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Mathematical Modeling of Antibacterial Activity of MoS2 (MX2) Transition Metal Dichalcogenides (TMDs) Nanotubes against Escherichia coli (E. coli): A Novel Approach to Combat Antibiotic Resistance using Stochastic Differential Equations

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Abstract

Antibiotic resistance poses a significant threat to global health, necessitating innovative strategies to combat bacterial infections. This study develops a mathematical model using stochastic differential equations to investigate the antibacterial activity of MoS2 nanotubes against Escherichia coli populations, accounting for bacterial growth, death, and interaction with MoS2 nanotubes, as well as intrinsic biological noise. The model is solved numerically using NumPy and SciPy libraries in Python, revealing the impact of varying parameters on the system dynamics. Simulation results demonstrate that increasing MoS2 concentration and controlling bacterial growth rates can effectively suppress E. coli populations, providing valuable insights into optimizing antibacterial interventions. The results are presented in time series plots, phase plane plots, and tables, showcasing the potential of mathematical modeling and simulation in developing robust strategies to combat antibiotic resistance.

Keywords: Antibacterial activity, MoS2 nanotubes, Stochastic differential equations, Escherichia coli, Antibiotic resistance, Mathematical modeling, Python simulation

INTRODUCTION

Antimicrobial resistance (AMR) poses a significant global health threat, rendering many antibiotics ineffective against common bacterial infections, including those caused by Escherichia coli (E. coli) (WHO n.d). The overuse and misuse of antibiotics have led to the emergence of multidrug-resistant bacteria, resulting in increased mortality and healthcare costs (CDC). E. coli is a particularly concerning pathogen due to its prevalence in various infections, including urinary tract infections, foodborne illnesses, and sepsis (Crooke et al., 2018). The emergence of multidrug-resistant (MDR) E. coli strains necessitates the development of novel, broad-spectrum antibacterial agents (McDougal & Wright, 2019). The urgent need for alternative antibacterial agents has sparked research into novel materials with unique properties, such as transition metal dichalcogenides (TMDs) like Molybdenum disulfide [MoS2] (MX2).

Transition metal dichalcogenides (TMDs), particularly molybdenum disulfide (MoS2), have emerged as promising candidates for novel antibacterial agents due to their unique properties. These materials possess high surface area, conductivity, and mechanical strength, contributing to their effectiveness (Mondal & De, 2022). Their antibacterial activity stems from two primary mechanisms: generation of reactive oxygen species (ROS) that induce oxidative stress, and sharp nanotube edges that disrupt bacterial cell membranes (Mondal & De, 2022, Zhao et al., 2021).
Recent research has extensively explored the antibacterial potential of MoS2 and other TMDs. Studies by Zhao et al. (2021) demonstrated the bactericidal capabilities of MoS2 nanosheets against E. coli, attributing their efficacy to oxidative stress and membrane damage. Similarly, a review by Shen et al. (2024) highlighted MoS2's promising antibacterial properties and mechanisms, suggesting further exploration for various biomedical applications.

Beyond MoS2, Pandit et al. (2016) investigated the antibacterial properties of functionalized two-dimensional chemically exfoliated MoS (ce-MoS) against ESKAPE pathogens, including Staphylococcus aureus (MRSA) and Pseudomonas aeruginosa. Their findings suggest that ce-MoS exhibits inhibitory and bactericidal properties against these pathogens, with a mechanism involving oxidative stress and rapid membrane depolarization. This study exemplifies the potential of 2D TMDs as a new class of antibiotics to combat antibiotic resistance.

The bactericidal mechanisms of TMDs extend beyond ROS generation and membrane disruption. Kim et al. (2019) explored the role of electrical conductivity and chemical oxidation in 1T-phase TMDs. Their research showed that MoS2's properties facilitate charge transfer from the bacterial membrane to the TMDs, leading to continuous bacterial disruption and loss of cellular components.
Despite the progress made through empirical and experimental research, these methods have limitations. They often rely on specific laboratory conditions that may not fully capture the complex interactions between TMDs and bacterial cells in real-world environments with diverse factors (Hu et al., 2018).

