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Heat conduction applied in 'River Pollutant Diffusion'

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Abstract:

Environment problems are a highly valued topic in today's society, where water pollution issue is one of the most significant that could threaten human's safety. Sources such as industrial wastewater and agricultural runoff are affecting the water quality. Rivers around the world suffer from varying degrees of pollution. In this paper, we investigate river heat pollution and employ a numerical model to investigate its evolution and impacts downstream by adapting the heat advection-diffusion equation. We explore the stability of our numerical solutions using von Neumann stability analysis of the forward and backward differencing method of discretization of the analytical equations. We further consider a setting where there are multiple sources of pollutant in the river to explore interaction of the two pollution sources. We use python to develop the model and plot temperature diffusion in the river as a function of time and location. Our model reflects the relationship between the speed of diffusion and thermal diffusivity, and how advection enhances pollutant. Our results show that heat pollution is very quickly transported to other locations and can affect water and food quality in many locations along the river. Additionally, pollution in rivers with fast currents will be more readily transported downstream, therefore both proximity to cities and speed of river water needs to be taken into account when addressing the problem of heat pollution in rivers near cities.

1.Introduction:

1a. Motivation:

The heat equation is a classic mathematical model that aims to address real-life problems by integrating with numerical models. This theory can be applied to several scientific fields. With the development of modern chemical industrialization, environmental problems such as pollutant diffusion require immediate attention. The heat equation can establish relationship between water temperature, air temperature, and stream discharge or flow velocity (Benyahya et al., 2007; Piotrowski et al., 2015; Sahoo et al., 2009). We hope to use the heat equation to solve the problem of 'River Pollutant Diffusion'. The spread of pollutants in water or air can be formulated as a heat conduction problem, particularly when considering concentration gradients and diffusion coefficients. Modeling diffusion adapting heat equations have also been studied in engineering where Myers, Fowkes and Ballim(2009) use heat equation to model the cooling of concrete by piped water. We want to study the river pollutant diffusion because it can help the release the environment problem, which is the most concerned topic. This project may help provide solutions to this issue.

1b. Limitation of current methods:

Let x denote the location and t denote the time. The analytical solution of heat equation can only address the temperature T (x, t) in the rod is determined from the boundary-value problem.

$$\partial T/\partial t = \alpha \nabla^2 T, 0 < x < L, t > 0$$
$$T(0,t) = 0, T(L,t) = 0, t > 0$$
$$T(x,0) = f(x), 0 < x < L$$

In real life, it is hard to apply the analytical method because the observed phenomena have more complicated conditions compared to a basic model. Moreover, the pollutant diffusion equation has an extra term of derivative, which amplifies the difficulty of analytical solution and requires a numerical approach that is faster and more practical.

1c. Extension of the heat diffusion problem:

To solve the problem of pollutant diffusion, using the heat equation is an effective method because it can describe similar diffusion processes. The form of the heat equation is

$$\frac{\partial T}{\partial t} = a \frac{\partial^2 T}{\partial x^2}$$

where a is thermal diffusivity (m^2/s). And the pollutant diffusion equation can be expressed as

$$\frac{\partial T}{\partial t} = a \frac{\partial^2 T}{\partial x^2} - v \frac{\partial T}{\partial x}$$

Where we have an additional parameter v which is the velocity. We will use the Forward differencing and Von Neuman stability analysis to solve the function and build numerical models in python.

1d. Outline of paper:

In section 2, we explain the different methods of applying finite difference schemes to the advection-diffusion equation and we apply von Neumann stability analysis. In section 3, we plot figures to indicate the result of diffusion downstream, and demonstrate the effect of advection as well as adding one more source of pollutant, explaining how advection enhances pollutant. In the last section of the paper, we will discuss the sensitivity of diffusion with the various sources and advection and conclude.

2. Methodology

2a. Finite difference scheme for the advection-diffusion problem

We have three types of derivatives that need to be discretized and studied for stability separately. First, the time derivative will be simulated using the forward differencing scheme to convert differential equations into algebraic equations. Von Neumann stability analysis can provide specific conditions for the stability for numerical methods and it helps ensure that the numerical solution remains stable over time by providing conditions that the discretization parameters must satisfy.

The first derivative in space (dT/dx) can be expressed in another form using the Taylor series expansion. The expansion around a point xxx is given by:

$$\varphi(x_i + \Delta x) = \varphi(x_i) + \Delta x \frac{\partial \varphi}{\partial x}\Big|_{x_i} + \frac{\Delta x^2}{2}\frac{\partial^2 \varphi}{\partial x^2}\Big|_{x_i} + \frac{\Delta x^3}{3}\frac{\partial^3 \varphi}{\partial x^3}\Big|_{x_i} + \cdots$$

Since each successive term in the series becomes smaller as the order of the derivative increases, we can simplify the calculation by neglecting higher-order terms and retaining only the first two terms. Thus, the approximation for the first derivative is:

$$\varphi(x_i + \Delta x) = \varphi(x_i) + \Delta x \frac{\partial \varphi}{\partial x}\Big|_{x_i}$$

This method is known as forward differencing because we use the value at the iiith point to estimate the derivative at the (i+1)(i+1)(i+1)th point.

