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Full Length Article

Modeling contaminant transport in riverbank filtration systems: A three-dimensional analysis with Green's function approach

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ABSTRACT

The utilization of Riverbank Filtration Systems (RBF) presents a promising approach for obtaining potable water from rivers or streams. However, the effectiveness of this technique relies significantly on two key factors: the width of the river and the presence of a clogging layer beneath the streambed, both of which influence the degree of contamination in the extracted water. Prior studies have predominantly relied on numerical models or simplistic one-dimensional flow assumptions to address these variables. In contrast, this research introduces a 3D analytical model utilizing the Green's function approach to analyze the movement of contaminants from the river towards the extraction well within RBF systems. By accounting for the dynamic interaction between river width and the clogging layer, this model offers a more accurate depiction of contaminant transport in three-dimensional water flow scenarios. The accompanying MATLAB code facilitates numerical integration of model equations, producing graphical representations for various hydrological inputs. Validation against MODFLOW software demonstrates a remarkable agreement, with outcomes aligning at 98–99%. Key findings underscore the exacerbation of pollutant concentrations with heightened clogging, increased river width, and optimal well placement. Moreover, the analysis underscores better predictive accuracy achieved by incorporating actual river width values compared to simple linear approximations. Notably, the research reveals minimal impact on contaminant concentrations when the distance between the river and the well exceeds twice the river's width, offering valuable insights for system design and management.

1. Introduction

Understanding the transport of solutes in groundwater systems is necessary for managing water resources and ensuring the safety of drinking water supply. In many real-world scenarios, such as near streams or rivers, the interaction between surface water and groundwater becomes a critical factor. Riverbank filtration (RBF) systems, also known as riverbank or riverbed filtration, are natural water treatment processes that depend on biological activities in riverbank sediments and the surrounding aquifer to enhance the quality of water supplies. The process involves the extraction of water from rivers or other surface water bodies by wells installed within riverbanks. As the water passes through the riverbank and into the aquifer, physical, chemical, and biological processes remove or transform contaminants, resulting in improved water quality. Where the water cannot be directly delivered to the public, this treatment method for highly polluted rivers is used. [1,2].

To simulate the solute movement in this system, several factors need to be considered, including river width and leakance coefficient of streambed. These are two critical river parameters that affect the water quality produced from the RBF system. The leakance coefficient is a function of hydraulic conductivity of streambed, which affects the amount of river water that passes through the streambed and, consequently, affects the level of contamination in the pumped water [3].

In the last two decades, most of the studies of the water quality on RBF systems focused on the surface water-groundwater interaction,

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pollutant migration and transformation, and evaluations of the water resource, etc., while studies on the relationship between the aforementioned topics and the river conditions (e.g. width and hydraulic conductivity of streambed) are relatively insufficient. These river parameters play crucial roles in calculating the distance between river and well, and in estimating the drawdown in the well which influences the level of water quality. Decreasing the distance between wells and the river increases the capture of surface water, while diminishing the purifying effects of the RBF system. Conversely, increasing drawdown facilitates greater water extraction, but leads to faster flow rates, potentially impeding pollutant removal [6,7]. Numerous case studies demonstrated the significant impact of the distance between wells and rivers on the volume of water reaching the well. It could also affect the recharge from the river [8,9]. After the pumping well is constructed and parameters like well depth and spacing are set, drawdown becomes the sole adjustable factor influencing both the quantity and quality of water from the pumping well [10]. However, the drawdown is affected by both river factors; the leakance coefficient and the width of the stream. Therefore, these factors should be fully considered in investigating the water quality of RBF.

Using mathematical modeling tools is necessary to determine the impact of clogging streambed and finite width stream on contaminant transport in RBF systems. Additionally, optimizing the ratio between river width and the distance from the well to the river edge is required to obtain high-quality water from RBF systems [11–15]. Huang, et al. [4] conducted an extensive review of existing analytical solutions for stream depletion rate. Their analysis highlighted some models that discussed the effect of river width and clogging on the drawdown in the well and consequently on water quality. To achieve realistic simulation of leakance coefficient, the ratio between the width of river and the distance between river and well should be greater than 1.0 [5]. This ratio is calculated to simulate the stream depletion rate, but not to evaluate the quality of water.

In recent years, there has been an increasing interest in modeling solute transport released from streams towards pumping wells in three-dimensional groundwater flow. Researchers, including Lu, et al. [16], Pan, et al. [7], Abd-Elaty, et al. [17], Knabe, et al. [18], Lee, et al. [9], Luo, et al. [19] and Jiang, et al. [20], have contributed to this interest. Nevertheless, the mentioned studies made the assumption that river is either a line contaminant source or completely penetrates the aquifer, and most of them are based on numerical solutions.

Several years ago, the theoretical foundations for contemporary groundwater models like the USGS's MODFLOW [Harbaugh, 2005[21]], or the California Department of Water Resources' IWFM [Dogrul, 2012 [22]], employing either finite difference (FD) or finite element (FE) formulations, were established. Although numerical solutions involve a discretization of the spatial–temporal aquifer domain and the consideration of irregular domain shapes, they may cause instability, and may need long programming and computing implementation periods. On the other hand, analytical solutions that describe contaminant behavior in groundwater system provide a thorough understanding of the system's underlying physics and allow for a clear understanding of how different parameters such as clogging, river width and well location affect the solution.

Therefore, analytical solutions are introduced to provide a better grasp of the mechanism of solute transport and an improved prediction of the contaminant plum movement. Singh and Chatterjee [23] investigated the solute transport behavior in groundwater with non-uniform flow analytically using Laplace transform. Sangani, et al. [24] produced an analytical model to investigate the behavior of solute transport in aquifer with plane sources of contamination. Although the two studies considered the river width in their three-dimensional contaminant transport model released from plane sources, they assumed that water moved to aquifer due to natural differences in water head without any existence of pumping well which is not the case of RBF systems.

Green's function approach is one of the prominent analytical strategies in groundwater modeling, notable for its adaptability in handling various boundary conditions [25–29]. Green's functions can serve as a foundation for efficient design, optimization, and control of mass transport processes [23,30]. In these applications, a dependable Green's function can replace approximate or empirical system models, enhancing the reliability and quality of a design or control procedure. It can be governed by a set of conservation laws and physical principles. Thus, the identification of a Green's function that accurately characterizes the system's spatial and temporal response to external influences brings forth a range of potent capabilities [31]. When addressing chemical transport within intricate and irregular domains, determining the temporal response at specific locations to a diverse array of spatially and temporally varying stimuli using Green's function becomes achievable [32,33].

Wang and Wu [34] implemented Green's function to address the contaminant transport released from rectangular source in two-dimensional groundwater flow. Also, Chen, et al. [35] produced analytical solutions based on Green's functions that deal with different sources including the plane sources like finite width streams. The previous two studies using Green's function considered only the width of the source but ignored the effect of pumping and clogging layer on contaminant transport. Several more researchers have utilized Green's function to analytically offer a set of solutions for the transit of pollutants in aquifers [26,27,34–42]. However, the majority of the existing models that utilized the Green's function technique in groundwater modelling either do not assume the existence of a pumping well close to the contaminated source or do not incorporate any degradation or adsorption of contaminants in their model. Additionally, earlier research neglected the width of stream and focused on rivers that completely infiltrates the aquifer. In order to simulate the movement of contaminants towards a pumping well located near stream that partially penetrates a homogenous aquifer, an analytical model utilizing Green's function is created in our previous study [39]. Despite taking into account the impact of stream width, we have modelled groundwater movement in a single direction.

In this article, the Green's function approach is chosen to simulate 3D pollutant transportation in RBF systems in 3D groundwater flow. This article aims to: (1) Construct a 3D model for contaminant transport originating from a stream near a pumping well in RBF systems using Green's function approach. (2) Analyze the effect of clogging, river width, and well location parameters on pollutant concentration in RBF systems, and (3) Determine the suitable ratio between river width and well-stream distance that required to obtain good quality water. In this model, the aquifer is supposed to be semi-infinite, initially has no contaminants and the stream just partially penetrates it. The layer of clogging beneath the streambed prevents the stream from penetrating it completely. Both finite depth aquifers and semi-infinite aquifers can be covered by the model. Contamination only comes from the river and the problem is formulated mathematically by assuming that the stream has finite width and the well has constant pumping rate. MATLAB software is used to calculate the numerical integral occurred in the proposed analytical solution obtained by using Green's function method. To validate the model, its results are compared with numerical results obtained using MODFLOW software which depends on finite difference method.

