i^2}}_{\text{Diffusive terms, } DT(\underline{x},t)} + Q(\underline{x},t) = S(\underline{x},t)\frac{\partial h(\underline{x},t)}{\partial t} \tag{6}$$

It may be assumed that at the regional scale the stochasticity of the random groundwater field, in equation (6), is mainly due to the stochasticity in the convective term, while the diffusive terms $DT(\underline{x},t)$ may contribute only to the mean behavior (Kavvas and Karakas, 1996; Tu et al., 2019). This assumption will be assessed later by comparison of the resulting LEFPE against Monte Carlo solutions. Thus, equation (6) may be recast into the form

$$\frac{\partial h(\underline{x},t)}{\partial t} - \frac{1}{S(\underline{x},t)}\frac{\partial T_i(\underline{x},t)}{\partial \underline{x}_i}\frac{\partial h(\underline{x},t)}{\partial \underline{x}_i} = \frac{1}{S(\underline{x},t)}\left[DT(\underline{x},t) + Q(\underline{x},t)\right] \tag{7}$$

Through the method of characteristics, the governing PDE (7) may be transformed into a system of stochastic ordinary differential equations (ODEs), where the following expressions represent the characteristic equations for unsteady confined groundwater flow

$$\frac{\partial x(t)}{\partial t} = -\frac{1}{S(\underline{x},t)}\frac{\partial T_x(\underline{x},t)}{\partial x} = \eta_1 \tag{8}$$

$$\frac{\partial y(t)}{\partial t} = -\frac{1}{S(\underline{x},t)}\frac{\partial T_y(\underline{x},t)}{\partial y} = \eta_2 \tag{9}$$

$$\frac{\partial h(\underline{x},t)}{\partial t} = \frac{1}{S(\underline{x},t)}\left[DT(\underline{x},t) + Q(\underline{x},t)\right] = \eta_3 \tag{10}$$

Equations (8) and (9) represent two velocity expressions that can be used to determine the evolution of the stochastic characteristic path $\underline{x}(t)$, while equation (10) describes the process behavior of the state variable $h(\underline{x},t)$ along $\underline{x}(t)$. Once the

dynamical system is described in terms of the system of ODEs, the upscaling technique proposed in Kavvas (2003) can be used. Thus, the point-scale system of conservation equations may be expressed as

$$\frac{\partial H(x,t)}{\partial t} = \eta(H, A, f) \tag{11}$$

with an initial condition

$$H(x, t = 0) = H_0 \tag{12}$$

where $H = \{h, x, y\}^T$ is the vector of all state variables of the hydrologic system of equations, A is the tensor of parameters, f is the vector of forcing functions, and $\eta = \{\eta_1, \eta_2, \eta_3\}^T$ is the governing function vector.

3 Ensemble-averaged equations for the stochastic unsteady confined groundwater flow

In this section, we introduce a novel methodology to solve the stochastic confined groundwater flow equation system as well as a well-suited numerical scheme to solve the resulting PDE in the form of a LEFPE. Thus, the time-space evolutionary PDF of the hydraulic head will be obtained. The following derivation assumes uncertainty in the transmissivity random field and in the source term. Nevertheless, stochasticity in the storativity and the boundary conditions could also be incorporated following similar steps.

3.1 Development of the Lagrangian-Eulerian Extension of the Fokker-Planck equation (LEFPE) for confined groundwater flow

Since $H = \{h, x, y\}^T$ could represent a point in the three-dimensional *h-x-y space*, equation (11) determines each point's velocity in the mentioned space. Conceptually, this could be interpreted as the path described by equation (11) 's solution for a given deterministic initial condition $H(x, t = 0) = H_0$. Nonetheless, the initial condition may be represented by a density $\rho(H, t = 0)$ in the *H phase space* to describe a cloud of deterministic initial conditions. Thus, the phase density $\rho(H, t)$ evolves according to a continuity equation, representing the conservation of all these points in the h-x-y space. The variation of $\rho(H, t)$ can be expressed in mathematical terms, as is shown in equation (11), following Kubo's stochastic Liouville equation (Kubo, 1963). This equation is a linear advective-transport stochastic PDE for the phase density ρ in the *H phase space.* Then, subject to the following initial condition,

$$\rho(H, t = 0) = \delta(H - H_0) \tag{13}$$

where δ is the three-dimensional Dirac delta function, equation (13) is the probabilistic rendering of the deterministic initial condition (12) in the phase density $\rho(H, t)$.

Kavvas & Karakas (1996), under a second-order cumulant expansion, derived the ensemble-averaged form of a stochastic purely convective transport equation (equation 11). This ensemble-averaged equation for the phase density $\rho(H,t)$ is expressed as

$$\frac{\partial \langle \rho(H(x_t,t),t)\rangle}{\partial t} = -\frac{\partial}{\partial H_i}\left\{\left[\langle \eta_j\left(H(x_t,t),A(x_t,t),f(x_t,t)\right)\rangle - \int_0^t Cov_0\left[\eta_j\left(H(x_t,t),A(x_t,t),f(x_t,t)\right);\ \frac{\partial}{\partial H_i}\eta_i\left(H(x_{t-s},t-s),A(x_{t-s},t-s),f(x_{t-s},t-s)\right)\right]ds\right]\cdot\langle\rho(H(x_t,t),t)\rangle\right\} + \frac{\partial}{\partial H_i}\left\{\int_0^t Cov_0\left[\eta_j\left(H(x_t,t),A(x_t,t),f(x_t,t)\right);\ \frac{\partial}{\partial H_i}\eta_i\left(H(x_{t-s},t-s),A(x_{t-s},t-s),f(x_{t-s},t-s)\right)\right]ds\cdot\frac{\partial}{\partial H_i}\langle\rho(H(x_t,t),t)\rangle\right\} \quad (14)$$

where the symbol $\langle\cdot\rangle$ denotes the ensemble averaging or expectation operation, s is the time displacement, and Cov_0 is the time-ordered covariance function defined by

$$Cov_0\left[\eta_j(x,t_1);\eta_i(x,t_2)\right] = \langle\eta_j(x,t_1)\eta_i(x,t_2)\rangle - \langle\eta_j(x,t_1)\rangle\langle\eta_j(x,t_1)\rangle \quad (15)$$

Equation (14) is a mixed Eulerian-Lagrangian partial differential equation. While x_t is known and represents the real space location at time *t*, the Lagrangian location x_{t-s} is unknown. However, this unknown Lagrangian location x_{t-s} can be determined from the known location x_t using the Lie operator defined by Kavvas and Karakas (1996) as

$$x_{t-s} = \overleftarrow{exp}\left[-\int_{t-s}^{t} d\tau\langle v_l(x_\tau,\tau)\rangle\frac{\partial}{\partial x_l}\right]x_t \quad (16)$$

where v_l is determined from the characteristic curve equations corresponding to a particular hydrologic/hydraulic system (equations 8 and 9) and $\overleftarrow{exp}$ denotes the time-ordered exponential, where within the exponential series of the integrals, the arguments within each integral are ordered in time. By considering a first-order approximation (Kavvas & Karakas, 1996), equation (16) may be expressed as

$$x_{t-s} = x_t - \int_{t-s}^{t} d\tau\langle v_l(x_\tau,\tau)\rangle \quad (17)$$