The second derivative in space can be derived from the first derivative using a similar approach. By applying the forward differencing method twice, we get:

$$\frac{\partial}{\partial x}\left(\frac{\partial T}{\partial x}\right) = \left(\frac{T_{i+1}^n - T_i^n}{\Delta x} - \frac{T_i^n - T_{i-1}^n}{\Delta x}\right)\frac{1}{\Delta x} = \frac{T_{i+1}^n - 2T_i^n + T_{i-1}^n}{\Delta x^2}$$

This formula provides an approximation for the second derivative based on the values of the function at three consecutive points

Our numerical model for River Pollutant Diffusion is robust to various conditions and do not require extensive calculations. This can help human predict the pollution in water and its diffusion at each period, assisting solving the environment problem. Moreover, we can use heat equation to calculate problems such as Electrical Conduction, Drug Diffusion, Information Diffusion, Sound Wave Propagation by adapting our method.

Methods

To solve the river pollutant diffusion problem, we mainly use three methods including heat equation, forward differencing and Von Neumann stability analysis. The one-dimensional heat equation is

$$\frac{\partial T}{\partial t} = a\frac{\partial^2 T}{\partial x^2}$$

$0 \le x \le L, t \ge 0$. Where T (x, t) is the dependent variable, the horizontal domain is the length L. Equation is a model of transient heat conduction in slab of material with thickness L. The solution to equation requires specification of boundary conditions at x=0 and x=L, and initial conditions at t=0. Simple boundary and initial conditions are $T(0,t) = T_0,\ T(L,t) = T_L,\ T(x,0) = f_0(x)$.

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We are going to use numerical methods to address the problem.

First of all, we do not consider the velocity condition. Approximately, we can express the river pollutant diffusion equation to ∂T/∂t =α*∇^2T. Let $r =\alpha\frac{\Delta t}{(\Delta x)^2}$. The forward differencing approximates the first order derivative as

$$\partial T/\partial t = (T_i^{n+1}\text{-}T_i^n)/\Delta t \text{ and } \partial T/\partial x = (T_{i+1}^n\text{-}T_i^n)/\Delta x$$

Similarly, we express ∂T/∂t=α*∇^2T as

$$T_i^{n+1}=r(T_{i+1}^n\text{-}2T_i^n+T_{i-1}^n) + T_i^n$$

For the condition with velocity, we use backward differencing

$$\partial T/\partial x = (T_i^n - T_{i-1}^n)/\Delta x$$

to express $v*\partial T/\partial x$ as $v\ (T_i^n - T_i^{n+1})/\Delta t$, let $s = v\frac{\Delta t}{\Delta x}$.

$$\frac{\partial T}{\partial t} = a\frac{\partial^2 T}{\partial x^2} - v\frac{\partial T}{\partial x}$$

can be expressed as

$$T_i^{n+1}=r(T_{i+1}^n\text{-}2T_i^n+T_{i-1}^n)+s(T_i^n - T_{i-1}^n)+ T_i^n$$

Because of approximation, Numerical methods always have the error term.
Von Neumann stability analysis can provide specific conditions for the stability for numerical methods and it helps ensure that the numerical solution remains stable over time by providing conditions that the discretization parameters must satisfy. This process is essential for the reliable and accurate numerical simulation of partial differential equations (PDE)'s.
The error also follows the same numerical formulas derived above.

Table 1

parameter	description	Value
α	thermal diffusivity (km^2/day)	0.02/0.2
v	Velocity of the river (km/day)	0.01/0.02
L	Length (km)	10/100/200
T	Temperature ($°C$)	
Δt	Grid point of time	1
Δx	Grid point of location	1

<u>2b. von Neumann stability analysis</u>

1. For the basic assumption, without considering the velocity.

we substitute in the error equation (1), we get

Technium Sustainability
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www.techniumscience.com

$$\varepsilon_i^{n+1} = r(\varepsilon_{i+1}^n - 2\varepsilon_i^n + \varepsilon_{i-1}^n) + \varepsilon_i^n \quad (1)$$

And we also assume the growth of error to be

$$\varepsilon_i^n = E_m(t)e^{i\omega x}$$

After substitute in the error equation (1), we get

$$\frac{E_n(t+\Delta t)}{E_n(t)} = r\left(e^{iw\Delta x} + e^{-iw\Delta x} - 2\right) + 1$$