Theoretical modeling offers a more robust framework for predicting and understanding the antibacterial activity of TMDs. Stochastic differential equations (SDEs) present a powerful tool in this regard. SDEs can account for the inherent randomness in biological systems, such as fluctuations in bacterial growth and mutation rates (Allen, 2017). By developing a mathematical model using SDEs, we can simulate the dynamics of the system and predict the effectiveness of MoS2 nanotubes under various conditions. This includes factors like varying concentrations, exposure times, and bacterial strain characteristics. Additionally, SDE models can help elucidate the underlying mechanisms of MoS2 nanotube action, leading to the identification of key factors influencing their effectiveness, such as surface area, functionalization, and interaction with bacterial membranes.

Previous research has demonstrated the potential of SDE modeling in the context of antibacterial activity. For instance, Akiyama and Kim (2021) investigated the stochastic response of bacterial cells to antibiotics and its implications for population and evolutionary dynamics. The study revealed insights into how these stochastic responses impact the population dynamics of bacteria and their evolutionary trajectories in the presence of antibiotics. Another study by Mansour (2023) developed a stochastic model based on deterministic equations to analyze the dynamics of bacterial populations under the influence of random fluctuations. The model demonstrated the stochastic effect of eradicating bacteria with antibiotics and provided insights into treatment outcomes. By building upon this existing work and applying SDEs to MoS2 nanotubes specifically, we can gain deeper insights and optimize their design for broad-spectrum antibacterial applications.

This study breaks new ground by employing stochastic differential equations (SDEs) to model the antibacterial activity of MoS2 nanotubes against E. coli. Unlike traditional methods, SDEs account for the inherent randomness in biological systems. This allows for a more nuanced understanding of MoS2 nanotube effectiveness by considering factors like bacterial population fluctuations and mutation rates. This novel approach can significantly enhance our ability to predict and optimize MoS2 nanotube design for broad-spectrum antibacterial applications.

The core of this study lies in developing a mathematical model using SDEs. These equations will incorporate variables like E. coli population state and MoS2 nanotube concentration. Deterministic terms will capture factors like bacterial growth and MoS2-mediated disruption. Stochastic terms will account for the inherent randomness in biological processes. By simulating these SDEs, we can predict the antibacterial activity of MoS2 nanotubes under diverse conditions. This analysis will allow us to identify key factors influencing their effectiveness and guide the design of next-generation antibacterial solutions.

METHODS

2.1. Overview Theoretical Concept

The interaction between MoS2 nanotubes and E. coli bacteria is a complex process influenced by various biological and physical factors (Yang et al., 2014). To understand and predict the antibacterial activity of MoS2, we employ a mathematical model that captures both the deterministic and stochastic nature of this interaction.

Deterministic Dynamics: Logistic Growth and Antibacterial Action

The logistic growth equation, a well-established mathematical representation of population dynamics (Verhulst, 1838), describes how the E.coli population, denoted by $X_E(t)$, grows in a controlled environment with limited resources. The growth rate (r_E) and the carrying capacity (K_E) are the key parameters, where the former dictates the speed of growth and the latter represents the maximum population size the environment can sustain (Murray, 2002). However, when MoS2 nanotubes, represented by $M_M(t)$, are introduced into the environment, they exert an antibacterial effect on the E. coli population, modeled by a term involving the rate constant (α_{EM}E) (Naskar et al., 2021).

Stochastic Dynamics: Accounting for Randomness

Biological systems are inherently random (Kampen and Reinhardt, 1983). This randomness arises from numerous sources, such as fluctuations in environmental conditions or random interactions at the molecular level. To incorporate this aspect into our model, we introduce a stochastic term characterized by the intensity (σX_E) and a white noise process ($\xi X_E(t)$) (Gardiner, 2009).

Coupled Dynamics: Interplay Between E. coli and MoS2

The coupled dynamics of E. coli and MoS2 are described by two linked differential equations (Keller et al., 2019). The first captures the changing E. coli population over time, considering both growth and antibacterial disruption (Braumann 2008). The second equation models the decay of MoS2 concentration, reflecting processes like aggregation or chemical reactions that reduce the availability of active nanotubes over time (Patel et al., 2021).