On the other hand, by using Van Kampen's lemma (Van Kampen, 1976), the phase density $\rho(H,t)$ is linked to the evolutionary probability density of the vector state variable $P(H,t)$, as follows

$$\langle\rho(H,t)\rangle = P(H,t) \quad (18)$$

Then, combining equations (8), (9), (10), (14), and (18) yields the following Lagrangian-Eulerian nonlocal extension to the Fokker-Planck equation (to be denoted as LEFPE) for confined groundwater flow, which would solve the hydraulic head's PDF, $P(H,t)$ as function of time and space as,

$$
\begin{aligned}
\frac{\partial P(h,x,y;t)}{\partial t} = & -\frac{\partial}{\partial x}\Bigg\{P(h,x,y;t)\Bigg[\langle \eta_1(x,y;t)\rangle + \int_0^t Cov_0\left[\frac{\partial \eta_1(x,y;t)}{\partial x};\ \eta_1(x,y;t-s)\right]ds \\
& + \int_0^t Cov_0\left[\frac{\partial \eta_1(x,y;t)}{\partial y};\ \eta_2(x,y;t-s)\right]ds + \int_0^t Cov_0\left[\frac{\partial \eta_1(x,y;t)}{\partial h};\ \eta_3(x,y;t-s)\right]ds\Bigg]\Bigg\} \\
& -\frac{\partial}{\partial y}\Bigg\{P(h,x,y;t)\Bigg[\langle \eta_2(x,y;t)\rangle + \int_0^t Cov_0\left[\frac{\partial \eta_2(x,y;t)}{\partial x};\ \eta_1(x,y;t-s)\right]ds \\
& + \int_0^t Cov_0\left[\frac{\partial \eta_2(x,y;t)}{\partial y};\ \eta_2(x,y;t-s)\right]ds + \int_0^t Cov_0\left[\frac{\partial \eta_2(x,y;t)}{\partial h};\ \eta_3(x,y;t-s)\right]ds\Bigg]\Bigg\} \\
& -\frac{\partial}{\partial h}\Bigg\{P(h,x,y;t)\Bigg[\langle \eta_3(x,y;t)\rangle + \int_0^t Cov_0\left[\frac{\partial \eta_3(x,y;t)}{\partial x};\ \eta_1(x,y;t-s)\right]ds \\
& + \int_0^t Cov_0\left[\frac{\partial \eta_3(x,y;t)}{\partial y};\ \eta_2(x,y;t-s)\right]ds + \int_0^t Cov_0\left[\frac{\partial \eta_3(x,y;t)}{\partial h};\ \eta_3(x,y;t-s)\right]ds\Bigg]\Bigg\} \\
& + \frac{\partial^2}{\partial x^2}\left\{P(h,x,y;t)\int_0^t Cov_0[\eta_1(x,y;t);\ \eta_1(x,y;t-s)]ds\right\} \\
& + \frac{\partial^2}{\partial y^2}\left\{P(h,x,y;t)\int_0^t Cov_0[\eta_2(x,y;t);\ \eta_2(x,y;t-s)]ds\right\} \\
& + \frac{\partial^2}{\partial h^2}\left\{P(h,x,y;t)\int_0^t Cov_0[\eta_3(x,y;t);\ \eta_3(x,y;t-s)]ds\right\} + \\
& cross-covariance\ dispersion\ terms
\end{aligned}
\tag{19}
$$

It is important to note that equation (19) has the structure of a linear advection-diffusion equation. For the advection terms, Liang and Kavvas (2008) defined the expected values of the η functions as the mean advection coefficients, while the integrals of the ordered covariance functions as the advection correction terms.

Even though equation (19) is a linear and deterministic PDE, it still presents substantial challenges for its solution. Therefore, some simplifications without losing the prime physical characteristics are examined. One of the complications arises in estimating the covariance terms in the advection and diffusion coefficients. However, the advection correction terms can be considered negligible compared to the mean advection terms. This assumption is based on the expected η_i magnitudes, which are much larger than those of the integral terms (Kavvas and Wu, 2002). Mathematically, this can be expressed as follows

$$
\langle \eta_i(x,y;t)\rangle \gg \int_0^t Cov_0\left[\frac{\partial \eta_i(x,y;t)}{\partial H_j};\ \eta_j(x,y;t-s)\right]ds \tag{20}
$$

Regarding diffusion terms, they can be defined into two categories. The first is the terms involving the ordered covariance between the same η functions. The second is the terms that consider the ordered covariance between two different η functions or also called cross-covariance dispersion terms. Liang & Kavvas (2008) showed that the autocovariance of the η function of

one state variable is considerably larger in magnitude than the covariance between any two different η functions. Therefore, all cross-covariance terms are neglected from equation (19) to simplify calculations. However, this assumption could break down depending on the behavior of the η functions. For η functions with similar periodicity and close frequencies, the cross-covariance terms could become more comparable in magnitude to the autocovariance values, contrary to the previous simplification (Dib and Kavvas, 2018). The resulting nonlocal LEFPE after simplifications previously mentioned is shown in equation (21) below:

$$\begin{aligned}\frac{\partial P(h,x,y;t)}{\partial t} = {} & \frac{1}{S(x,y)}\frac{\partial}{\partial x}\left\{P(h,x,y;t)\langle\frac{\partial T_x(x,y;\,t)}{\partial x}\rangle\right\} + \frac{1}{S(x,y)}\frac{\partial}{\partial y}\left\{P(h,x,y;t)\langle\frac{\partial T_y(x,y;\,t)}{\partial y}\rangle\right\} \\ & - \frac{1}{S(x,y)}\frac{\partial}{\partial h}\{P(h,x,y;t)\langle[DT(x,y;t)+Q(x,y;t)]\rangle\} \\ & + \frac{1}{S(x,y)^2}\frac{\partial^2}{\partial x^2}\left\{P(h,x,y;t)\int_0^t Cov_0\left[\frac{\partial T_x(x,y;\,t)}{\partial x};\,\frac{\partial T_x(x,y;\,t-s)}{\partial x}\right]ds\right\} \\ & + \frac{1}{S(x,y)^2}\frac{\partial^2}{\partial y^2}\left\{P(h,x,y;t)\int_0^t Cov_0\left[\frac{\partial T_y(x,y;\,t)}{\partial y};\,\frac{\partial T_y(x,y;\,t-s)}{\partial y}\right]ds\right\} \\ & + \frac{1}{S(x,y)^2}\frac{\partial^2}{\partial h^2}\left\{P(h,x,y;t)\int_0^t Cov_0[Q(x,y;t);\,Q(x,y;t-s)]ds\right\}\end{aligned} \tag{21}$$

In equation (21), transmissivity and the source/sink terms are treated as random functions, while storativity is assumed to be a deterministic constant. Accordingly, storativity was moved outside of the expectations and ordered covariance terms. This assumption agrees with several studies, indicating that storativity has low variability (Freeze, 1975; Dagan and Rubin, 1988; Meier et al., 1998; Castagna et al., 2011). Nonetheless, the inclusion of storativity as a random function is possible.

Moreover, it is essential to note that the diffusive term $DT(x,y;t)$ is not considered inside of the covariance terms. This absence can be explained by the previous assumption that stated that the diffusive terms $DT(x,y;t)$ in the stochastic point-scale confined groundwater flow equation fundamentally contributes only to the mean behavior. Therefore, since $DT(x,y;t)$ is deemed deterministic, it will imply a null correlation against any random function.

Following the notation established by Garabedian (1986), the final form of the LEFPE (equation 21) can be written as shown in equation (22). Terms F^i denote the advection terms, while diffusion terms are expressed by D^i. In addition, $P(h,x,y;t)$ is substituted by P to increase the readability and simplicity of large equations.

$$\frac{\partial P}{\partial t} = \frac{1}{S(x,y)}\frac{\partial}{\partial x}F^xP + \frac{1}{S(x,y)}\frac{\partial}{\partial y}F^yP + \frac{\partial}{\partial h}F^hP + \frac{1}{S(x,y)^2}\frac{\partial^2}{\partial x^2}D^xP + \frac{1}{S(x,y)^2}\frac{\partial^2}{\partial y^2}D^yP + \frac{\partial^2}{\partial h^2}D^hP \tag{22}$$

where,

$$F^x = \langle \frac{\partial T_x(x,y;t)}{\partial x} \rangle \quad (23)$$

$$F^y = \langle \frac{\partial T_y(x,y;t)}{\partial y} \rangle \quad (24)$$

$$F^h = -\frac{1}{S(x,y)} \langle [DT(x,y;t) + Q(x,y;t)] \rangle \quad (25)$$

$$D^x = \int_0^t Cov_0 \left[\frac{\partial T_x(x,y;t)}{\partial x}; \frac{\partial T_x(x,y;t-s)}{\partial x} \right] ds \quad (26)$$

$$D^y = \int_0^t Cov_0 \left[\frac{\partial T_y(x,y;t)}{\partial y}; \frac{\partial T_y(x,y;t-s)}{\partial y} \right] \mathrm{ds} \quad (27)$$

$$D^h = \frac{1}{S(x,y)^2} \int_0^t Cov_0 [Q(x,y;t);\ Q(x,y;t-s)]\, ds \quad (28)$$

Equation (22) represents the resulting Lagrangian-Eulerian extension to the Fokker-Planck equation, which is a deterministic second-order PDE. The probability density function for the hydraulic head in the h-x-y phase through time can be obtained based on the solution of this nonlocal LEFPE. Hence, the spatio-temporal evolution of the hydraulic head's mean and standard deviation behavior (in the horizontal two-dimensional x-y space) can also be obtained, as well as any of its statistical moments.