2. Methodology: Analytical model

2.1. Mathematical formulation

Fig. 1 illustrates the location of pumping well next to river in RBF system. Assume that the river extends in y direction from $-y_0$ to y_0 and its width extends from 0 to x_0 on horizontal direction. The pumping well, which has a constant pumping rate Q, is located at a distance L from the river in a finite depth aquifer d. Due to pumping process, the contaminants induced to move from river towards the well.

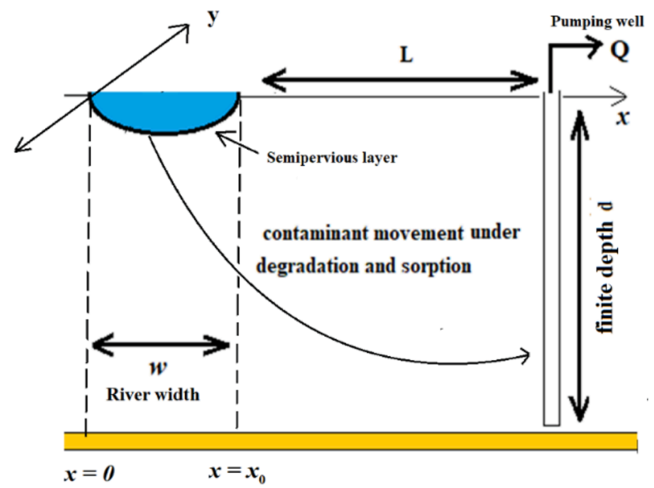

Fig. 1. Cross sectional view for the release of contaminants from streams of finite width.

Assume that the pumping well's concentration of pollutants is equal to $C_w(t)$ and that the initial concentration emitted from the river is equal to C_0. Based on the balance equation, the value of $C(x,y,z,t)$ which represents pollutants concentration during their movement from the river to the well is equal to:

$$C(x,y,z,t) = C_0(t) - C_w(t), \tag{1}$$

Since the 3D transport of contaminants with degradation rate is usually described by using advection dispersion equation, then Equation (1) with initial and boundary conditions can be written as:

$$R\frac{\partial C}{\partial t} - D_x\frac{\partial^2 C}{\partial x^2} - D_y\frac{\partial^2 C}{\partial y^2} - D_z\frac{\partial^2 C}{\partial z^2} + U_x\frac{\partial C}{\partial x} + U_y\frac{\partial C}{\partial y} + U_z\frac{\partial C}{\partial z} + \nu RC = C_0(t) - C_w(t), \tag{2}$$

$$C(\pm\infty, y, z, t) = 0 \quad -\infty \le y \le \infty,\ 0 \le z \le d \quad \text{and}\ t \ge 0 \tag{2a}$$

$$C(x, \pm\infty, z, t) = 0 \quad -\infty \le x \le \infty,\ 0 \le z \le d \quad \text{and}\ t \ge 0 \tag{2b}$$

$$\frac{\partial C(x,y,0,t)}{\partial z} = \frac{\partial C(x,y,d,t)}{\partial z} = 0 \quad -\infty \le x \le \infty,\ -\infty \le y \le \infty \ \text{and}\ t \ge 0, \tag{2c}$$

$$C(x,y,z,0) = 0 \quad -\infty \le x \le \infty,\ -\infty \le y \le \infty \ \text{and}\ 0 \le z \le d \tag{2d}$$

where $C(x,y,z,t)$ is the pollutants concentration (M/L^3),U_x, U_y, U_z are the seepage velocities in x, y and z directions (L/T), D_x, D_y,D_z are the dispersion factors in x, y and z directions (L^2/T), ν is decay constant (1/T) and R is the linear retardation factor. Initially, the aquifer is presumed to be uncontaminated. As one moves far from the river in both the x and y directions, contamination levels diminish to zero. In the z direction, the top and lower borders are presumed to be impenetrable by contaminants.

The function $C_0(t)$ can be calculated using the formula below by assuming that the river has the following dimension: $x \in [0,\ x_0]$, $y \in [-y_0, y_0]$ and $z \in [z_0, z_1]$. The function is defined as the mass of pollutants emitted from the source and disintegrated in a unit water volume in a unit time amount (M/(L^3.T)).

$$C_0(t) = \begin{cases} S_o f(t)/\phi & 0 < x < x_0, -y_0 < y < y_0,\ z_0 < z < z_1 \\ 0 & \text{otherwise} \end{cases}, \tag{3}$$

where S_0 (M/(L3.T)) is source concentration constant, $f(t)$ is a dimensionless function of time and ϕ is the porosity. The model integrates the impact of river width using equation (3), where the variable x_0 represents the river's width, denoted as w. According to Dillon, et al. [43] the following equation can be used to get the value of concentration at pumping well:

$$C_w(t_w) = \frac{q}{Q}[S_o exp(-\nu t)], \tag{4}$$

where time t (T) at which the pollutants enter the well (T), Q is the value of pumping amount (L^3/T) and q is stream depletion rate (L^3/T). To model the impact of clogging in the streambed, the equation proposed by Hunt [44] is employed to calculate the ratio q/Q when the stream partially interacts with the aquifer:

$$\frac{q}{Q} = erfc\left(\sqrt{\frac{S_x L^2}{4Tt_p}}\right) - Exp\left(\frac{\lambda^2 t_p}{4S_x T} + \frac{\lambda L}{2T}\right) erfc\left(\sqrt{\frac{\lambda^2 t_p}{4S_x T}} + \sqrt{\frac{S_x L^2}{4Tt_p}}\right), \tag{5}$$

where λ is the leakage coefficient of the stream bed (L/T), L represents the river's distance from the pumping well (L), S_x represents the storage coefficient, t_p represents the pumping duration (T) and T represents transmissivity (L^2/T). The following transformations are needed to resolve Equation (1):

$$x^* = x - \frac{U_x t}{R};\quad y^* = y - \frac{U_y t}{R},\quad z^* = z - \frac{U_z t}{R}, C_s(t) = C_0(t) - C_w(t)$$

$\overline{C}_w(t) = C_w(t)e^{\nu t}$, $\overline{C}_0(t) = C_0(t)e^{\nu t}$, $\overline{C}_s(t) = [\overline{C}_0(t) - \overline{C}_w(t)]$, $\overline{C}(x,y,t) = C(x,y,t)e^{\nu t}$;

Also these dimensionless relations are required:

$$t_D = D_z t/\left(Rd^2\right);\quad C_D = D_z\overline{C}/\left(RS_0 d^2\right);\quad C_{s_D}(t) = \overline{C}_s(t)/(S_0 R);$$

$$y_D^* = \frac{y^*\left(\sqrt{D_z/D_y}\right)}{d};\quad z_D^* = \frac{z^*}{d};\quad x_D^* = \frac{x^*\left(\sqrt{D_z/D_x}\right)}{d}; \tag{6}$$

$$U_{x_D} = U_x d\Big/\sqrt{D_z D_x};\quad U_{z_D} = U_z d\Big/D_z;\quad U_{y_D} = U_y d\Big/\sqrt{D_z D_y}$$

Thus Equations (1) is converted to (see Appendix A):

$$\frac{\partial C_D}{\partial t_D} - \frac{\partial^2 C_D}{\partial x_D^{*2}} - \frac{\partial^2 C_D}{\partial y_D^{*2}} - \frac{\partial^2 C_D}{\partial z_D^{*2}} = C_{s_D}(t_D) \tag{7}$$

$$C_D(\pm\infty, y_D^*, z_D^*, t_D) = 0 \quad -\infty \le y_D^* \le \infty,\ -U_{z_D}t_D \le z_D^* \le 1 - U_{z_D}t_D \ \text{and}\ t_D \ge 0 \tag{7a}$$

$$C_D(x_D^*, \pm\infty, z_D^*, t_D) = 0 \quad -\infty \le x_D^* \le \infty,\ -U_{z_D}t_D \le z_D^* \le 1 - U_{z_D}t_D \ \text{and}\ t_D \ge 0 \tag{7b}$$

$$\frac{\partial C_D(x_D^*, y_D^*, -U_{z_D}t_D, t_D)}{\partial z_d} = \frac{\partial C_D(x_D^*, y_D^*, 1 - U_{z_D}t_D, t_D)}{\partial z_d} = 0 \quad -\infty \le y_D^* \le \infty,\ -\infty \le x_D^* \le \infty, \quad \text{and}\ t_D \ge 0 \tag{7c}$$

$$C_D(x_D^*, y_D^*, z_D^*, 0) = 0 \quad -\infty < x_D^* < \infty,\ -\infty \le y_D^* \le \infty,\ -U_{z_D}t_D \le z_D^* \le 1 - U_{z_D}t_D \tag{7d}$$