Master Equation: Probability Distribution

To fully understand the system's behavior, we derive the master equation, known as the Fokker-Planck equation in the context of stochastic processes (Risken, 1996). This equation governs the evolution of the probability distribution of the system's states, providing a comprehensive picture of the possible outcomes of the interaction between E. coli and MoS2 (Lamperti, 1977)

2.2. Development of the Mathematical Model

In this section we develop a mathematical model for the membrane disruption of E. coli induce by the concentration of MoS2 and environmental fluctuation at the point of interaction.

The Stochastic Differential Equation Model

We introduced the stochastic Differential Equations thus;

The logistic growth term for the E. coli population, denoted by $X_E(t)$, is given by:

$$Logistic\ growth_E = \frac{dX_E}{dt} = r_E \cdot X_E \cdot \left(1 - \frac{X_E}{K_E}\right) \quad (1)$$

r_E is the intrinsic growth rate of E. coli, $X_E(t)$ is the concentration of E. coli at time (t) and K_E is the carrying capacity of the environment for E. coli.

The MoS2-mediated disruption term, which models the antibacterial effect of MoS2 nanotubes on E. coli, is given by:

$$\text{Disruption}_{EM} = \frac{dX_{EM}}{dt} = -\alpha_{EM} \cdot X_E(t) \cdot M_M(t) \quad (2)$$

α_{EM} is the rate constant for the interaction between E. coli and MoS2 and $M_M(t)$ is the concentration of MoS2 nanotubes at time (t).

The SDE that describes the change in the bacterial population dX_E over a small-time interval (dt), influenced by the noise intensity σ_{X_E} population size $X_E(t)$ and random noise process $\xi_{X_E}(t)$ is given as:

$$Stochastic\ Noise_E = \frac{dX_E}{dt} = \sigma_{X_E} \cdot X_E(t) \cdot \xi_{X_E}(t) \quad (3)$$

Combining (1),(2) and (3), we find the full SDE for the concentration of E. coli in the presence of MoS2 nanotubes:

$$\frac{dX_E(t)}{dt} = Logistic\ growth_E + \text{Disruption}_{EM} + Stochastic\ Noise_E$$

$$\frac{dX_E(t)}{dt} = r_E \cdot X_E(t) \cdot \left(1 - \frac{X_E(t)}{K_E}\right) - \alpha_{EM} \cdot X_E(t) \cdot M_M(t) + \sigma_{X_E} \cdot X_E(t) \cdot \xi_{X_E}(t)$$

$$dX_E(t) = \left[r_E \cdot X_E(t) \cdot \left(1 - \frac{X_E(t)}{K_E}\right)\right] dt - [\alpha_{EM} \cdot X_E(t) \cdot M_M(t)]dt + \left[\sigma_{X_E} \cdot X_E(t) \cdot \xi_{X_E}(t)\right]dt \quad (4)$$

Eqn (4) is of the form $\boldsymbol{dX(t) = f(X(t), t)dt + g(X(t), t)dW(t)dt}$ where $f(X(t), t)$ represents the deterministic part of the dynamics and $g(X(t), t)$ represents the stochastic noise.

Eqn (4) describes the dynamics of the E. coli population under the influence of logistic growth, antibacterial disruption by MoS2, and stochastic environmental variations.

Concentration Dynamics of MoS2 Nanotubes

To model the concentration dynamics of MoS2 nanotubes, we assume a simple decay process with a rate proportional to the current concentration. This can be represented mathematically as:

$$\frac{dM_M(t)}{dt} = -\beta_M \cdot M_M(t) + \eta \cdot dW(t) \quad (5)$$

β_M is the decay rate constant of MoS2 nanotubes. $\eta \cdot dW(t)dt$ noise term, where η is the noise intensity (a constant), and $dW(t)$ is a Wiener process (a random process with Gaussian increments). This term represents the random fluctuations in MoS2 concentration due to external factors.