3.2 Numerical solution for the Lagrangian-Eulerian Extension of the Fokker-Planck equation (LEFPE)

Once the LEFPE is derived (equation 22), it must be solved using a well-suited numerical scheme. However, significant computational resources are required to solve this equation, especially to compute the tail probabilities of the distribution (Johnson et al., 1997). To date, most of the studies have used the Finite Element Method (Arif Masud and Bergman, 2005; Galán et al., 2007; Král and Náprstek, 2017) and the Finite Difference Method (Fok et al., 2002; Sepehrian and Radpoor, 2015; Qian et al., 2019) to solve the conventional FPE numerically.

According to Masud and Bergman (2005), solving the conventional FPE for high dimensional problems (≥ 3) requires fine resolution in the time integration scheme. This requirement is even more critical at early times in the simulation to accurately resolve features in the rapidly evolving probability flow. The difficulties at the beginning of the simulation are associated with sharp changes occurring in small spatial regions, which can strongly influence the global properties of the system (Wei, 2000). Moreover, numerical algorithms can be highly sensitive to sharp gradients and quickly lead to numerically induced spatial and/or temporal chaos (Ablowitz et al., 1996)

Pichler et al. (2013) addressed comparative studies between the Finite Element Method (FEM) and Finite Difference Method (FDM), motivated by the high dimensionality in engineering dynamical systems. In this study, four widely used Finite Element and Finite Difference schemes to solve the transient FPE were reviewed by means of various numerical examples. They stated that FEM is preferable over FDM in terms of accuracy. However, the FEM is only suitable for dimensions ≤3 due to the significant numerical effort required. Park and Petrosian (1996) examined six Finite Difference Methods, three fully implicit and three semi-implicit commonly used to solve the FPE. Each method was evaluated in terms of its stability, accuracy, and efficiency. They concluded that the most robust FDM was the fully implicit Chang-Cooper method (Chang and Cooper, 1970).

Nowadays, the Chang-Cooper method is still considered one of the most popular tools to tackle the FPE due to its desirable properties (Larsen et al., 1985; Buet and Thanh, 2007; Buet and Dellacherie, 2010; Butt, 2021). This scheme ensures second-order accuracy, the positiveness of the solution, conservation of the probability mass, and the exact representation of the analytical solution upon equilibration. While having the above-mentioned good characteristics, the Chang-Cooper scheme is based on the advection coefficients' positiveness ($F^i > 0$). Therefore, its solution is not guaranteed for the FPE of the confined groundwater flow. In equation (22), the drift coefficients can be negative for this particular problem since their sign depends on the transmissivity field, flux conditions, and the source term. Hence, an appropriate numerical scheme must be selected, different from Chang and Cooper's scheme, to tackle this problem.

The LEFPE of our study closely resembles an advection-diffusion equation (ADE), widely studied in the computational fluid dynamics (CFD) field. Hence, several researchers have used common numerical schemes used in the CFD field to solve the conventional FPE. Even though the ADE is a linear PDE, difficulties arise due to its dual nature. If the ADE is diffusion-dominated, the equation behaves as a second-order parabolic equation. At the same time, if the ADE is advective-dominated, this equation behaves as a first-order hyperbolic equation. Therefore, to accurately solve the ADE, the numerical scheme needs to handle the mixed parabolic-hyperbolic behavior of the physical system (Yeh et al., 1992). Further details about the numerical method used to solve the advection-diffusion equation can be found in Zheng and Bennett (2002).

Motivated by the drift coefficients' negativity, Ohara et al. (2008) used an explicit Finite Volume Method (FVM) to solve their LEFPE for the snowmelt process. The FVM was used to handle the boundary conditions that present potential difficulty for the snowmelt process. Ohara et al. (2008) pointed out that there is no universal scheme to solve the LEFPE since the selected numerical scheme depends on each problem.

Ceyhan and Kavvas (2018) developed a one-dimensional LEFPE for the transient confined groundwater flow to a well. They used the explicit Lax-Wendroff scheme, a second-order FDM, to solve the advective term. Additionally, a flux delimiter was included to mitigate artificial oscillation while preserving sharp concentration fronts using the upwind method (Shu and LeVeque, 1991). For the diffusive term, an implicit second-order centered difference approximation was used, which resulted

in a one-dimensional implicit-explicit (IMEX) scheme to be solved. Selecting implicit schemes for solving diffusive terms and explicit schemes for advective terms is common practice in the CFD field (Ascher et al., 1995; Chaudhry et al., 2015). Mixing implicit and explicit schemes allows specialized numerical methods for systems formed by operators with different time scales. Refer to Ascher et al. (2006) for additional details about IMEX methods to solve PDEs.

ULTIMATE QUICKEST (Leonard, 1991) is another widely used explicit numerical scheme to tackle the advection-diffusion equation in the CFD field. This scheme has not just been successfully applied in open-channel systems (Kashefipour and Zahiri, 2010; Yoshimura and Fujita, 2019) and subsurface hydrology (Lin and Falconer, 1997; Neumann et al., 2011) but also for solving the LEFPE (Tu et al., 2019). Tu et al. (2019) developed a one-dimensional LEFPE for a solute transport model under uncertain open-channel flow conditions. The ULTIMATE QUICKEST (UQ) and an explicit second-order centered difference approximation were used to discretize the advective and diffusive terms, respectively. Their results suggest that the UQ numerical scheme can generally handle both small and significant variability in the flow fields with satisfactory results. Therefore, this numerical scheme could be used to solve advective-dominated as well as diffusive-dominated problems. While Leonard (1991) developed and applied the UQ scheme to a one-dimensional problem, Tu et al. (2020) generalized it to solve a two-dimensional LEFPE.

The ULTIMATE QUICKEST is based on the QUICKEST (Quadratic Upwind Interpolation for Convective Kinematics with Estimated Streaming Terms) scheme and the ULTIMATE (Universal Limiter for Transient Interpolation Modeling of the Advective Transport Equation) limiter. The QUICKEST scheme (Leonard, 1979) is an explicit third-order accurate upwind scheme. Leonard (1979) designed this scheme for reducing numerical oscillations and truncations problems on highly advective unsteady flows. This scheme was derived using a finite difference approach for temporal discretization and a control volume approach for spatial discretization. This derivation implies calculating the discrete fluxes entering and leaving the control volume, which are estimated using an average quadratic upstream interpolation over a time increment. Even though the QUICKEST method has little numerical dispersion and a large stability region, even minimal oscillations can corrupt the solution, especially near sharp gradients (Leonard, 1991; Neumann et al., 2011).

Leonard (1991) proposed the ULTIMATE (the Universal Limiter for Transient Interpolation Modeling of the Advective Transport Equations) to overcome the problem associated with the numerical oscillations by the QUICKEST scheme. ULTIMATE is a total variation diminution (TVD) algorithm that uses flux limiters to preserve the local monocity of the solution, even close to the sharp discontinuities and shocks. Thus, the local monotonicity is preserved, which is crucial for our problem since negative values would indicate negative probabilities, losing our problem's physical meaning. This scheme was derived using the Normalized Variation Diagram (NVD) concept, based on normalized variables to set the nodal boundaries to suppress oscillations. Several authors have indicated improved stability near steep fronts due to non-oscillatory behavior and reduced numerical dispersion by using ULTIMATE (Lin and Falconer, 1997; Harris et al., 2002; Neumann et al., 2011).

In addition to the ULTIMATE limiter's desirable characteristics, this algorithm involves minimal extra computational load, and it is particularly attractive for point sources (deterministic conditions) in the Lagrangian-Eulerian Fokker-Planck Equation framework.