The concentration in the aquifer at the site caused by a point instantaneous pollutants source (x', y', z', τ) is represented by Green's function G in this model. At first, the value of G equals the Solution to the following equation.

$$\frac{\partial^2 G}{\partial x_D^{*2}} + \frac{\partial^2 G}{\partial y_D^{*2}} + \frac{\partial^2 G}{\partial z_D^{*2}} - \frac{\partial G}{\partial t_D} = \delta(x_D^* - x_D')\delta(y_D^* - y_D')\delta(z_D^* - z_D')\delta(t_D - \tau_D) \tag{8}$$

where δ is called Dirac delta function. The following integral must then be solved in order to arrive at the solution of Equation (8):

$$C_D(x_D^*, y_D^*, z_D^*, t_D) = \int_0^{t_D} C_{s_D}(\tau_D) \int_\Delta G(x_D^*, y_D^*, z_D^*, t_D - \tau_D) d\Delta d\tau_D,$$
$$= \int_0^{t_D} C_{s_D}(\tau_D) SF(x_D^*, y_D^*, z_D^*, t_D - \tau_D) d\tau_D, \tag{9}$$

The source function in Equation (9) is denoted by SF that is equal to the integration of G over the domain of the source Δ. Thus the three dimensional function G that satisfied Equation (8) can be obtained by evaluating the products of 1D Green's functions in the main directions x, y and z [26]:

$$G(x_D^*, y_D^*, z_D^*, t_D - \tau_D) = G(x_D^*, t_D - \tau_D) G(y_D^*, t_D - \tau_D) G(z_D^*, t_D - \tau_D) \tag{10}$$

and,

$$SF(x_D^*, y_D^*, z_D^*, t_D - \tau_D) = SF(x_D^*, t_D - \tau_D) SF(y_D^*, t_D - \tau_D) SF(z_D^*, t_D - \tau_D) \tag{11}$$

Now, the source function for x axis is [26]:

$$SF(x_D^*, t_D - \tau_D) = 1/(2\sqrt{\pi}) \int_{-U_{xD}\tau_D}^{x_{0_D} - U_{x_D}\tau_D} \frac{1}{\sqrt{t_D - \tau_D}} exp\left(\frac{-(x_D^* - \psi_D)^2}{4(t_D - \tau_D)}\right) d\psi_D$$

$$= \frac{1}{2}(\text{erfc}\left(\frac{x_D^* - x_{0_D} + U_{x_D}\tau_D}{2\sqrt{t_D - \tau_D}}\right) - \text{erfc}\left(\frac{x_D^* + U_{x_D}\tau_D}{2\sqrt{t_D - \tau_D}}\right) \tag{12}$$

For y direction, the integration of Green's function is:

$$SF(y_D^*, t_D - \tau_D) = 1/(2\sqrt{\pi}) \int_{-y_{0_D} - U_{yD}\tau_D}^{y_{0_D} - U_{y_D}\tau_D} \frac{1}{\sqrt{t_D - \tau_D}} exp\left(-\frac{(y_D^* - \zeta_D)^2}{4(t_D - \tau_D)}\right) d\zeta_D$$

$$= \frac{1}{2}\left(\text{erfc}\left(\frac{y_D^* - y_{0_D} + U_{y_D}\tau_D}{2\sqrt{t_D - \tau_D}}\right) - \text{erfc}\left(\frac{y_D^* + y_{0_D} + U_{y_D}\tau_D}{2\sqrt{t_D - \tau_D}}\right)\right) \tag{13}$$

Since the aquifer has finite depth d, then the integration along z direction is evaluated as follows [26]:

$$SF(z_D^*, t_D - \tau_D) = \int_{z_{0_D} - U_{z_D}\tau_D}^{z_{1_D} - U_{z_D}\tau_D} [1 + 2\sum_{n=1}^{\infty} cosn\pi\eta_D cosn\pi z_D^* exp(-n^2\pi^2(t_D - \tau_D)) d\eta_D$$

$$= z_{1_D} - z_{0_D} + \frac{2}{\pi}\sum_{n=1}^{\infty} \frac{1}{n}[sin(n\pi(z_{1_D} - U_{z_D}\tau_D)) - sin(n\pi(z_{0_D} - U_{z_D}\tau_D))] cosn\pi z_D^* exp(-n^2\pi^2(t_D - \tau_D)) \tag{14}$$

Equation (11) is changed by using Equations (12), (13) and (14) to give the following result:

$$SF(x_D^*, y_D^*, z_D^*, t_D - \tau_D) = \left[\frac{1}{2}\left(\text{erfc}\left(\frac{x_D^* - x_{0_D} + U_{x_D}\tau_D}{2\sqrt{t_D - \tau_D}}\right) - \text{erfc}\left(\frac{x_D^* + U_{x_D}\tau_D}{2\sqrt{t_D - \tau_D}}\right)\right)\right]$$
$$\times \left[\frac{1}{2}\left(\text{erfc}\left(\frac{y_D^* - y_{0_D} + U_{y_D}\tau_D}{2\sqrt{t_D - \tau_D}}\right) - \text{erfc}\left(\frac{y_D^* + y_{0_D} + U_{y_D}\tau_D}{2\sqrt{t_D - \tau_D}}\right)\right)\right]$$
$$\times \left[z_{1_D} - z_{0_D} + \frac{2}{\pi}\sum_{n=1}^{\infty}\frac{1}{n}[sin(n\pi(z_{1_D} - U_{z_D}\tau_D)) - sin(n\pi(z_{0_D} - U_{z_D}\tau_D))] cosn\pi z_D^* exp(-n^2\pi^2(t_D - \tau_D))\right] \tag{15}$$

Thus, from Equation (9), the solution is:

$$C_D(x_D^*, y_D^*, z_D^*, t_D) = \frac{1}{4}\int_0^{t_D} C_{s_D}(\tau_D) \times \left[\left(\text{erfc}\left(\frac{x_D^* - x_{0_D} + U_{x_D}\tau_D}{2\sqrt{t_D - \tau_D}}\right) - \text{erfc}\left(\frac{x_D^* + U_{x_D}\tau_D}{2\sqrt{t_D - \tau_D}}\right)\right)\right]$$
$$\times \left[\left(\text{erfc}\left(\frac{y_D^* - y_{0_D} + U_{y_D}\tau_D}{2\sqrt{t_D - \tau_D}}\right) - \text{erfc}\left(\frac{y_D^* + y_{0_D} + U_{y_D}\tau_D}{2\sqrt{t_D - \tau_D}}\right)\right)\right]$$
$$\times [z_{1_D} - z_{0_D} + \frac{2}{\pi}\sum_{n=1}^{\infty}\frac{1}{n}[sin(n\pi(z_{1_D} - U_{z_D}\tau_D)) - sin(n\pi(z_{0_D} - U_{z_D}\tau_D))] cosn\pi z_D^* exp(-n^2\pi^2(t_D - \tau_D))] d\tau_D, \tag{16}$$

When presented in dimensional form, the answer is

$$C(x, y, z, t) = 1/4dR \int_0^t C_s(\tau) \exp(-\nu(t - \tau))$$
$$\times \left[\text{erfc}\left[\frac{\sqrt{R}(x - x_0 - U_x(t - \tau)/R)}{2\sqrt{D_x(t - \tau)}}\right] - \text{erfc}\left[\frac{\sqrt{R}(x - U_x(t - \tau)/R)}{2\sqrt{D_x(t - \tau)}}\right]\right]$$
$$\times \left[\text{erfc}\left[\frac{\sqrt{R}(y - y_0 - U_y(t - \tau)/R)}{2\sqrt{D_y(t - \tau)}}\right] - \text{erfc}\left[\frac{\sqrt{R}(y + y_0 - U_y(t - \tau)/R)}{2\sqrt{D_y(t - \tau)}}\right]\right]$$
$$\times \left[z_1 - z_0 + \frac{2}{\pi}\sum_{n=1}^{\infty}\frac{1}{n}[sin\left(\frac{n\pi(z_1 - U_z\tau/R)}{d}\right) - sin\left(\frac{n\pi(z_0 - U_z\tau/R)}{d}\right)\right] cos\left(\frac{n\pi(z - U_z t/R)}{d}\right)$$
$$exp\left(\frac{-n^2\pi^2 D_z(t - \tau)}{Rd^2}\right)] d\tau \tag{17}$$