Coupled Dynamics:
Now, we combine the E. coli growth and disruption dynamics with the MoS2 concentration dynamics. The coupled system of differential equations is:

$$\begin{Bmatrix} dX_E(t) = \left[r_E \cdot X_E(t) \cdot \left(1 - \frac{X_E(t)}{K_E}\right)\right] dt - [\alpha_{EM} \cdot X_E(t) \cdot M_M(t)]dt + \left[\sigma_{X_E} \cdot X_E(t) \cdot \xi_{X_E}(t)\right]dt \\ dM_M(t) = -\beta_M \cdot M_M(t)dt + \eta \cdot dW(t)dt \end{Bmatrix} \quad (6)$$

In this coupled system:
The Eqn (4) describes the change in E. coli concentration over time, incorporating logistic growth, MoS2-mediated disruption, and stochastic environmental noise.

The Eqn (5) describes the decay of MoS2 concentration over time.
Together, these equations model the interaction between E. coli and MoS2 nanotubes, taking into account the antibacterial activity of MoS2 and the environmental variability affecting the system.

Modelling the Probability Distribution of the System's State

To fully capture the stochastic nature of the system and the interactions between the species, we derived a Master Equation that describes the probability distribution of the system's states, offering a more comprehensive understanding of the system's behavior over time.

We define the transition probabilities $P(X_E, M_M, t + \Delta t \mid X'_E, M'_M, t)$ which describe the probability of the system transitioning from state (X'_E, M'_M) at time (t) to state ((X_E, M_M)) at time ($t + \Delta t$).

The Chapman-Kolmogorov equation (Tarasov, 2007) relates the transition probabilities at different times:

$$P(X_E, M_M, t + \Delta t) = \int\int P(X_E, M_M, t + \Delta t \mid X'_E, M'_M, t)P(X'_E, M'_M, t)dX'_E dM'_M \quad (7)$$

By Taylor Series Expansion

$$P(X_E, M_M, t + \Delta t \mid X'_E, M'_M, t) = P(X'_E, M'_M, t) + \left(\frac{\partial}{\partial X'_E} P(X'_E, M'_M, t)\right)(X_E - X'_E) + \left(\frac{\partial}{\partial M'_M} P(X'_E, M'_M, t)\right)(M_M - M'_M) + \cdots$$

integrating this expansion over all possible values of X'_E, M'_M *and truncating at the* 2nd term

$$\frac{\partial P(X_E, M_M, t)}{\partial t} = -\frac{\partial}{\partial X_E}[\alpha(X_E, M_M, t)P(X_E, M_M, t)] + \frac{\partial^2}{\partial X_E^2}\left[\frac{1}{2}\beta(X_E, M_M, t)P(X_E, M_M, t)\right] \quad (8)$$

Where α *and* β Kramers-Moyal coefficients are defined as the moments of the transition rates:

$$\alpha(X_E, M_M, t) = \frac{1}{1!}\int (X_E - X'_E)^n W(X_E \mid X'_E, M'_M, t)dX'_E$$

$$\beta(X_E, M_M, t) = \frac{1}{2!}\int (X_E - X'_E)^n W(X_E \mid X'_E, M'_M, t)dX'_E$$

Here, $\alpha(X_E, M_M, t)$ is the drift coefficient, which represents the deterministic part of the process, and $\beta(X_E, M_M, t)$ is the diffusion coefficient, which represents the stochastic part.

Eqn (8) describes the time evolution of the probability distribution ($P(X_E, M_M, t)$) for the system's states and is used to analyze the overall behavior of the system in terms of probabilities. The equation takes into

account both the deterministic dynamics (growth and decay) and the stochastic fluctuations due to random environmental factors.

2.3. Solution of the Derived Models

1. Solution of the Coupled SDE

To numerically solve the coupled SDE (Eqn 6) the Euler-Maruyama method is employed:

$$X_{n+1} = X_n + f(X_n, t_n)\Delta t + g(X_n, t_n)\Delta\xi$$

where X_n is the population size at the $n-th$ time step, Δt is the time step size, and $\Delta\xi_n$ is the Wiener process increment during the $n-th$ step.