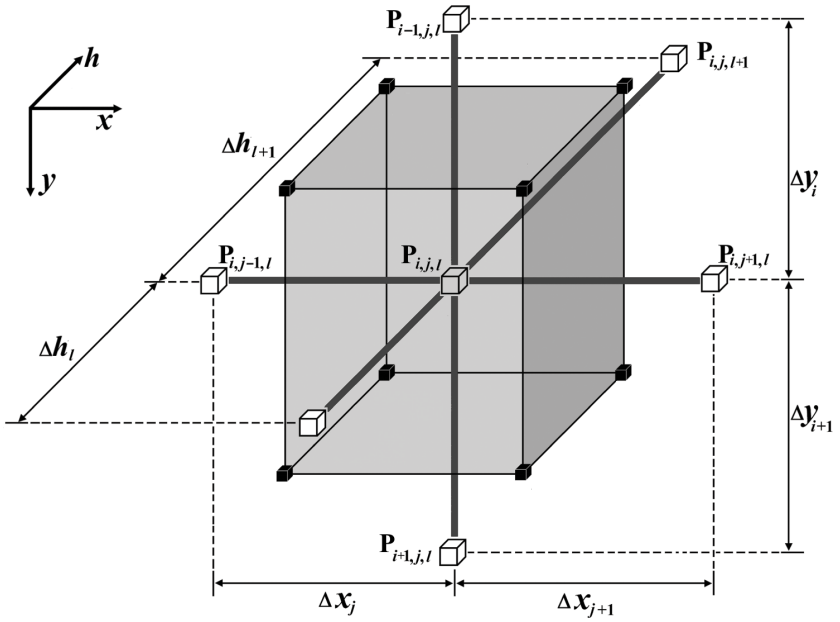

Figure 1: Grid cell for a 3D domain. The probability density function value P is defined at the cell center, whereas the probability fluxes are defined in the cell faces.

The numerical method selected to solve the three-dimensional LEFPE (equation 22) needs to achieve two main objectives: (1) to have a potential to be parallelized and also (2) it needs to control the numerical dispersion. The importance of parallelizing the numerical scheme relies on the high computational times required to solve multi-dimensional FPE (Masud and Bergman, 2005). In addition, parallelization will allow dealing with larger domains in space and probability sense. Furthermore, the main goal of this study is to estimate the ensemble mean and variance of the hydraulic head under uncertain parameters. A numerical scheme that causes numerical dispersion would result in overestimating the variance. Therefore, accurate numerical simulation without numerical dispersion plays a vital role in the goodness of the results.

In this study, the UQ is adopted to solve the advective terms. Like Tu et al. (2020), who generalized the UQ to solve a two-dimensional LEFPE, an attempt is made here to generalize this scheme to three-dimensional problems. An explicit scheme for advective terms was preferred over an implicit scheme for mainly two reasons: (1) implicit schemes for advection tend to be more numerically diffusive than explicit schemes (Dawson, 1995), and (2) implicit schemes for advection lead to a nonsymmetric matrix, which could be challenging to invert (Ascher et al., 1995) and convergence of many iterative solvers

will suffer (Wang et al., 2015). In addition, Cahyono (1993) tested more than 30 schemes for discretizing the advection term. He concluded that the UQ was the most attractive since it was more general than the other schemes. However, the stability region imposed by the Courant-Friedrich-Lewy (CFL) condition is a severe restriction of standard explicit numerical methods. This restriction implies a much smaller time step than permitted by accuracy considerations (Casulli, 1990; Dehghan, 2004).

A typical practice to rectify the CFL condition's limitation involves using an implicit discretization for diffusive terms in the ADE. Thus, the resulting implicit-explicit scheme will be less restrictive regarding the time step required for stability (Bürger et al., 2020). In addition to the desirable properties of IMEX schemes previously mentioned, it is essential to mention that the resulting linear 7-diagonal system of equations is symmetric, sparse, and strictly diagonally dominant, with positive elements on the main diagonal and negative elements elsewhere (Ascher et al., 1995). Therefore, this system is positively defined and has a unique solution. Furthermore, preconditioned conjugate gradient methods can solve a 7-diagonal sparse system of equations very efficiently (Casulli, 1990) .

Then, by applying forward finite difference formulas for the time derivative and the previously discussed schemes for the first and second spatial derivatives on a staggered grid, as shown in Figure (1), the proposed LEFPE (equation 22) can be discretized by the following IMEX scheme:

$$\begin{aligned}\frac{P_{j,i,l}^{t+1}-P_{i,j,l}^{t}}{\Delta t} = {} & F^{x,t}\frac{P_{j-0.5,i,l}^{t}-P_{j+0.5,i,l}^{t}}{\Delta x_j} + F^{y,t}\frac{P_{j,i+0.5,l}^{t}-P_{j,i-0.5,l}^{t}}{\Delta y_i} + F^{h,t}\frac{P_{j,i,l+0.5}^{t}-P_{j,i,l-0.5}^{t}}{\Delta h_l} \\ & + \frac{(D^xP)_{j-1,i,l}^{t+1}-2(D^xP)_{j,i,l}^{t+1}+(D^xP)_{j+1,i,l}^{t+1}}{\Delta x_j^2} + \frac{(D^yP)_{j,i-1,l}^{t+1}-2(D^yP)_{j,i,l}^{t+1}+(D^yP)_{j,i+1,l}^{t+1}}{\Delta y_i^2} \\ & + \frac{(D^yP)_{j,i,l-1}^{t+1}-2(D^yP)_{j,i,l}^{t+1}+(D^yP)_{j,i,l+1}^{t+1}}{\Delta h_l^2}\end{aligned} \tag{29}$$

Where Δt, Δx_j, Δy_i, and Δh_l are discretization intervals for *t, x, y, h* dimensions, respectively; the subscripts {*j, i, l*} denote the nodes in *x*, *y*, and *h* domains, while the superscript *t* denotes the current time step of the probability density P, and t+1 denotes the next time step. Note that in equation (29), each subscript {*j, i, l*} followed by a ± 0.5 may be interpreted as the probability flux or probability current, whereas *P* (the probability density function) is considered as the state variable.

It is important to note that while the drift coefficients $F^{x,t}$, $F^{y,t}$, and diffusion coefficients $D^{x,t}$, $D^{y,t}$, and $D^{h,t}$ depend on external input such as the transmissivity random field and the source term, the drift coefficient $F^{h,t}$ depends on the curvature in the x-y space at the current time t. Hence, we estimate this term in the current time "t" through the solution obtained in the

last time "t-1" by assuming that small changes in the curvature occur between a time step Δt. Then, the diffusive term $DT(\underline{x}, t)$ can be estimated as follows:

$$DT(\underline{x}, t) = T_x(\underline{x}, t)\frac{\partial^2 h(\underline{x}, t)}{\partial x^2} + T_y(\underline{x}, t)\frac{\partial^2 h(\underline{x}, t)}{\partial y^2} \approx T_{i,j}^{x}\frac{h_{j-1,i}^{t-1} - 2h_{j,i}^{t-1} + h_{j+1,i}^{t-1}}{\Delta x_j^2} + T_{i,j}^{y}\frac{h_{j,i-1}^{t-1} - 2h_{i,j}^{t-1} + h_{j,i+1}^{t-1}}{\Delta y_i^2} \quad (30)$$

Due to its control-volume formulation for spatial gradients, this scheme is sensitive to the flow direction. Hence, the probability fluxes of each face consider the flux direction to carry out the calculations. Thus, the probability fluxes in the advection terms, represented by $P_{j-0.5,i,l}$, $P_{j+0.5,i,l}$, $P_{j,i-0.5,l}$, $P_{j,i+0.5,l}$, $P_{j,i,l-0.5}$ and $P_{j,i,l+0.5}$ are estimated based on the one-dimensional ULTIMATE QUICKEST scheme. Assuming that the velocity in node $\{j, i, l\}$ is positive in the x-direction ($F^{x,t} > 0$), the flux at the face $\{j+0.5, i, l\}$ can be summarized as follows:

(1) Compute the upwind-biased second-order difference *CURV* and the normalization difference *DEL* as:

$$CURV_j = C_j = P_{i+1,i,l}^{t} - 2P_{j,i,l}^{t} + P_{j-1,i,l}^{t} \quad (31)$$

$$DEL_j = D_j = P_{j+1,i,l}^{t} - P_{j-1,i,l}^{t} \quad (32)$$

(2) Set the probability flux as

$$P_{j+0.5,i,k}^{t} = \begin{cases} P_{j,i,l}^{t} & ,If\ |C_j| \geq |D_j| \\ \frac{\left(P_{j+1,i,l}^{t} + P_{j,i,l}^{t}\right)}{2} - \frac{|c_x|\left(P_{j+1,i,l}^{t} - P_{j,i,l}^{t}\right)}{2} - \frac{(1-c_x^2)}{6}CURV_j & ,If\ |C_j| < |D_j| \end{cases} \quad (33)$$