We get $r \leq 1/2$

2. For the situation with velocity,

$$\varepsilon_i^{n+1} = r(\varepsilon_{i+1}^n - 2\varepsilon_i^n + \varepsilon_{i-1}^n) + s(\varepsilon_i^n - \varepsilon_{i-1}^n) + \varepsilon_i^n$$

We consider the range of r and s separately, the r is the same as the last one r$\leq 1/2$, for s, we use same methods before to derive

$$\frac{E_n(t+\Delta t)}{E_n(t)} = 1 - s\left(1 - e^{-i\theta}\right)$$

After calculation, we found s is consistently unconditional stable for all the $s < 0$

3.Result:

In this section, we show the results of simulated data using our methods First of all, we plot the figure of the setting where there is one source of pollutant without advection, where L=10km and a=0.02km2/day.

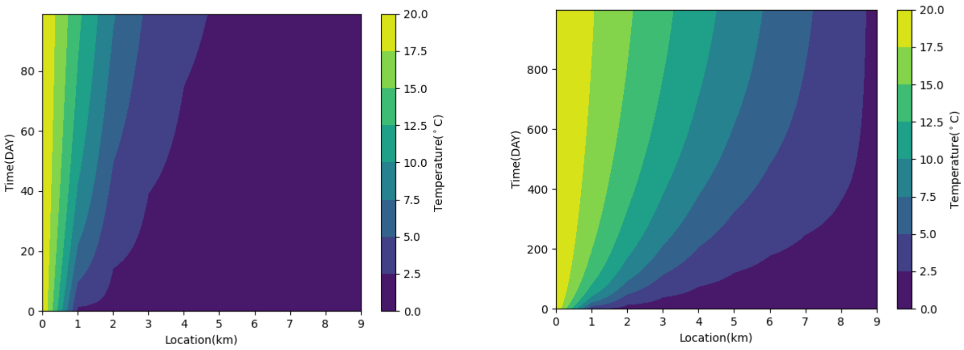

Figure 1. Diffusion of temperature at t=100days (left panel) and t=1000days (right panel)

In Figure 1, we can see the diffusion moves slowly and it takes more than 100 days to affect 5km downstream. Next, we add the advection where v=0.02km/day

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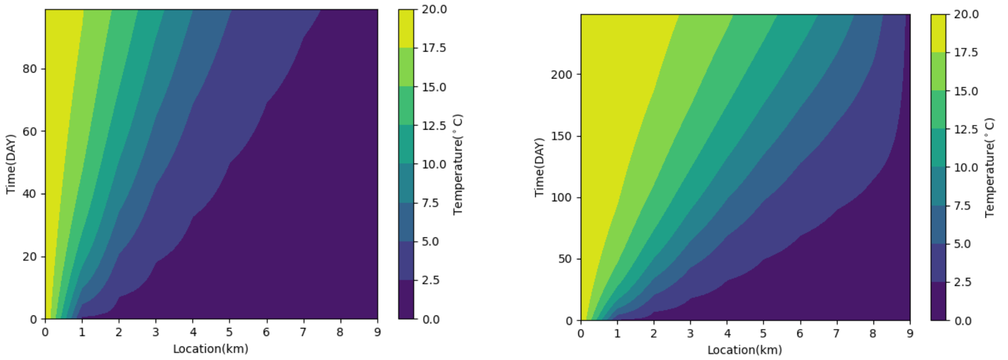

Figure 2. Diffusion of temperature at t=100days (left panel) and t=250days (right panel)

Comparing to the setting without advection, the Figure 2 shows that the diffusion become faster and takes around 50days to spread 5km downstream. The pollutant will affect the whole river in fewer days.

If we put another source of pollutant in the middle of the river, where the location=L/2 For the situation without advection. L=100km and a=0.2km2/day.

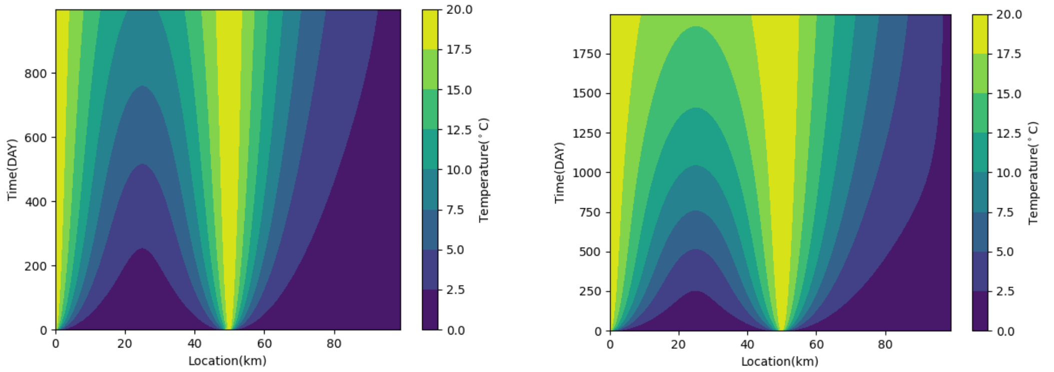

Figure 3. Diffusion of temperature at t=1000days (left panel) and t=2000days (right panel)

Comparing to the previous setting where there is one source of pollutant, we observed two areas of high concentration that show symmetric spread on both sides.