When the integration parameter is changed from τ to $\tau' = t - \tau$ we get:

$$C(x,y,z,t) = \frac{1}{4dR}\int_0^t C_s(t-\tau')\exp(-\nu\tau') \times \left[\mathrm{erfc}\left[\frac{\sqrt{R}\left(x-x_0-\frac{U_x\tau'}{R}\right)}{2\sqrt{D_x\tau'}}\right] - \mathrm{erfc}\left[\frac{\sqrt{R}\left(x-\frac{U_x\tau'}{R}\right)}{2\sqrt{D_x\tau'}}\right]\right]$$
$$\times\left[\mathrm{erfc}\left[\frac{\sqrt{R}\left(y-y_0-U_y\tau'/R\right)}{2\sqrt{D_y\tau'}}\right] - \mathrm{erfc}\left[\frac{\sqrt{R}\left(y+y_0-U_y\tau'/R\right)}{2\sqrt{D_y\tau'}}\right]\right] \times \left[z_1 - z_0 + \frac{2}{\pi}\sum_{n=1}^{\infty}\frac{1}{n}\left[sin\left(\frac{n\pi(z_1-U_z(t-\tau')/R)}{d}\right)\right.\right.$$
$$\left.\left. - sin\left(\frac{n\pi(z_0-U_z(t-\tau')/R)}{d}\right)\right] cos\left(\frac{n\pi(z-U_zt/R)}{d}\right)\ exp(\frac{-n^2\pi^2D_z\tau'}{Rd^2})\right]d\tau' \tag{18}$$

The solutions in Equation (18) considered that at the aquifer's lower and higher limits, there is no flow, then $U_z = 0$ at $z = 0$ and $z = d$.

In the case that the aquifer has infinite depth, then the Equation (14) will become similar to Equation (13) which provides the following solution:

$$C(x,y,z,t) = \frac{1}{4dR}\int_0^t C_s(t-\tau')\exp(-\nu\tau')$$
$$\times\left[\mathrm{erfc}\left[\frac{\sqrt{R}(x-x_0-U_x\tau'/R)}{2\sqrt{D_x\tau'}}\right] - \mathrm{erfc}\left[\frac{\sqrt{R}(x-U_x\tau'/R)}{2\sqrt{D_x\tau'}}\right]\right]$$
$$\times\left[\mathrm{erfc}\left[\frac{\sqrt{R}(y-y_0-U_y\tau'/R)}{2\sqrt{D_y\tau'}}\right] - \mathrm{erfc}\left[\frac{\sqrt{R}(y+y_0-U_y\tau'/R)}{2\sqrt{D_y\tau'}}\right]\right]$$
$$\times\left[\mathrm{erfc}\left[\frac{\sqrt{R}(z-z_0-U_z\tau'/R)}{2\sqrt{D_{yz}\tau'}}\right] - \mathrm{erfc}\left[\frac{\sqrt{R}(z-z_1-U_z\tau'/R)}{2\sqrt{D_z\tau'}}\right]\right] \tag{19}$$

Equations (18) and (19) can be used to simulate contaminant transport in finite depth and infinite depth aquifers respectively.

3. Results and discussion

This article employs Green's function to develop an analytical model for pollutants emitted by rivers of finite width. The model aims to examine the effect of clogging and river width on contaminant transport behavior in the system and to investigate the suitable ratio between river width and well-stream distance that required to obtain good quality water.

$$\phi_x(x,t) = \exp\left[\frac{U_x(x-x_0)}{2D_x}\left(1-\sqrt{1+\frac{4(k-\nu)D_x}{U_x^2}}\right)\right]\mathrm{erfc}\left[\frac{x-x_0-U_xt\sqrt{1+\frac{4(k-\nu)D_x}{U_x^2}}}{2\sqrt{D_xt}}\right]$$
$$\exp\left[\frac{U_x(x-x_0)}{2D_x}\left(1+\sqrt{1+\frac{4(k-\nu)d_x}{U_x^2}}\right)\right]\mathrm{erfc}\left[\frac{x-x_0+U_xt\sqrt{1+\frac{4(k-\nu)D_x}{U_x^2}}}{2\sqrt{D_xt}}\right] \tag{22}$$

3.1. Model validation

Initially, the results are compared with a previous analytical solution in the literature and with numerical simulations due to the non-availability of real data. Subsequently, the model is applied to real riverbank filtration sites in Malaysia. Therefore, validation of the proposed model relies on analytical solutions from previous years. Since these former solutions did not consider at least the river width, clogging, or three-dimensional flow parameters, our model must be adjusted to align with the assumptions of these earlier models to ensure a proper comparison. Three literature studies have been selected: Sangani, et al. [24], Singh and Chatterjee [23] and Chen, et al. [35].

Additionally, based on our knowledge, there is no analytical model in the literature accounting for the impact of river width and partial interaction between riverbed and aquifer on contaminant transport in three-dimensional water flow. Consequently, a numerical simulation is undertaken to validate the model.

3.1.1. Comparing with previous analytical models

The outcomes of the developed analytical model are first compared with the approximate closed-form analytical solutions presented by Sangani, et al. [24] using Dirichlet boundary conditions. The following two expressions are provided in their results for groundwater contaminants transport analytical solution released from area pulse sources in infinite depth aquifer [24]:

$$C(x,y,z,t) = \frac{C_0}{8}[\phi_x(x,t) - \phi_x(x,t-t_s)]f_y(y,\tau)f_z(z,\tau) \tag{20}$$

where

$$f_y(y,\tau) = \mathrm{erf}\left[(y+y_0)/\left(2\sqrt{D_y\tau}\right)\right] - \mathrm{erf}\left[(y-y_0))/\left(2\sqrt{D_y\tau}\right)\right]$$
$$f_z(z,\tau) = \mathrm{erf}\left[(z-z_1)/\left(2\sqrt{D_z\tau}\right)\right] - \mathrm{erf}[(z-z_0))/\left(2\sqrt{D_z\tau}\right)] \tag{21}$$

where t_s is the time duration of the input from the pulse source, k and ν are the plume and source decay rates coefficient. Since the aquifer was assumed with infinite depth in their model, the comparison is conducted with Equation (19). Additionally, the source dimension is assumed the same as considered by Sangani, et al. [24] where $y \in [-y_0, y_0]$, and $z \in [-z_0, z_0]$ and $x = 0$. Table 1 summarizes the differences between the assumptions of the two models and how the equation is adjusted in these models.

Table 1
The differences between the assumptions of the proposed model and Sangani, et al. [24] model.

Sangani, et al. [24] solution Equation (20)	The proposed solution Equation (19)	The new terms of equation
The groundwater flow is unidirectional through x-axis	Three- dimensional groundwater flow	Equation (19) includes the terms U_y and U_z for water velocity in y and z directions.
The dispersion is expressed in terms of both k and ν plume and source decay rates coefficient.	It is assumed k and ν are equal. However the retardation factor is involved.	In Equation (22), If $k = \nu$and if it is assumed $R = 1$, then Equation (19) expression is recovered.
The transverse dispersion terms $f_y(y,\tau)$ and $f_z(z,\tau)$ are written in terms of error functions	The transverse dispersion terms $f_y(y,\tau)$ and $f_z(z,\tau)$ are written in terms of complementary error functions	If the following relation is implemented $\mathrm{erfc}(t) = 1 - \mathrm{erf}(t)$. Then two expression are similar.
The plane source dimensions are $y \in [-y_0, y_0]$, $z \in [z_0, z_1]$ and $x = 0$.	The source dimension is $y \in [-y_0, y_0]$, $z \in [z_0, z_1]$ and $x \in [0, x_0]$.	In Equation (19), the solution takes into account the river's width along the x-axis. Thus the Green's functions is integrated from 0 to x_0 in Equation (12). If the river is line source then the Green's function over x-axis remains in exponential form leading to a similarity between the two solutions."
The source boundary is assumed to be a pulse, with the boundary condition being enforced only for a limited duration.	The river is considered as a continuous source of contaminant.	To handle the continuous source, the solution of Equation (19) is integrated over time.