(3) Compute the reference face value:

$$P_{ref-j}^{t} = P_{j-1,i,l}^{t} + (P_{j,i,l}^{t} - P_{j-1,i,l}^{t})/c_x \quad (34)$$

(4) If $DEL_j > 0$, limit the fluxes according to:

$$if\ P_{j+0.5,i,l}^{t} \leq P_{j,i,l}^{t} \ \Rightarrow\ P_{j+0.5,i,l}^{t} = P_{j,i,l}^{t} \quad (35)$$

Then,

$$if\ P_{j+0.5,i,k}^{t} \geq min\{P_{ref-j}^{t}; P_{j+1,i,l}^{t}\} \ \Rightarrow\ P_{j+0.5,i,l}^{t} = min\{P_{ref-j}^{t}; P_{j+1,i,l}^{t}\} \quad (36)$$

(5) Similar to step (4), if $DEL_j < 0$, limit the fluxes according to:

$$if\ P^t_{j+0.5,i,l} > P^t_{j,i,l} \ \Rightarrow\ P^t_{j+0.5,i,l} = P^t_{j,i,l} \tag{37}$$

Then,

$$if\ P^t_{j+0.5,i,l} < max\{P^t_{ref-j}; P^t_{j+1,i,l}\} \ \Rightarrow\ P^t_{j+0.5,i,l} = max\{P^t_{ref-j}; P^t_{j+1,i,l}\} \tag{38}$$

Like the flux calculation at the face $P_{j+0.5,i,l}$, the fluxes at the other five faces can be estimated by following steps (1) to (5). Once all probability fluxes faces are estimated, they must be substituted into the discretized LEFPE (equation 29). Thus, the probability density function at the next step can be calculated by solving the resulting system of linear equations. Moreover, the probability mass in the *x-y-h space* must be conserved since the proposed LEFPE is an evolutionary probability density function transport equation. Therefore, non-flux boundary conditions are applied to the boundaries in the *x-y-h space*. Furthermore, since an explicit numerical scheme is used to deal with the advective terms, the Courant–Friedrich–Lewy (CFL) condition is required at each computational node to achieve stable solutions. The CFL condition can be expressed in mathematical terms as follows

$$Courant\ Number = C = \frac{F^x \cdot \Delta t}{\Delta x_j} + \frac{F^y \cdot \Delta t}{\Delta y_i} + \frac{F^h \cdot \Delta t}{\Delta h_l} \leq C_{max} \leq 1 \tag{39}$$

The solution of this LEFPE results in the joint PDF of the state variables in the *x-y-h space*. Thus, it is possible to obtain a hydrologic system's ensemble behavior and variability defined by the point-scale stochastic confined groundwater flow equations under uncertainty in the transmissivity field and the source term. However, the proposed methodology may also be expanded to problems with uncertainties in storativity and boundary conditions.

4 Results and discussion

In this section, a two-dimensional numerical experiment is performed to illustrate the potential and capabilities of the novel proposed stochastic model for groundwater flow in confined aquifers. Hence, the probabilistic behavior of the hydraulic head under uncertainty in the transmissivity random field is investigated by solving the LEFPE (equation 21). The solution of the LEFPE will obtain the ensemble behavior and variability of the confined groundwater system in one shot by computing the hydraulic head's PDF over time and space. The performance of the stochastic model proposed is evaluated by comparison with the results from the corresponding Monte Carlo simulations. The numerical scheme used to carry out the MC simulation for the discretized governing equation (4) was the Control-Volume Finite-Difference (CVFD) method. This scheme is the same one used by MODFLOW, which is currently the most popular numerical model to deal with groundwater flow-transport

problems. Thus, the computation of 100,000 groundwater flow realizations with a randomized transmissivity field comprises the MC simulation. For further details about the CVFD numerical scheme, please see (Hughes et al., 2017).

This study considers a log-normal distribution to represent the transmissivity random field, the most widely accepted assumption for this parameter. The model proposed by Zárate-Miñano and Milano (2016) was used to represent the stochasticity in the transmissivity field. This model uses stochastic differential equations (SDEs) employing the equivalence between the Langevin and the Fokker–Planck equations and the regression theorem. To generate the transmissivity random field, the only information needed is the mean and variance of the transmissivity as well as its correlation length. Thus, generating stochastic processes with a specific probability distribution and exponentially decaying autocorrelation function is possible. This model can be expressed as follows:

$$dT(x) = a[T(x), x] \cdot dx + b[T(x), x] \cdot dW(x) \tag{40}$$

where the drift term $a[T(x), x]$, and the diffusion term $b[T(x), x]$ are expressed as follows

$$a[T(x), x] = -\alpha \left(T(x) - exp\left[\mu + \frac{\sigma^2}{2}\right]\right) \tag{41}$$

$$b[T(x), x] = \sqrt{b_1[T(x), x] \cdot b_2[T(x), x]} \tag{42}$$

with

$$b_1[T(x), x] = \sqrt{2\pi} \cdot \alpha \cdot \sigma \cdot T(x) \cdot exp\left[\mu + \frac{\sigma^2}{2} + \frac{[\ln(T(x)) - \mu]^2}{2\sigma^2}\right] \tag{43}$$

$$b_2[T(x), x] = erf\left(\frac{\mu + \sigma^2 - \ln(Tx))}{\sqrt{2}\sigma}\right) - erf\left(\frac{\mu - \ln(Tx))}{\sqrt{2}\sigma}\right) \tag{44}$$

where $W(x)$ represents a standard Wiener process., $erf(\cdot)$ is the error function, T is transmissivity, α is the autocorrelation coefficient, and μ and σ are the mean and the standard deviation of the natural logarithm of variable T, respectively. To generate the transmissivity random field implies the numerical integration of the stochastic differential equation (40). The implicit Milstein scheme is used to solve the SDE numerically (Mil'shtejn, 1975). This scheme is based on the truncated Ito-Taylor expansion, and it has a convergence error of order 1 ($\mathcal{O}(h)$) in both the weak and the strong sense. This scheme can be expressed as follows:

$$T(x+\Delta h) = T(x) + \frac{\Delta h}{2}\left[a[T(x+\Delta h), x+\Delta h] + a[T(x), x]\right] + b[T(x), x]\cdot \Delta W(x)$$

$$+\frac{1}{2}\, b[T(x), x]\cdot \frac{\partial b[T(x), x]}{\partial T(x)}\left[\left(\Delta W(x)\right)^2 - \Delta h\right] \quad (45)$$

where Δh is the integration spatial step and $\Delta W(x) \sim \mathrm{N}(\Delta h)$ are random increments of the Wiener process.

For this hypothetical problem, the total simulation time is T = 3 hours which consists of a two-dimensional confined aquifer of 2000 [m] by 2000 [m] extent (figure 2) and 15 [m] thickness. For the initial conditions, the hydraulic head h is set at 20 [m], while the boundary conditions at the corners are set at 23 [m] at x=0 and y=0, h=21 [m] at x=0 and y=2000, h=20 [m] at x=2000 and y=0, h=20 [m] at x=2000 and y=2000 and linearly interpolated between the corners to impose constant gradient at the boundaries.

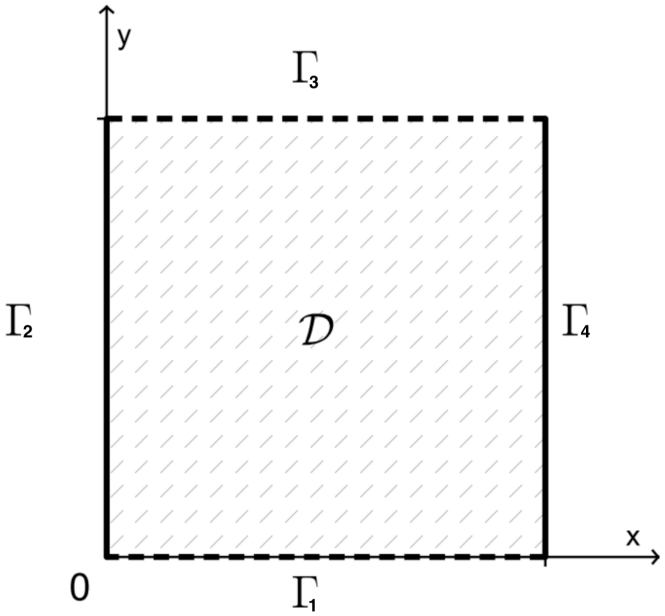

Figure 2. Illustration of the two-dimensional physical domain.