Discretization of Eqn (6) with the Euler-Maruyama Method

$$X_{E,n+1} = X_{E,n} + \left[r_E \cdot X_{E,n}\left(1 - \frac{X_{E,n}}{K_E}\right) - \alpha_E \cdot M_{M,n} \cdot X_{E,n}\right]\Delta t + \sigma_{X_E} \cdot X_{E,n} \cdot \sqrt{\Delta t} \cdot N(0,1) \cdot \xi_{E,n}$$

$X_{E,n}$ is the population of E. coli at the n-th time step $\xi_{E,n}$is a random variable from a standard normal distribution, $\xi_{E,n}$~N(0,1)

The MoS2 Nanotube Concentration becomes;

$$M_{M(n+1)}(t) = M_{M,n} - \beta_M \cdot M_{M,n}\Delta t + \eta \cdot dW(t)dt$$

The Numerical Solution becomes:

$$\begin{Bmatrix} X_{E,n+1} = X_{E,n} + \left[r_E \cdot X_{E,n}\left(1 - \frac{X_{E,n}}{K_E}\right) - \alpha_E \cdot M_{M,n} \cdot X_{E,n}\right]\Delta t + \sigma_{X_E} \cdot X_{E,n} \cdot \sqrt{\Delta t} \cdot N(0,1) \cdot \xi_{E,n} \\ M_{M,n+1} = M_{M,n} - \beta_M \cdot M_{M,n}\Delta t + \eta \cdot dW(t)dt \end{Bmatrix}$$

This solution is set-up with Python Algorithms to simulate the behavior of the system under stochastic influences and determine how the antibacterial activity of MoS_2 affects the bacterial population over time.

2. Solution of the Probability Distribution

The general form of the Fokker-Planck equation, which describes the time evolution of the probability density function ($P(X,t)$) of a state variable (X) under the influence of deterministic and stochastic processes.

$$\frac{\partial P(X,t)}{\partial t} = -\frac{\partial}{\partial X}[A(X,t)P(X,t)] + \frac{\partial^2}{\partial X^2}[B(X,t)P(X,t)]$$

For our specific model, the equation modifies to Equ (8)

$$\frac{\partial P(X_E, M_M, t)}{\partial t} = -\frac{\partial}{\partial X_E}[\alpha(X_E, M_M, t)P(X_E, M_M, t)] + \frac{\partial^2}{\partial X_E^2}\left[\frac{1}{2}\beta(X_E, M_M, t)P(X_E, M_M, t)\right]$$

$P(X_E, M_M, t)\ is\ the$ Probability density function of the state variables $X_E\ and\ M_M\ at\ time\ t$

- $\alpha(X_E, M_M, t)$ is the Drift term, which represents the deterministic part of the dynamics.
- $\beta(X_E, M_M, t)$ Diffusion term, which represents the stochastic part of the dynamics.

Expanding the expression:

$$\frac{\partial P(X_E, M_M, t)}{\partial t} = -\alpha\frac{\partial}{\partial X_E}(X_E, M_M, t)\frac{\partial}{\partial X_E}P(X_E, M_M, t) + \frac{\beta}{2}\frac{\partial^2}{\partial X_E^2}(X_E, M_M, t)\frac{\partial^2}{\partial X_E^2}P(X_E, M_M, t)$$

$$\Rightarrow \frac{\partial P(X_E, M_M, t)}{\partial t} = -\alpha \frac{\partial}{\partial X_E}(X_E, M_M, t) + \frac{\beta}{2}\frac{\partial^2}{\partial X_E^2}(X_E, M_M, t)$$

By Characteristic method:

The Drift Term becomes;

$$\frac{\partial P}{\partial t} = -\alpha \frac{\partial}{\partial X_E}$$

This is a linear first-order PDE, which can be solved by the method of characteristics. The characteristic equations are:

$$\frac{\partial X_E}{\partial t} = \alpha \qquad and \qquad \frac{\partial P}{\partial t} = 0$$

Solving these gives:

$$X_E(t) = X_E(0) - \alpha t$$

Thus, the solution for P is:

$$P(X_E, M_M, t) = P_0(X_E(0) - \alpha t, M_M) \tag{9}$$

The Diffusion Term:

$$\frac{\partial P}{\partial t} = \frac{\beta}{2}\frac{\partial^2 P}{\partial X_E^2}$$

This is a standard heat equation with a diffusion coefficient $\frac{\beta}{2}$. The general solution is a Gaussian distribution:

$$P(X_E, t) = \frac{1}{\sqrt{2\pi\beta t}} \exp\left(-\frac{(X_E - \mu)^2}{2\beta t}\right) \tag{10}$$