In summary, both solutions become identical if the following assumptions are made in Equation (19): no groundwater flow along the y and z directions, equal decay rates for the plume and source, a river characterized as a pulse and line source, implying that $U_y = U_z = 0$, $k = \nu$, R = 1, $\mathrm{erfc}(t) = 1 - \mathrm{erf}(t)$ and no integration is necessary over the x-domain and time.

The Proposed model in Equation (18) is also compared with the solution obtained by Singh and Chatterjee [23] who modeled the 3D transport of solutes from planned sources in a semi-infinite aquifer. The same values for dispersion and velocity parameters used by Singh and Chatterjee [23] are employed, with groundwater velocities$U_x = 0.33$ m/d, $U_y = 0.27$ m/d, and$U_z = 0.027$ m/d, and with parameters of dispersion $D_x = 6.5$ m^2/d, $D_y = 5.48$ m^2/d, and$D_z = 10.4$ m^2/d. The aquifer parameters values assumed in the comparison are $R = 1$, $\phi = 0.2$, D_x=0.2, $D_y = 0.1$, $D_z = 0.01$, $C_0 = 0.2$, $d = 1$, $U_x = 1$, and $\lambda = 0.12$. However, the primary limitation of the solution derived by Singh and Chatterjee [29] is that the shape of the source influences the pollutant flow, resulting in a unidirectional flow when the plane is $x = 0$, effectively reducing their solution to one-dimensional in this scenario. To maintain a three-dimensional perspective, our solution accommodates this challenge by assuming a slight inclination of the plane source with the x-axis, rather than a perpendicular arrangement. Another concern with the solution proposed by Singh and Chatterjee [23] is that the water velocities they assumed are low, implying that the pumping rate must also be considered very small during the comparison. Both models continue to display similar profile shapes and behavior, and over time, the two answers merge into one. As noticed in Fig. 2, both solutions exhibit similar profile shapes and behavior, and over time, the two solutions become identical. During the initial 30 days, there appears to be no contamination in the produced water, suggesting that the river water has not yet reached the well, most likely due to the assumed small pumping rate. This observation provides insight into the validity of the proposed model. Another finding is that after 450 days, the concentration does not surpass 0.6 mg/l. While this value may pose a risk for certain contaminants, such as nitrate that should not exceed 0.5 mg/l, it remains manageable, and the treatment cost is lower than treating water from the river directly. Overall, employing minimal pumping allows for an extended utilization of the well. This obviously supports the validation of the model.

The current model is also compared with another analytical solution developed by Chen, et al. [35] specifically for one dimensional flow (Fig. 3). Since Chen, et al. [35] produced one dimensional solution models, the parameters U_z and U_y were set equal to zero in our 3D model. In fact, Chen, et al. [35] produced a collection of analytical techniques for pollutant released from various sources. However, we compared only with the solution for horizontally rectangular source. x_0, y_0, z_0 and z_1 have the values 1, 0.5, 4.75 and 5.25 m, respectively. The

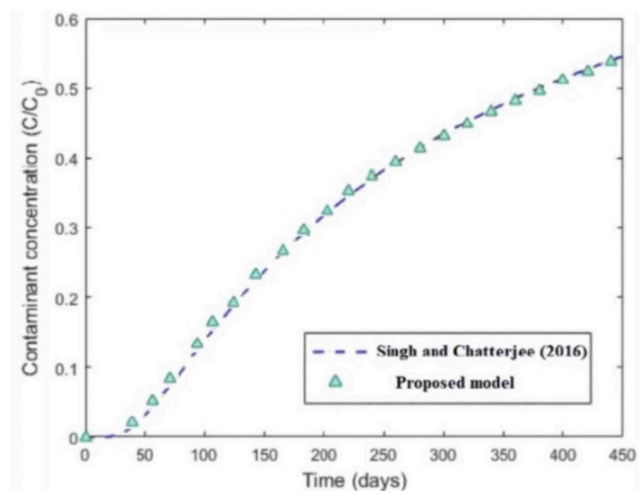

Fig. 2. The concentration profiles of the proposed solution using Green's function Singh and Singh and Chatterjee [23] solution.

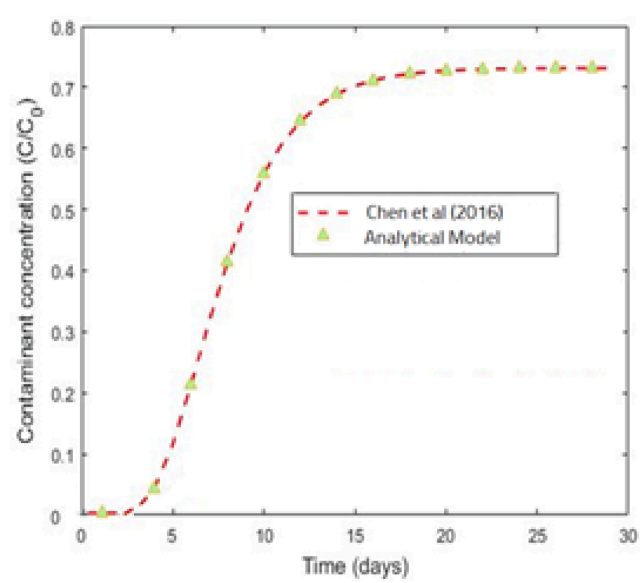

Fig. 3. Solute concentration values for the proposed model and Chen et al. (2016) solutions.

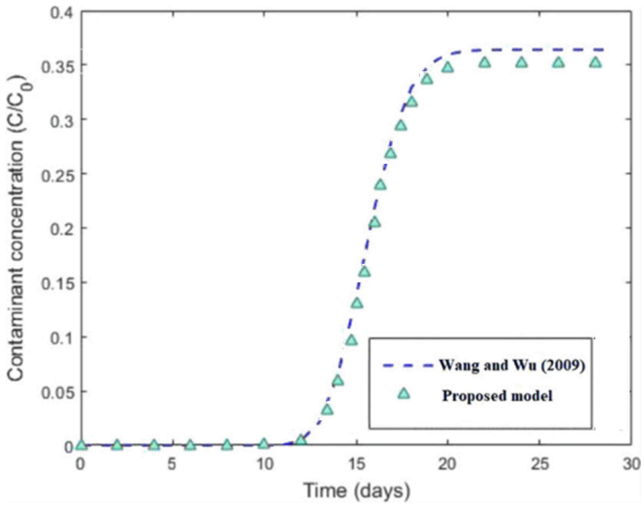

Fig. 4. A comparison between the proposed solution and Wang and Wu (2009) solution.

profile of concentration for $x = 10$ m, $z = 5$ m and $y = 0$ are presented in Fig. 3. Our solutions completely match with those provided by Chen, et al. [35]. The water inside the well starts to be contaminated after 3 days of pumping and the level of contamination continues to rise until it reaches more than 0.7 mg/l after 15 days only. This level is considered dangerous for human health due to the rise of different pollutants, such as nitrates.

Wang and Wu [34] put forward collection of analytical solutions that addressed volumetric and rectangular source types. These solutions only include a single solution that takes into account both vertical and horizontal velocities (U_x and U_z) and this particular solution focuses on a rectangular source situated horizontally in the *x-y* plane. At the beginning, Wang and Wu (2009) made an assumption in their solution; there is no water movement in the direction of y. Consequently, in our solution, we also assume that $U_y = 0$. The disparities between these two solutions are illustrated in Fig. 4. It is clear that the two profiles closely align and exhibit the same behaviour. During first 10 days, the concentration is observed to be zero, probably because the contaminant has not yet reached the area that is being examined and it is presumed that no additional sources of contamination are there. After 20 days, Fig. 4 shows a small difference between the two solutions, which can be attributed to an error function incorporated in Wang and Wu's (2009) solution, resulting in approximate values compared to the precise values obtained from an exponential function. Nonetheless, this discrepancy is negligible, and both solutions demonstrate similar performance.