A Hydraulic conductivity mean equal to $\mu_K = 2 \cdot 10^{-3}\ [m/s]$ is used, which is a representative hydraulic conductivity value for gravel aquifers (Domenico and Schwartz, 1998). A coefficient of variation equal to $C.V. = 1.5$ was considered, and a correlation length equal to $L = 100\ [m]$ was used for its correlation structure. Nevertheless, the correlation is independent along each spatial dimension. This independence in the transmissivity field occurs by the use of independent SDEs in the x

and y directions, which is a drawback for the used transmissivity generation model. For specific storage S_s, typical values in confined aquifers range from $5 \cdot 10^{-5}\ [1/m]$ to $5 \cdot 10^{-3}\ [1/m]$ (Todd, 1980). Thus, numerical tests in this study consider a specific storage equal to $S_s = 10^{-4}\ [1/m]$, consistent with the range reported by Todd (1980).

Regarding the numerical discretization for the MC and LEFPE, both models were implemented using the same spatial grid $\Delta x = 10\ [m]$ In the case of the time discretization, while the time step in the MC simulation was fixed $\Delta t = 1\ [s]$, the LEFPE was variable to satisfy the Courant constraint (Equation 39) This time step restriction is crucial at the beginning of the simulation due to the high gradients in the probability domain $(P - x - y - h)$, which add extra numerical diffusion to the system These high gradients are due to incorporating deterministic conditions by means of Dirac delta pulses. However, as time goes, the simulation tends to smooth the probability mass in the $x - y - h$ domain, reducing the probability gradients. A resume of the parameters used to carry out this application can be found in table (1) below.

Parameter	Symbol	Value
Hydraulic conductivity mean	$\overline{K_x} = \overline{K_y}$	$2 \cdot 10^{-3}\ [m/s]$
Coefficient of Variation	$C.V.$	1.5
Correlation length	$L_x = L_y$	$100\ [m]$
Specific storage	S_s	$10^{-4}\ [1/m]$
Aquifer length	L	$2000\ [m]$
Aquifer width	B	$15\ [m]$
I.C. at t=0	h_0	$20\ [m]$
B.C. at y=0	Γ_1	$23 - 0.0015x\ [m]$
B.C. at x=0	Γ_2	$23 - 0.001y\ [m]$
B.C. at y=L	Γ_3	$21 - 0.0005x\ [m]$
B.C. at x=L	Γ_4	$20\ [m]$
x-y-grid size	$\Delta x = \Delta y$	$10\ [m]$
h-grid size	Δh	$2.5\ [cm]$
Simulation time	T	$3\ [hours]$

Table 1. Physical parameters values of the numerical experiment.

The variable time step used for solving numerically the LEFPE was calculated dynamically to satisfy the CFL condition at each solution step. Devkota and Imberger (2009) reported a good agreement between 1D and 2D analytical solutions for pure advection of the Gaussian tracer distribution and the numerical solution provided by the ULTIMATE-QUICKEST scheme

using a C_{max} close to one. However, they reported the presence of numerical diffusion. Similar behavior was shown by Lin and Falconer (1997) for the simulation of pure advection of a column in a 2-D. Therefore, we imposed a more restrictive C_{max} equal to 10% to reduce numerical diffusion effects.

Moreover, this variable time step helps reduce the computation time since the LEFPE has an extra dimension compared to the original groundwater flow equation, implying a higher computational cost. This extra dimension is associated with the hydraulic head in the probability space, and it shows up due to the probabilistic nature of the LEFPE. Since the state variable in this equation is the PDF (P) instead of the groundwater flow equation (4) in which the state variable is the hydraulic head (h).

Figure (3) shows the hydraulic head's ensemble average obtained by the LEFPE and MC approaches at the simulation time t = {T/3; 2T/3; T }. These figures indicate water fluxes through the x and y axes. The comparison shows a good match in terms of the ensemble mean of the hydraulic head. However, it is possible to note an overestimation of this quantity as time goes on. This behavior is probably due to the influence of boundaries through the h-axis, which tends to advect probability mass through the positive direction of the h-axis, increasing the ensemble mean at the boundaries.

The corresponding standard deviation profiles for this example are shown in Figure (4) to evaluate the performance of the LEFPE methodology. This figure indicates that the proposed framework correctly portrays the ensemble variability, providing a good representation of the patterns. Even though the LEFPE was derived by employing a second-order cumulant expansion, it is essential to note that it tends to smooth its solutions (Ohara, 2003). This behavior of the LEFPE reported by Ohara (2003) makes the PDF flatter, artificially increasing the standard deviation estimation. Similar issues were faced by Diaz (2019), where the standard deviation estimation suffers from a lack of accuracy next to the boundary condition.

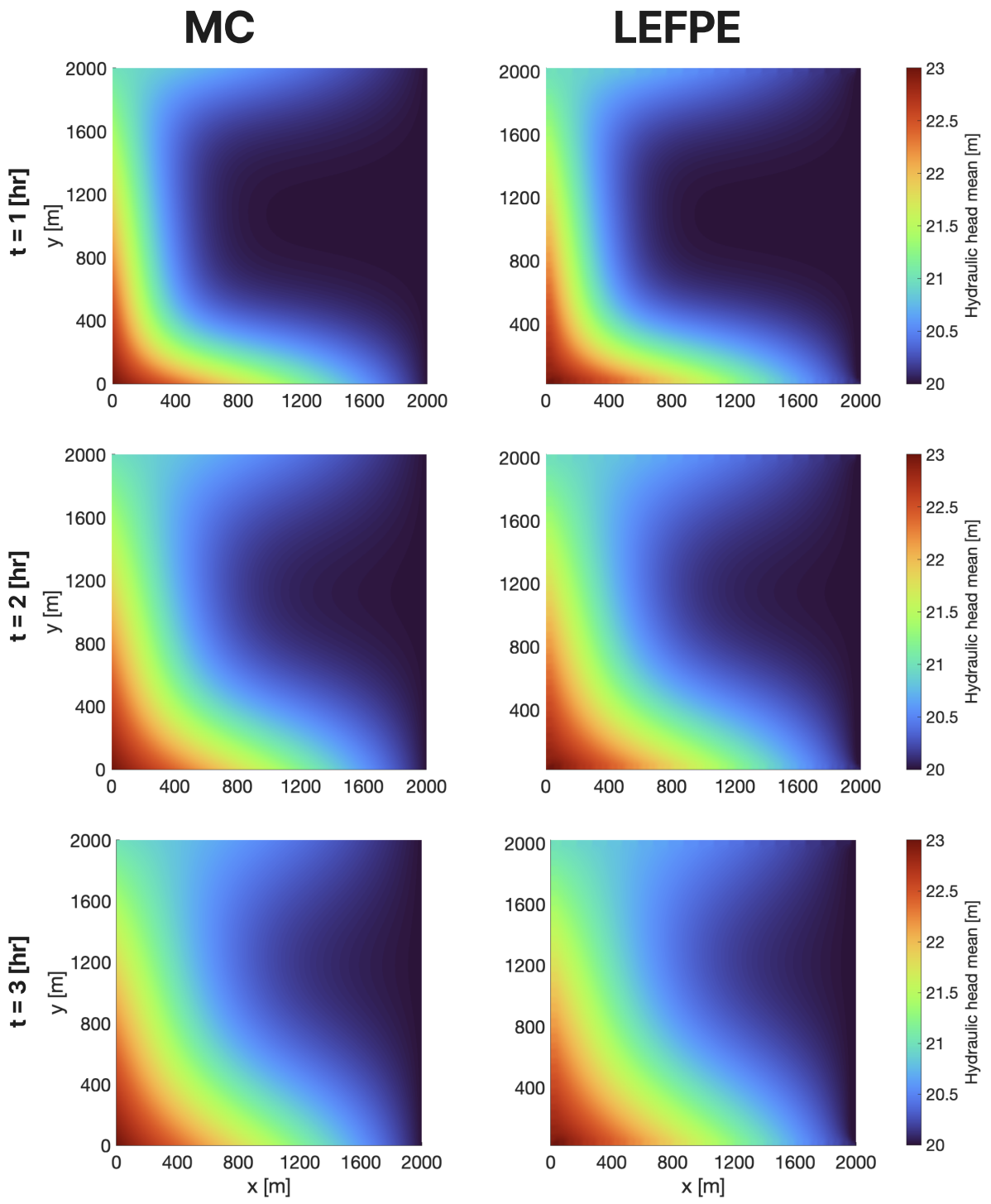

Figure 3: Plan view of the Hydraulic head's ensemble average with respect to position and time for the results obtained by the MC method (left panel) and those obtained by the LEFPE method (right panel).