Combining Eqn. (9) and (10)

$$P(X_E, M_M, t) = \int_{-\infty}^{\infty} \frac{1}{\sqrt{2\pi\beta t}} \exp\left(-\frac{(X_E - \xi - \alpha t)^2}{2\beta t}\right) P_0(\xi, M_M)\, d\xi \tag{11}$$

Solving (11) Numerically:

To solve the Fokker-Planck equation numerically using the Finite Difference Method (FDM), we discretize the time and space into a grid and then approximate the derivatives in the equation with finite differences

$$\frac{\partial P}{\partial X} \approx \frac{P[j+1][i] - P[j-1][i]}{2\Delta X}$$

$$\frac{\partial^2 P}{\partial X^2} \approx \frac{P[j+1][i] - 2P[j][i] + P[j-1][i]}{\Delta X^2}$$

The solution is simulated in Python. The Algorithm is attached.

RESULTS

The results of the stochastic differential equation modeling are presented below, featuring time series plots, phase plane plots, and tables that highlight the key findings and trends in the data.

The phase plane plot (figure 1) of our model reveals a dynamic interaction between the E. coli population and MoS2 concentration. The trajectories indicate that the system does not settle into a steady state but rather exhibits fluctuations that suggest a sensitive dependence on initial conditions and parameters.

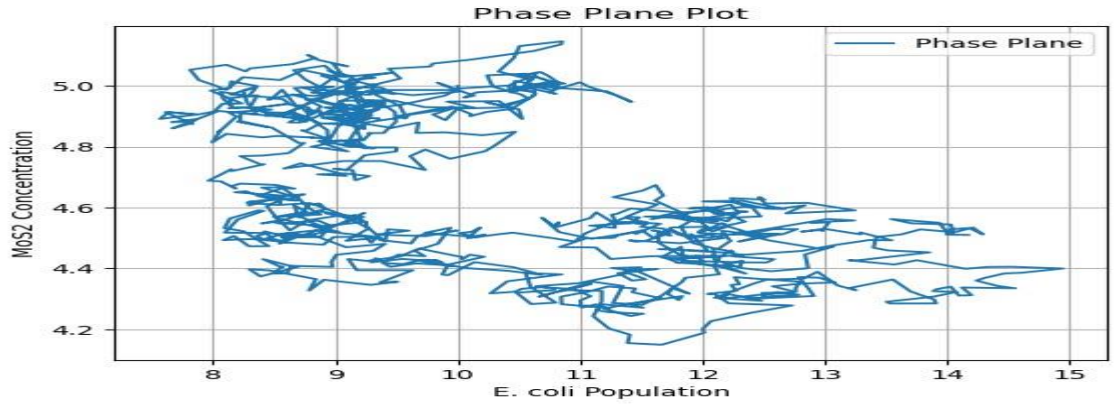

Figure 1: Phase Plane plot of the MoS2 – E.Coli Interaction

This stochastic behavior highlights the complexity of biological systems where even a small change in the environment can lead to significantly different outcomes.

Figure 2 shows four line graphs, each representing a sample path with different values of beta (β) and eta (η), which are parameters in the stochastic differential equations modeling the antibacterial activity. The x-axis on all graphs represents time (hours), ranging from 0 to 10, while the y-axis represents bacterial population size for E. coli and MoS2 concentration, both measured in arbitrary units.

In each graph, there are two lines: one for E. coli population size and another for MoS2 concentration. The first graph has $\beta = 0.3$ and $\eta = 0.4$, the second has $\beta = 0.6$ and $\eta = 0.4$, the third has $\beta = 0.3$ and $\eta = 0.8$, and the fourth has $\beta = 0.6$ and $\eta = 0.8$.