In Figs. 2 and 4, contaminations appear in the well after 15 to 25 days, whereas it is noticeable after only 4 days in Fig. 3 when the values of U_z and U_y were set equal to zero. This means assuming the unidirectional groundwater flow reduces the travelling time of pollutants from river to the well. Consequently, the well's age will be shorter. Additionally, it is observed that assuming three-dimensional flow of groundwater in Fig. 2 results in a longer travel time for solutes toward the well compared to the two-dimensional flow depicted in Fig. 4. Thus, we can conclude that assuming three-dimensional water flow in the model indicates that the well can be used for a longer duration.

3.1.2. Comparing with MODFLOW simulation

Within this section, a comparison is conducted between our proposed solution and MODFLOW model that is based on numerical solution. This comparison is carried out because, to the best of our understanding, there is currently no available analytical solution that addresses the influence of river width, well location, and clogging on contaminant transport within a three-dimensional groundwater flow field. The MODFLOW software employs a Finite Difference approach as its underlying methodology. The combination of MODFLOW with the MT3D (3D contaminant transport model simulator) allows for the simulation of contaminant concentration changes, accounting for advection, dispersion, and certain chemical reactions. The model grid has a size of 500 m by 500 m with 10 m as the standard grid spacing between each row and column. To ensure adherence to the assumptions of infinite aquifer, the model dimension is selected to be large enough to stop the boundaries from being influenced by the pumping well. This can be achieved by either shifting the boundary further away from the extraction point or utilizing the boundary of head to be general in MODFLOW [30]. The streambed is considered to be 10 m long and 1 m thick for each cell, with a hydraulic conductivity value of 0.5 m/d. The additional input parameters required for the numerical simulation in MODFLOW are $\lambda = 0.5$, $\phi = 0.3$, $U_x = 10$ m/d, $U_y = 1$ m/d, $U_z = 1$ m/d, $C_0 = 16$ mg/l, $d = 20$ m, $S_x = 0.00034$, $T = 1000$ m^2/d, $Q = 3072$ m^3/d, $L = 40$ m.

Fig. 5 illustrates the concentration distributions obtained from

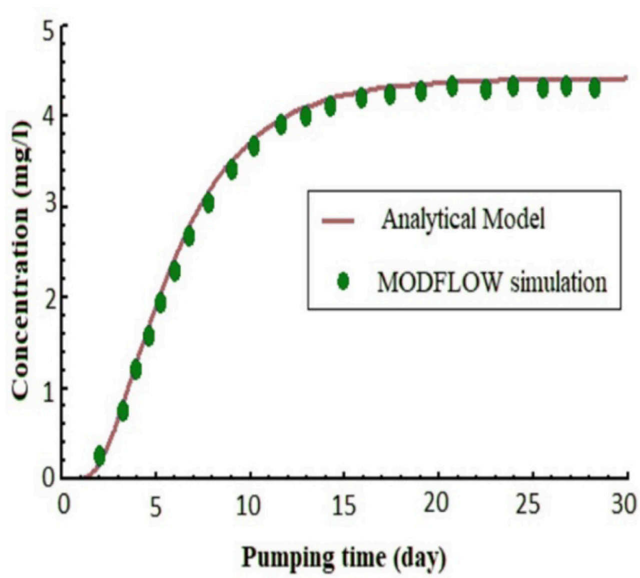

Fig. 5. MODFLOW and analytical models for pollutant concentration over 30 pumping days.

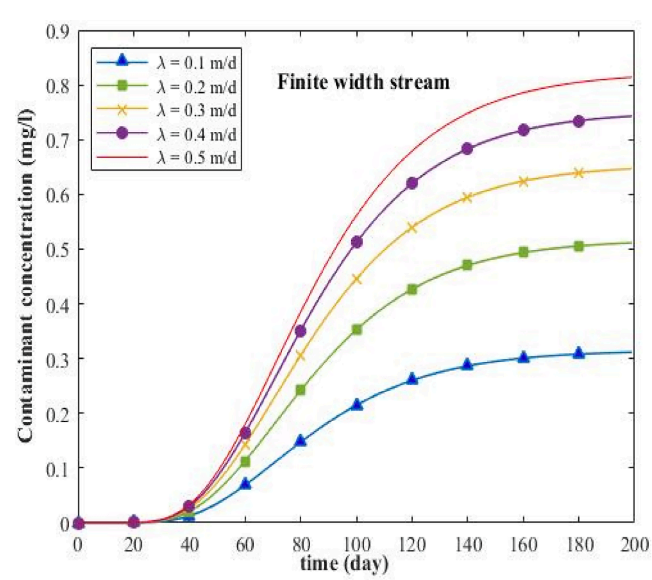

Fig. 6. Contaminants Profile with different leakance coefficients.

simulations conducted over a 30-day pumping period. The well's water was initially considered to be uncontaminated. Both models displayed similar profiles with an overall agreement of 98–99%. Within the first 10 days, there was a significant rise in concentration, with values can be reach up to 4 mg/l as the pumping duration increased. Subsequently, the increase in concentration became less pronounced, indicating a reduced influx of river water into the well after the initial 10 days.

3.2. Analyzing the effect of clogging on contaminant transport

Another factor that controls the contaminant transport process in riverbank filtration systems is the leakage coefficient of the streambed. In real-life scenarios, the presence of clogging in riverbed sediments can impact the movement of contaminants from the river to the well. For small clogging values, more water can penetrate the aquifer, allowing more contaminants to enter with the water movement toward the well. Fig. 6 examines how the clogging parameter affects the concentration of contaminants in the produced water. The leakance coefficient, denoted as λ, was varied across values of 0.1, 0.2, 0.3, 0.4, and 0.5 m/d. In the simulation, we assumed that the aquifer was initially uncontaminated, and we set the value of D_y/D_x to 0.1. The other parameters values are $\lambda = 0.5$, $\phi = 0.3$, $U_x = 10$ m/d, $U_y = 1$ m/d, $U_z = 1$ m/d, $C_0 = 16$ mg/l, $d = 20$ m, $S_x = 0.00034$, $T = 1000$ m^2/d, $Q = 3072$ m^3/d, $L = 40$ m.

A higher leakance coefficient indicates lower levels of clogging in the area. The highest levels of contamination were observed at a leakance coefficient of 0.5 m/d, where contaminant concentrations exceeded 0.7 mg/l. Overall, there is a significant and rapid increase in contaminant concentration after the first 40 days. The rapid increase in contaminations is noticed in the period between 50 to 100 days. After this, the concentration of pollutants still increases at a slower rate. However, the water is considered unsafe after 80 days for areas with less clogging, while the well can produce quality water for 200 days in cases of more clogging.

3.3. Analyzing the effect of river width on contaminant transport

Fig. 7 presents a comparison of the concentration profiles for contaminants released from a stream with a fixed width and a line stream. Initially, the water at the well was uncontaminated, and the concentration began to rise after 5 days for the finite width stream and 10 days for the line stream. After 20 days, the concentration increased by 0.1 when considering the width of the stream in the model, whereas for the line stream, this value was only 0.02. Overall, it is noticeable that the finite width stream leads to a higher level of contamination in the produced water compared to the line width stream. It is more realistic to consider the impact of river width in the model because it will assist decision-makers in taking the correct actions regarding the safety of produced water for human health. For example, the line stream model indicated that the contamination level remains acceptable after 50 days, not exceeding 0.03 mg/l. However, assuming the finite width stream model showed that contamination levels rapidly increased to unsafe levels within just 10 days.

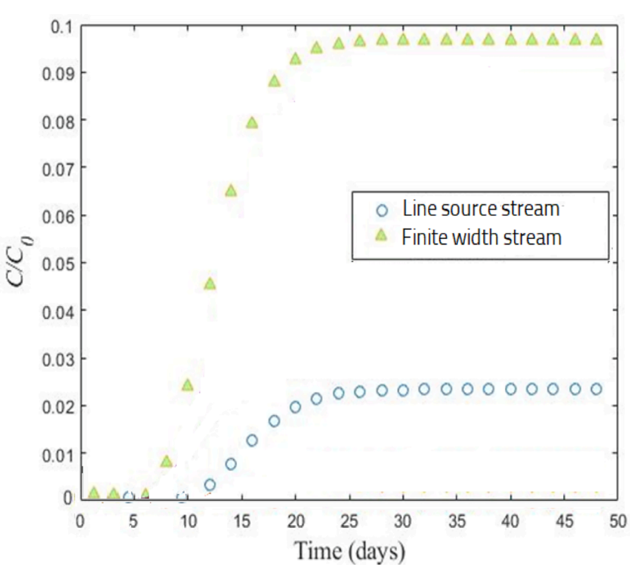

Fig. 7. Contaminants profile for finite width stream sand line stream.