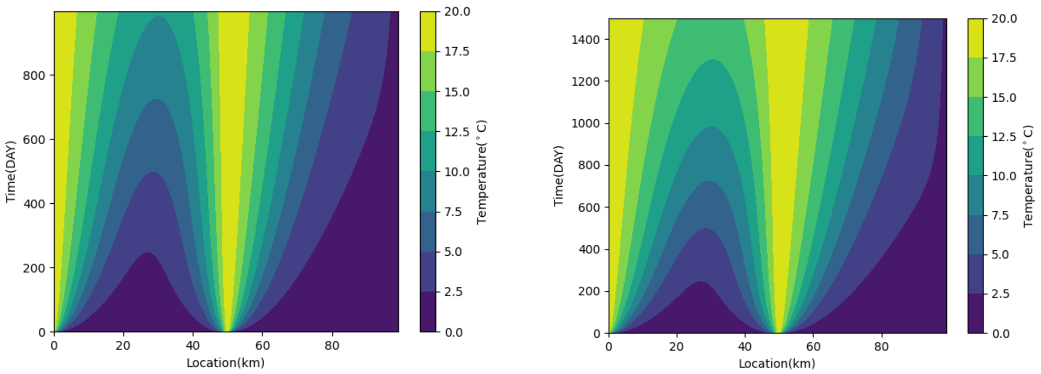

Figure 4. Diffusion of temperature at t=1000days (left panel) and t=1500days (right panel)

Comparing to Figure 3 and Figure 4, it is clear that the half of the river's temperature changes in fewer days because of the velocity. Moreover, the image is not symmetrical and is right shifted. The water between two sources of the pollutant is affected in about 250days, where it takes 400 days without velocity.

4.Discussion

The slope of Figure 1 is 25 days/km, and the slope of Figure 2 is 14.3 days/km. This shows that the river with advection takes fewer days to spread per kilometer. As a result, we can see that the speed of diffusion and the velocity of the water have a positive relationship. Consequently, advection is one of the most significant factors influencing diffusion. Faster advection leads to a faster spread of pollutants.

However, due to the stability analysis conditions, the velocity value we use is much lower than the real data. For example, the Amazon River, which is the largest river by volume, has an average flow rate of 7,400,000 cubic feet per second, an average water depth of 45 meters, and a flow velocity of 0.9313 m/s. This velocity is much higher than 0.01 km/day. Therefore, pollutant diffusion will spread downstream faster in real rivers. Compared to the model in our assumptions, the whole river's temperature would be affected in fewer days. Moreover, the depth, width, and shape of the river will influence diffusion. Yang et al. (2022) shows that methane concentration and diffusive flux were mainly co-regulated by water temperature, water depth, and water productivity (Chla, trophic status). We assume that the river is straight, but in reality, not all rivers are straight. We need to consider the shape of the river, which also affects diffusion. Besides, external factors such as climate temperature and wind velocity also influence diffusion. We need to consider more conditions when analyzing real rivers.

5.Conclusions

This study underscores the effective application of the heat equation to model the diffusion of thermal pollutants in river systems, demonstrating its capability to establish relationships among critical parameters such as water temperature, time, and stream location. By accurately simulating the temporal and spatial dispersion of pollutants, the model provides valuable predictive insights into pollutant dynamics. Employing numerical methods like forward and backward differencing and Von Neumann stability analysis ensures accurate and stable simulations, considering factors such as thermal diffusivity and river velocity. The model's strengths include its predictive capabilities and adaptability to various scenarios, aiding in environmental impact assessments and mitigation strategies. However, the reliance on simplifying assumptions and sensitivity to thermal diffusivity and velocity parameters pose certain limitations. Future research should aim to enhance the accuracy of parameters by incorporating real-world data, such as the river's average flow, width, and depth, to calculate a more accurate average velocity. These values can then be integrated into the relevant equations to develop models that should be validated against empirical observations. Additionally, investigating advanced numerical methods to improve accuracy and extend the model's applicability is essential. Incorporating additional parameters, such as the river's width and depth, can further refine the model's realism and predictive

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capacity. Overall, this study highlights the crucial role of numerical modeling in addressing environmental challenges and promoting sustainable practices

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