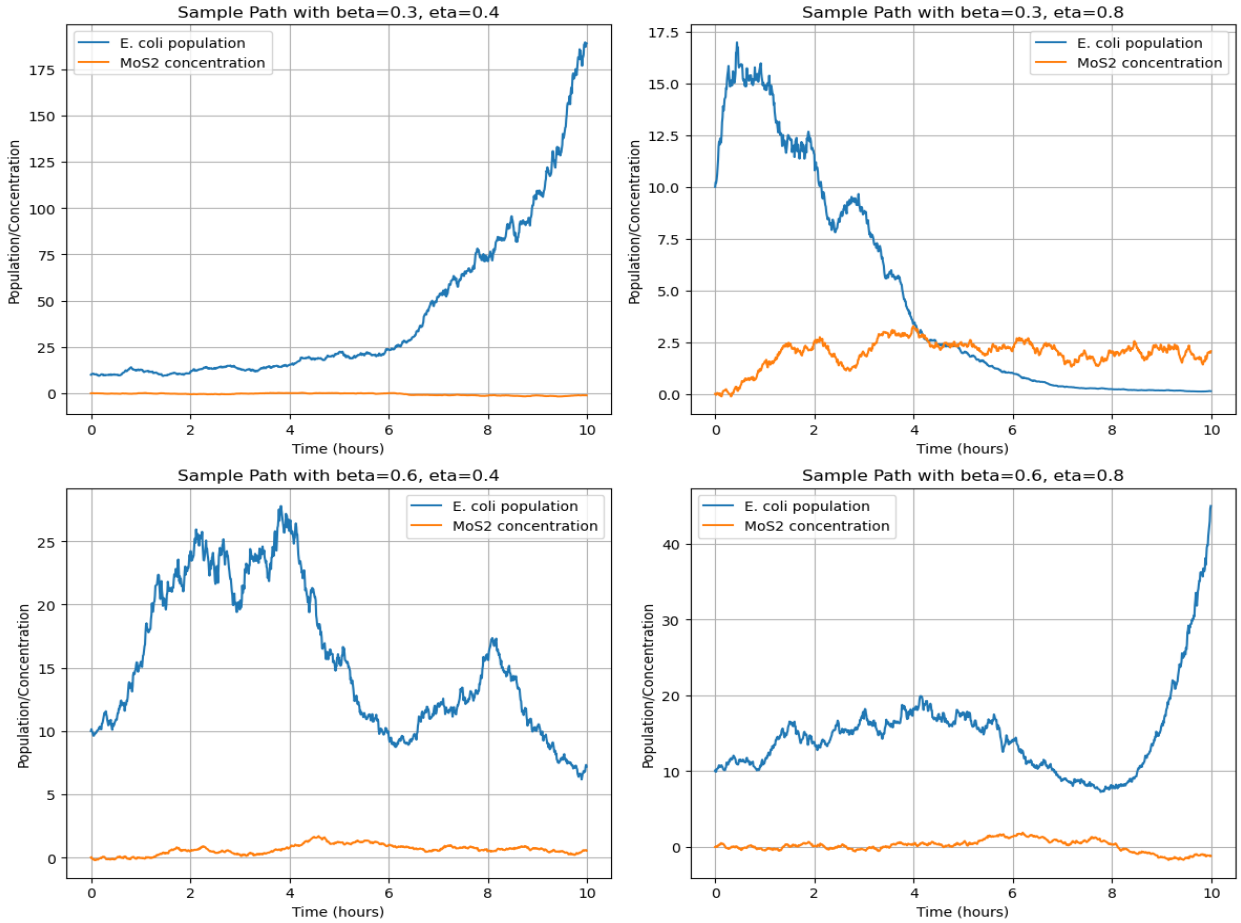

Figure 2: Dynamic Interplay of E. coli Population and MoS2 Concentration

The results from these plots indicate that as the value of beta (β) increases from 0.3 to 0.6 while keeping eta (η) constant at 0.4, there is a more pronounced fluctuation in both E.coli population size and MoS2 concentration over time with higher peaks observed in bacterial reduction followed by recovery phases.
Figure 2 shows that an increase in η leads to a more significant decrease in E.coli population size along with higher MoS2 concentrations over time.

Figure 3 is a plot of the growth of E. coli population over time, measured in hours, with three different growth rates indicated by three distinct lines. The x-axis represents time in hours, ranging from 0 to 10, and the y-axis represents the E. coli population, ranging from 0 to 70. There are three lines representing different values of the parameter r (growth rate): $r = 0.1$ (red line), $r = 0.2$ (orange line), and $r = 0.3$ (green line). As time progresses, each line shows an increase in E. coli population with varying slopes indicating that a higher growth rate results in a steeper slope and thus a faster-growing population.