Figures (5) and (6) show the ensemble average and variability for the hydraulic head at x = y and x=2y, respectively. From the left panel, it can be easily seen that the proposed stochastic framework's mean behavior of the hydraulic head and the Monte Carlo simulation indicate good matches, with a slight overestimation in the area with the higher curvature. In the variability case (right panel figure), the LEFPE methodology shows excellent agreement with only light deviations concerning the MC simulations.

The overestimation of the ensemble variability of the proposed LEFPE methodology over the MC simulations can be attributed to three factors. The first one is associated with the derivation of the LEFPE. Even though a second-order cumulant expansion was used for its derivation, the solution tends to be smooth (Ohara, 2003). Second, the numerical diffusion inherent to any numerical model, especially with advection schemes. The previous factors mentioned diffusing the state variable P, making it flatter and consequently increasing its variability. In addition, as a third factor, modeling deterministic conditions as Dirac delta pulses introduces high gradients into the system. These high gradients result in extra numerical diffusion in these areas compared to zones far from the boundaries.

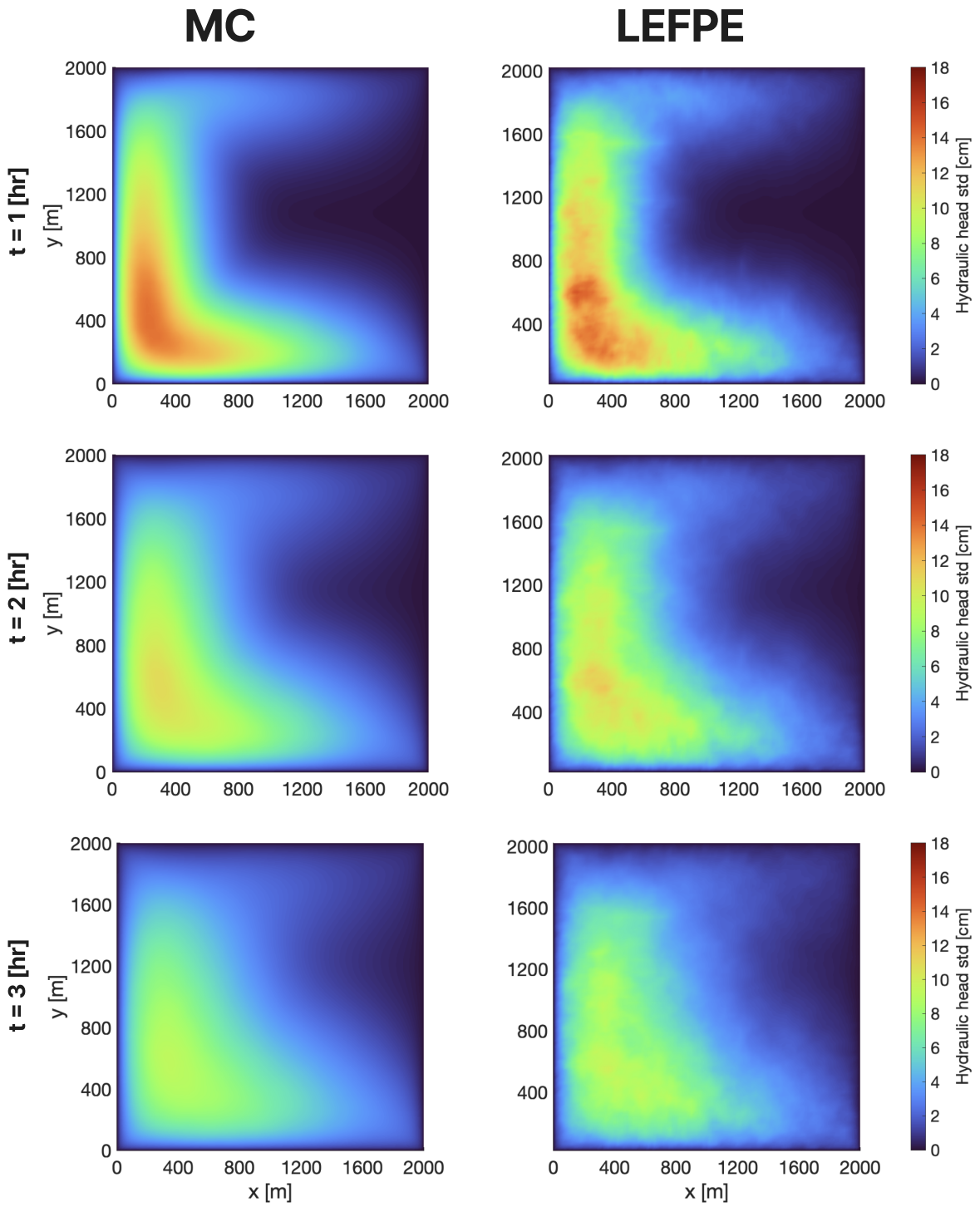

Figure 4: Plan view of the Hydraulic head's ensemble variability (in terms of its standard deviation) with respect to position and time for the results obtained by the MC method (left panel) and those obtained by the LEFPE method (right panel).

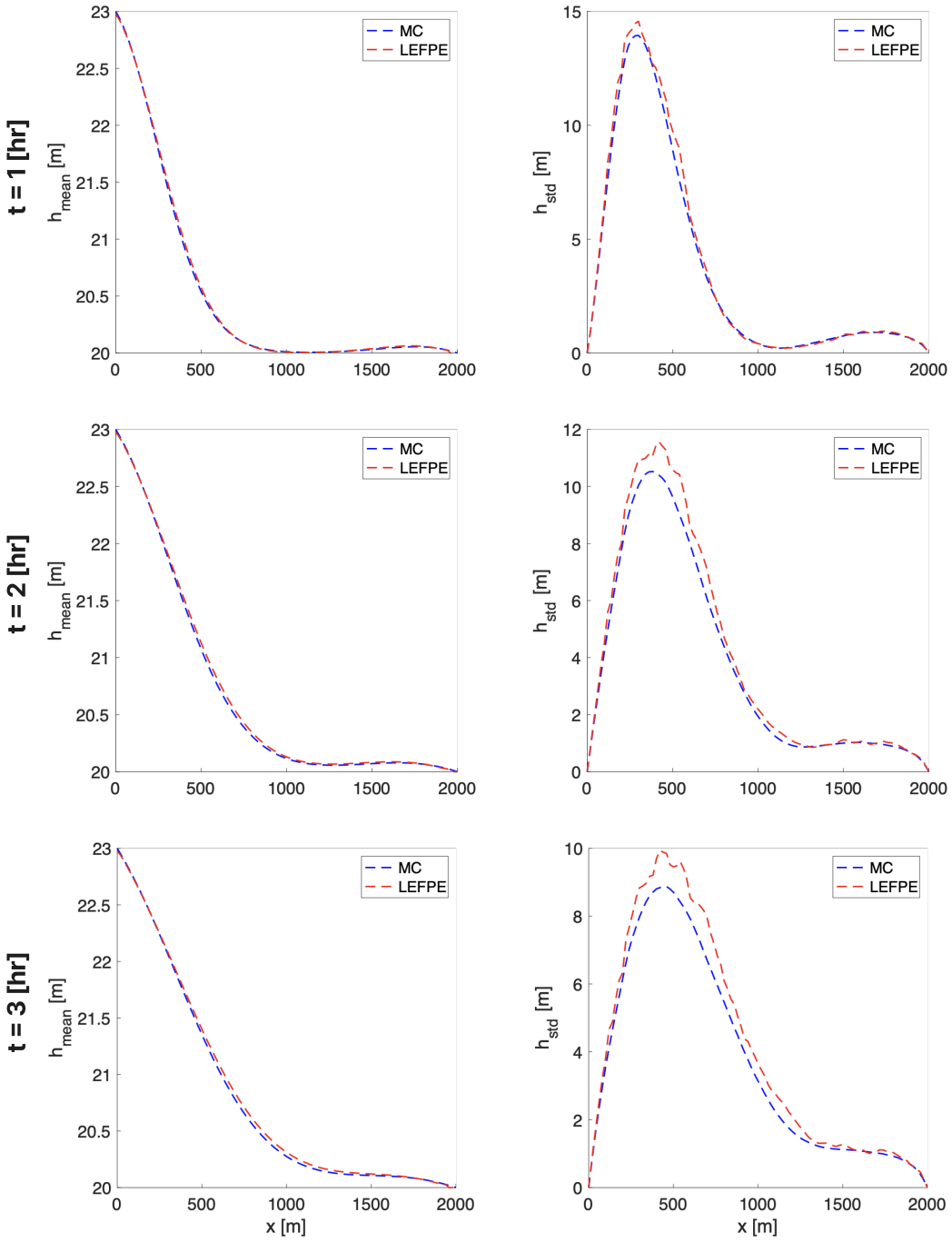

Figure 5: Comparison of the hydraulic head ensemble average and variability (standard deviation) by LEFPE method and the MC approach at locations x = y at different times.