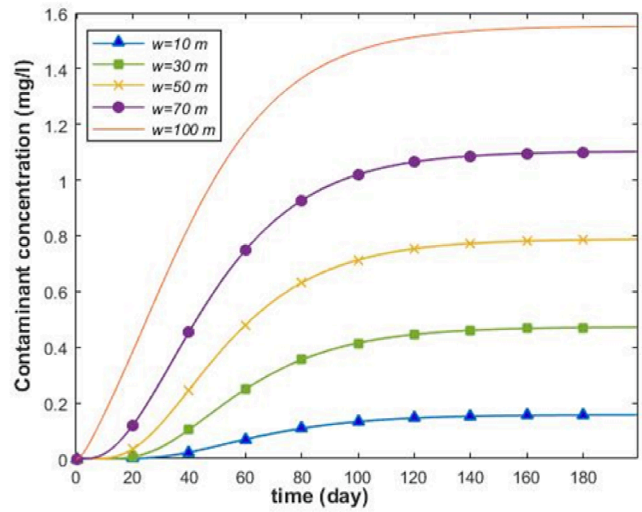

Fig. 8. Contaminants Profile with different width stream values.

The importance of stream width on the concentration level in the pumped water, as observed in Fig. 7, is highlighted by considering different values of widths. Initially, a small river with a width of only 10 m was considered. Subsequently, the width was increased to 30 m, 50 m, 70 m, and finally 100 m. The concentration profiles for each width value are illustrated in Fig. 8. In the case of the small width, contamination was observed after 20 days. However, for larger widths, contamination was detected in the produced water from the initial days. Moreover, for a small width of the stream, such as 10 m, the concentration of contaminants does not exceed 0.2 mg/l even after 180 days. On the other hand, more treatment processes should be conducted for water produced from wells near wide streams like 100 m, where it reaches unacceptable contamination levels only in the first few days. This finding verifies the significance of the river width factor in determining the efficiency of the system.

3.4. Analyzing the ratio between stream width and well location

Before establishing new riverbank filtration sites, determining the suitable distance to drill the well to get high quality water for long time period is required. To investigate the impact of well position with respect to the river on contaminant transport model, two different locations were examined within the two models: line stream model and finite width river model. The first location was near the stream border and at a distance of 40 m that is smaller than the width of stream (W = 50), while the second site was situated 100 m from the stream, and this value is twice the breadth of the stream. The outputs depicted in Fig. 9 demonstrate the considerable influence of a streams with finite widths on the contamination levels. At a distance of 40 m and within 20 days, the concentrations in mg/l were approximately equal to 1.5 for the line river, while the contamination was higher than 4.5 mg/l in case of river that has finite width. This rapid growth of contamination can be due to the well's close proximity to the stream. Conversely, at a distance of 100 m, the positioning of the pumping well distance from the river resulted in pollution levels that were fewer than 0.5 mg/l for both models.

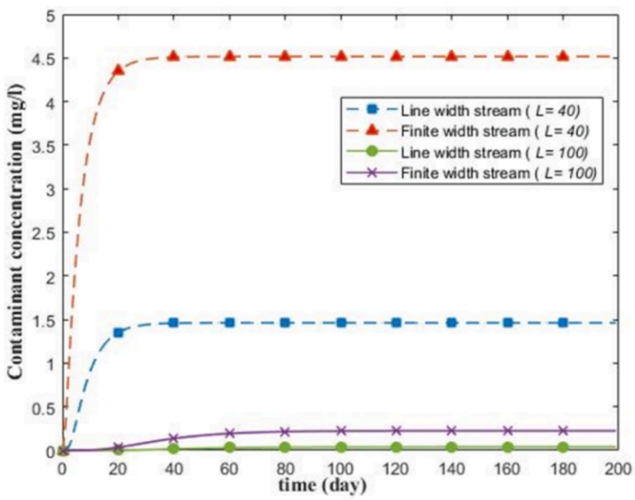

Fig. 9. Line and finite stream width profiles for pollutant concentrations.

Furthermore, the difference in concentration values by using the two stream types was not significant, showing that the impact of stream width can be disregarded.

Hence, at longer distances, the solution of both stream types yield acceptable concentration estimates since they yield relatively small concentration values. Specifically, to neglect the impact of the width of the stream on pollution, the distance from well to the edge of river should be at least twice the stream width.

3.5. Applying the model in real RBF site in Malaysia

This model can be used by decision makers to manage RBF sites. To investigate the impact of the river width and Leakance coefficient parameters on the transport of solutes, we applied our model to the dataset related to Langat River area in Malaysia to nearby wells. The study area consisted of an aquifer with a 20-meter thickness that is very permeable and uniform. Two vertical extraction wells placed 40 m and 18 m apart from the stream, respectively. The aquifer is confined and consists of sand and gravel. Notably, these wells were not influenced by one another because they were spread out along the river in different locations. In the simulation, we assumed that the aquifer was initially uncontaminated, and we set the value of D_y/D_x to 0.1. The other parameters values are $\lambda = 0.5$, $\phi = 0.3$, $U_x = 10$ m/d, $U_y = 1$ m/d, $U_z = 1$ m/d, $C_0 = 16$ mg/l, $d = 20$ m, $S_x = 0.00034$, $T = 1000$ m^2/d, $Q = 3072$ m^3/d, and $L = 40$ m.

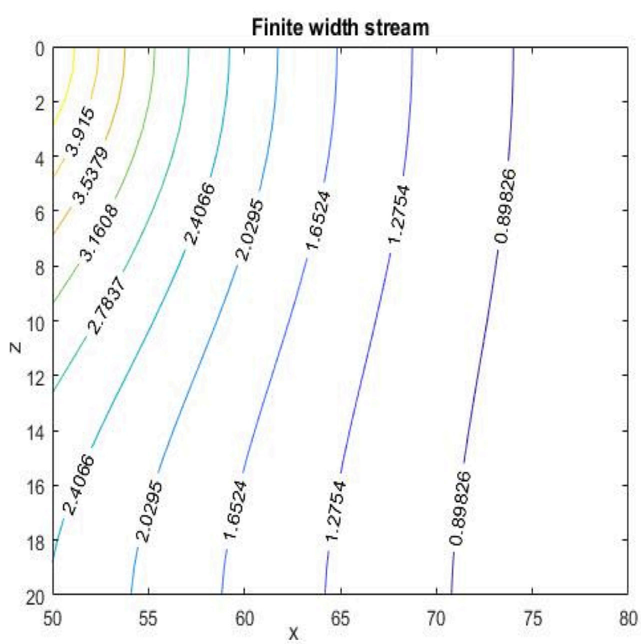

Fig. 10. Contaminants contour lines in *xz* plane.

The acquired results are presented as contour lines illustrating the distribution of pollutants concentration on *xz* surface (Fig. 10). The area closest to the stream exhibited the highest concentration, measuring approximately 3.9 mg/l. However, as the pollutants approached the well, their concentration decreased to 0.89 mg/l. This reduction can be attributed to the activities of bacteria present in the sediments of the riverbed. Additionally, the concentrations are reduced along the depth of aquifer especially near the river area where a zone of active bacteria is present. However, the contamination still reaches the well which means that the water produced from the well is unsafe. Based on these results, action should be taken from the government either by reducing the pumping rate or implementing additional treatment processes before supplying water to the public. This example can show how the model can be applied to manage the RBF site to ensure supplying a high-quality drinking water.

4. Conclusion

A Green's function-based analytical model is produced in order to simulate the potential impact of extracting water next to river on the three-dimensional movement of contaminants from river to nearby wells, specifically in cases where streambeds are clogged. The model investigates the effect of river width and clogging on pollutants movement process through aquifer. The results are compared with four different analytical solutions from existing literature, each based on different assumptions. The comparison showed well agreement between our results and the findings of previous analytical models. Additionally, we compared our model with a numerical simulation that incorporates all these factors. The numerical solution is conducted using MODFLOW software. The high matching between the analytical and numerical results have affirmed the effectiveness of proposed model in simulating the movement of contaminants within a 3D domain. The results of this study highlight the following main conclusion remarks:

1. The models designed for the flow of groundwater along the x-axis alone suggest that wells will become contaminated more rapidly compared to models that account for three-dimensional groundwater flow.
2. The amount of river water and the concentration of pollutants inside the well are both decreased by the presence of a clogging layer.
3. Finite-width solutions provide a more accurate estimation of solute distribution from line stream solutions when the pumping well is situated close to the stream. The models that ignored the effect of river width show less contamination in the well area from the finite width stream models. Moreover, larger width of streams makes a significant increase in pollution around the well.
4. For greater distances between the river and pumping well, both models yield low concentration values. This means that the effect of river width can be neglected if the distance between well and river is more than twice the river width.
5. Applying the proposed model to real riverbank filtration site in Malaysia demonstrates that this model has the potential for further development in managing groundwater extraction from pumping wells, particularly in urban areas characterized by high levels of contamination.