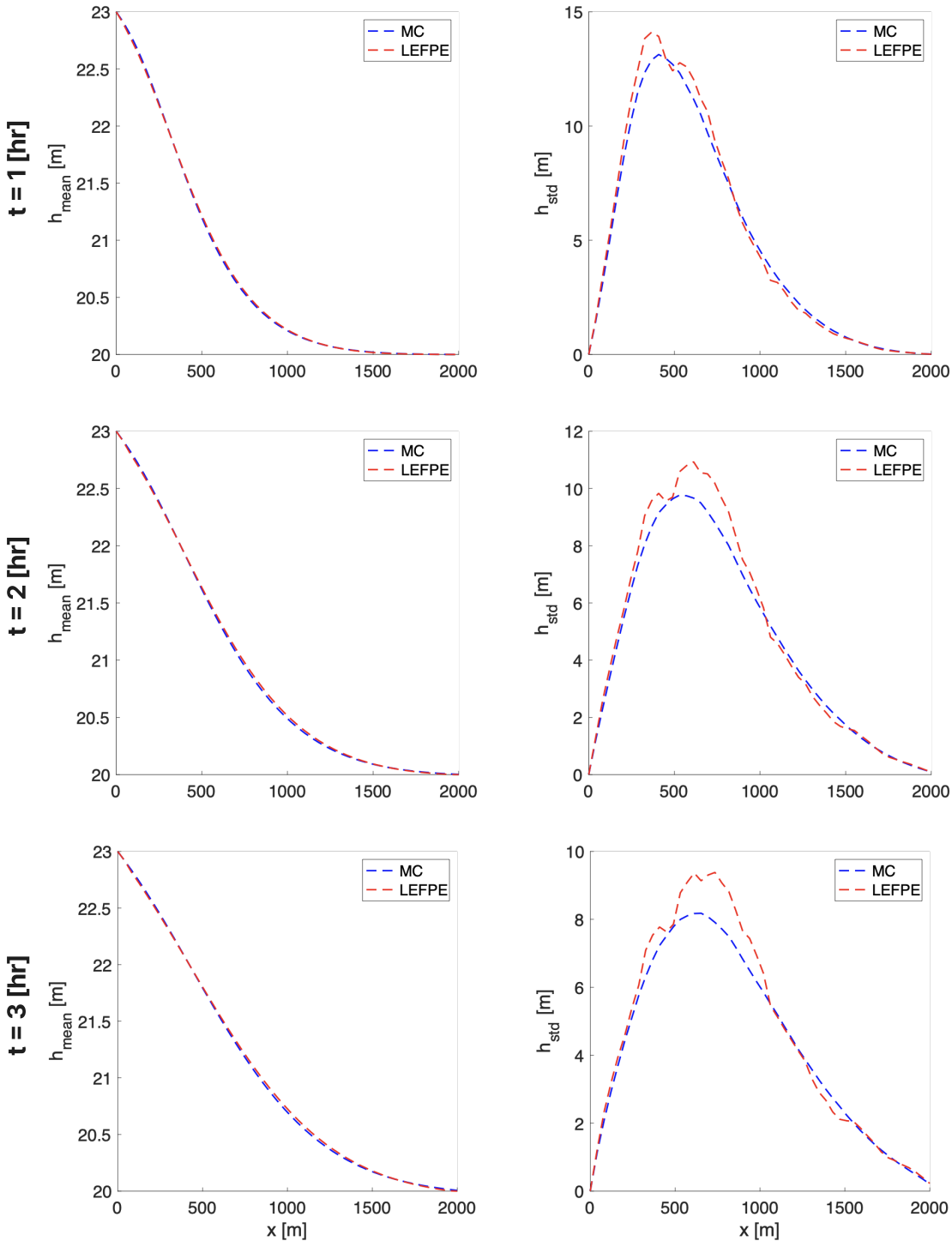

Figure 6: Comparison of the ensemble average and variability by LEFPE method and the MC approach at locations x = 2y at different times.

5 Summary and conclusions

Due to the heterogeneity in geomaterials and the stochasticity of the source/sink process, the governing subsurface flow equation in confined aquifers at the point-scale becomes a stochastic PDE at the field scale. Therefore, this governing equation needs to be upscaled to the corresponding field scale to predict its behavior correctly. One of the most popular approaches to carry out this task has been developing their ensemble average forms. Although the MC and Perturbation methods have been widely used for upscaling the groundwater flow equation in confined aquifers, they have essential drawbacks regarding computational cost and small variance constraints.

For this purpose, this study developed a second-order expression for the mean and probabilistic behavior of the groundwater flow equation in confined aquifers. The resulting expression (22) is a deterministic PDE in the form of a Lagrangian-Eulerian extension to the Fokker-Planck equation (LEFPE), while the original governing equation, described by equation (4), was a stochastic PDE. The solution of the LEFPE under the appropriate initial and boundary conditions describes the time-space evolution of the hydraulic head's PDF. Therefore, it is possible to determine the ensemble averages and variances of the hydraulic head in confined aquifers in one shot, unlike numerical analysis based on a Monte Carlo approach. The ensemble average is then obtained from a standard expectation operation using the system's already calculated PDF.

Obtaining the probabilistic ensemble behavior by a single simulation is one of the most advantageous characteristics of the proposed methodology. This characteristic is fundamental in (1) high-dimensional problems and (2) simulations where tails' responses are essential to estimate accurately. Thus, the computational time could be reduced significantly in both cases since larger sample sizes are required for Monte Carlo simulations. Furthermore, the LEFPE approach does not suffer from the "closure problem" associated with the traditional perturbation approach or limitations associated with high random parameter variability.

The resulting linear and deterministic LEFPE was discretized by using the explicit ULTIMATE QUICKEST algorithm (Leonard, 1991) for the advective terms, while an implicit second-order centered difference approximation was used for diffusive terms. Thus, the LEFPE is solved numerically using an implicit-explicit (IMEX) scheme to determine the confined aquifer system's ensemble behavior and variability. The election of the numerical scheme was based on two points. The scheme needed the potential to be parallelized to speed up the calculations and to model large domains. In addition, the numerical scheme had to control the numerical dispersion. The latter is a crucial factor since extra diffusion in the system would artificially increase its variance estimation.

Results obtained by solving the LEFPE were compared against the Monte-Carlo solutions to evaluate the performance of the proposed methodology. Despite minor differences, the comparison showed a good agreement in terms of the ensemble mean and variance in the solution domain, characterizing the first and second moments of the hydraulic head in confined aquifers. Thus, the LEFPE solution gives a good representation of the general patterns, the decreasing and increasing trend, and the ranges of the ensemble mean and variability.–The developed methodology can also potentially include variability in the storativity and boundary conditions. Subsequently, this stochastic framework shows good promise in dealing with high-dimensional problems and including correlated structures in the random field variables. Current work is progressing in that direction.

Even though the proposed stochastic framework can effectively capture the shapes of the standard deviation behavior, the ensemble variability tends to be overestimated by the LEFPE methodology. Three reasons can explain the overestimation of this statistical parameter: (1) the second-order cumulant expansion used to derive the LEFPE, (2) the numerical diffusion inherent to any numerical model, and (3) the representation of deterministic conditions by means of Delta pulses. The developed methodology can also include variability in the storativity and boundary conditions. Subsequently, this stochastic framework shows good promise in dealing with high-dimensional problems and including correlated structures in the random field variables.

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