In summary, our model offers more precise predictions than other analytical models by examining the influences of river width, clogging, and well location. Disregarding any of these parameters can result in obtaining inaccurate information about contamination levels, potentially impacting human health. The proposed model is valuable in detecting contamination in confined and unconfined aquifers that are partially intersected by a stream.

CRediT authorship contribution statement

Shaymaa Mustafa: Conceptualization, Formal analysis, Methodology, Supervision. **Fahid K.J. Rabah:** . **Mohamad Darwish:** Visualization, Writing – review & editing. **Arifah Bahar:** Investigation, Resources. **Zainal Abdul Aziz:** Supervision.

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.

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Appendix A

In this Appendix, we'll demonstrate the mathematical equations detailing the conversion of Equation (2) to Equation (7). The following is Equation (2)

$$R\frac{\partial C}{\partial t}-D_x\frac{\partial^2 C}{\partial x^2}-D_y\frac{\partial^2 C}{\partial y^2}-D_z\frac{\partial^2 C}{\partial z^2}+U_x\frac{\partial C}{\partial x}+U_y\frac{\partial C}{\partial y}+U_z\frac{\partial C}{\partial z}+\nu RC=C_0(t)-C_w(t)$$

By using the following transformation:

$$x^*=x-\frac{U_x t}{R};\quad y^*=y-\frac{U_y t}{R},\quad z^*=z-\frac{U_z t}{R},\quad C_s(t)=C_0(t)-C_w(t)$$

$$\overline{C}_w(t)=C_w(t)e^{\nu t},\quad \overline{C}_0(t)=C_0(t)e^{\nu t}\overline{C}_s(t)=[\overline{C}_0(t)-\overline{C}_w(t)],\quad \overline{C}(x,y,t)=C(x,y,t)e^{\nu t};$$

Also these dimensionless:

$$t_D=D_z t\Big/\left(Rd^2\right);\qquad C_D=D_z\overline{C}\Big/\left(RS_0d^2\right);\qquad C_{s_D}(t)=\overline{C}_s(t)/(S_0R);$$

$$y_D^*=\frac{y^*\left(\sqrt{D_z/D_y}\right)}{d};\qquad z_D^*=\frac{z^*}{d};\qquad x_D^*=\frac{x^*\left(\sqrt{D_z/D_x}\right)}{d};$$

$$U_{x_D}=U_xd\Big/\sqrt{D_zD_x};\qquad U_{z_D}=U_zd\Big/D_z;\qquad U_{y_D}=U_yd\Big/\sqrt{D_zD_y}$$

We got:

$$\begin{aligned}\frac{\partial C_D}{\partial t_D}&=\frac{\partial C_D}{\partial t}\frac{\partial t}{\partial t_D}=\frac{Rd^2}{D_z}\frac{\partial C_D}{\partial t}=\frac{1}{S_0}\frac{\partial\overline{C}}{\partial t}\\&=\frac{1}{S_0}\frac{\partial}{\partial t}(C(x,y,t)e^{\nu t})\\&=\frac{1}{S_0}\left[\nu e^{\nu t}C(x,y,t)+e^{\nu t}\left(\frac{\partial C}{\partial t}+\frac{\partial C}{\partial x}\frac{\partial x}{\partial t}+\frac{\partial C}{\partial y}\frac{\partial y}{\partial t}+\frac{\partial C}{\partial z}\frac{\partial z}{\partial t}\right)\right]\\&=\frac{1}{S_0}e^{\nu t}\left[\nu C(x,y,t)+\left(\frac{\partial C}{\partial t}+\frac{U_x}{R}\frac{\partial C}{\partial x}+\frac{U_y}{R}\frac{\partial C}{\partial y}+\frac{U_z}{R}\frac{\partial C}{\partial z}\right)\right]\end{aligned}\tag{A1}$$

Also,

$$\begin{aligned}\frac{\partial C_D}{\partial x_D^*}&=\frac{\partial C_D}{\partial x}\frac{\partial x}{\partial x^*}\frac{\partial x^*}{\partial x_D^*}=\frac{d}{\sqrt{D_z/D_x}}\frac{\partial C_D}{\partial x}\\&=\frac{d}{\sqrt{D_z/D_x}}\left[\frac{D_z}{RS_0d^2}e^{\nu t}\frac{\partial C}{\partial x}\right]\end{aligned}\tag{A2}$$

$$\begin{aligned}\frac{\partial^2 C_D}{\partial x_D^{*2}}&=\frac{\partial}{\partial x_D^*}\left[\frac{\partial C_D}{\partial x_D^*}\right]=\frac{\partial}{\partial x}\frac{\partial x}{\partial x^*}\frac{\partial x^*}{\partial x_D^*}\left[\frac{\partial C_D}{\partial x_D^*}\right]\\&=\frac{D_x}{S_0}\frac{1}{R}e^{\nu t}\frac{\partial^2 C}{\partial x^2}\end{aligned}\tag{A3}$$

By similar way

$$\frac{\partial^2 C_D}{\partial y_D^2}=\frac{D_y}{RS_0}e^{\nu t}\frac{\partial^2 C}{\partial y^2}\tag{A4}$$

And

$$\frac{\partial^2 C_D}{\partial z_D^2}=\frac{D_z}{RS_0}e^{\nu t}\frac{\partial^2 C}{\partial z^2}\tag{A5}$$

Additionally.

$$C_{S_D}(t_D) = \frac{1}{S_0R}\overline{C}_s(t_D) = \frac{1}{S_0R}e^{\nu t}C_s(t_D) \tag{A6}$$

Multiplying Equation (2) by $\frac{1}{S_0R}e^{\nu t}$

$$\frac{1}{S_0R}e^{\nu t}\left[R\frac{\partial C}{\partial t} - D_x\frac{\partial^2 C}{\partial x^2} - D_y\frac{\partial^2 C}{\partial y^2} + U_x\frac{\partial C}{\partial x} + U_y\frac{\partial C}{\partial y} + U_z\frac{\partial C}{\partial z} + \beta C\right] = \frac{1}{S_0R}e^{\nu t}C_s(t) \tag{A7}$$

By comparing Equations (A.1)−(A.6) with Equation (A.7) we get

$$\frac{\partial C_D}{\partial t_D} - \frac{\partial^2 C_D}{\partial {x_D^*}^2} - \frac{\partial^2 C_D}{\partial {y_D^*}^2} - \frac{\partial^2 C_D}{\partial {z_D^*}^2} = C_{s_D}(t_D)$$

And

$$C_D(\pm\infty, y_D^*, z_D^*, t_D) = 0 - \infty \le y_D^* \le \infty,\ -U_{z_D}t_D \le z_D^* \le 1 - U_{z_D}t_D \quad \text{and}\ t_D \ge 0$$

$$C_D(x_D^*, \pm\infty, z_D^*, t_D) = 0 - \infty \le x_D^* \le \infty,\ -U_{z_D}t_D \le z_D^* \le 1 - U_{z_D}t_D \quad \text{and}\ t_D \ge 0$$

$$\frac{\partial C_D(x_D^*, y_D^*, -U_{z_D}t_D, t_D)}{\partial z_d} = \frac{\partial C_D(x_D^*, y_D^*, 1 - U_{z_D}t_D, t_D)}{\partial z_d} = 0 \quad -\infty \le y_D^* \le \infty,\ -\infty \le x_D^* \le \infty, \qquad \text{and}\ t_D \ge 0$$

$$C_D(x_D^*, y_D^*, z_D^*, 0) = 0 - \infty < x_D^* < \infty,\ -\infty \le y_D^* \le \infty,\ -U_{z_D}t_D \le z_D^* \le 1 - U_{z_D}t_D$$

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