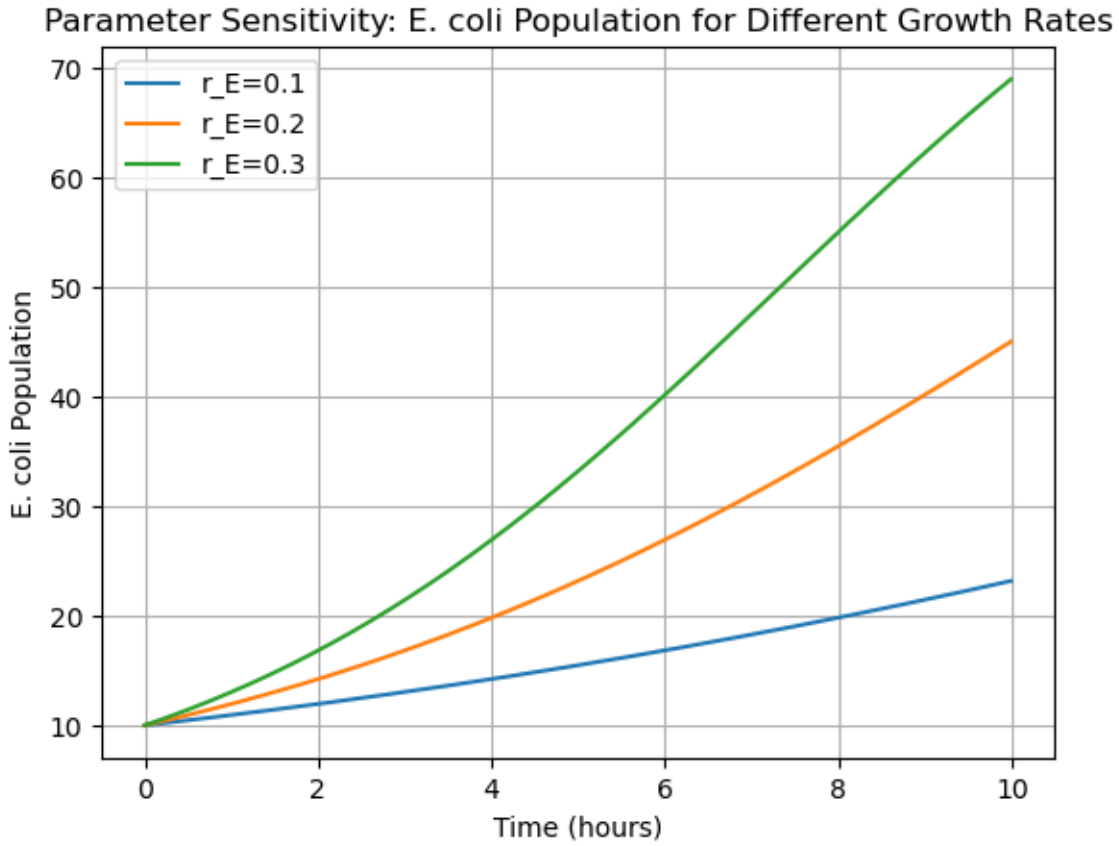

Figure 3: Impact of Growth Rate on E. coli Population Dynamics in MoS2 Nanotubes

The analysis of Figure 3 reveals that the growth rate parameter 'r' significantly influences the proliferation of Escherichia coli within MoS2 nanotubes over time. For a lower growth rate value of $r = 0.1$, the increase in bacterial population is gradual and linear, reaching approximately 20 units after 10 hours. When the growth rate parameter is doubled to $r = 0.2$, there is a notable acceleration in bacterial expansion with the final count nearing 40 units at the same time point—a twofold increase compared to $r = 0.1$ scenario.

Figure 4 shows the Stochastic Simulations of E. coli Population over time. There are three lines represents the different realizations or simulations of E. coli population growth over time: Realization 1 (blue), Realization 2 (green), and Realization 3 (orange). Each line fluctuates, showing variability in the population size at different time points, which is characteristic of stochastic models.

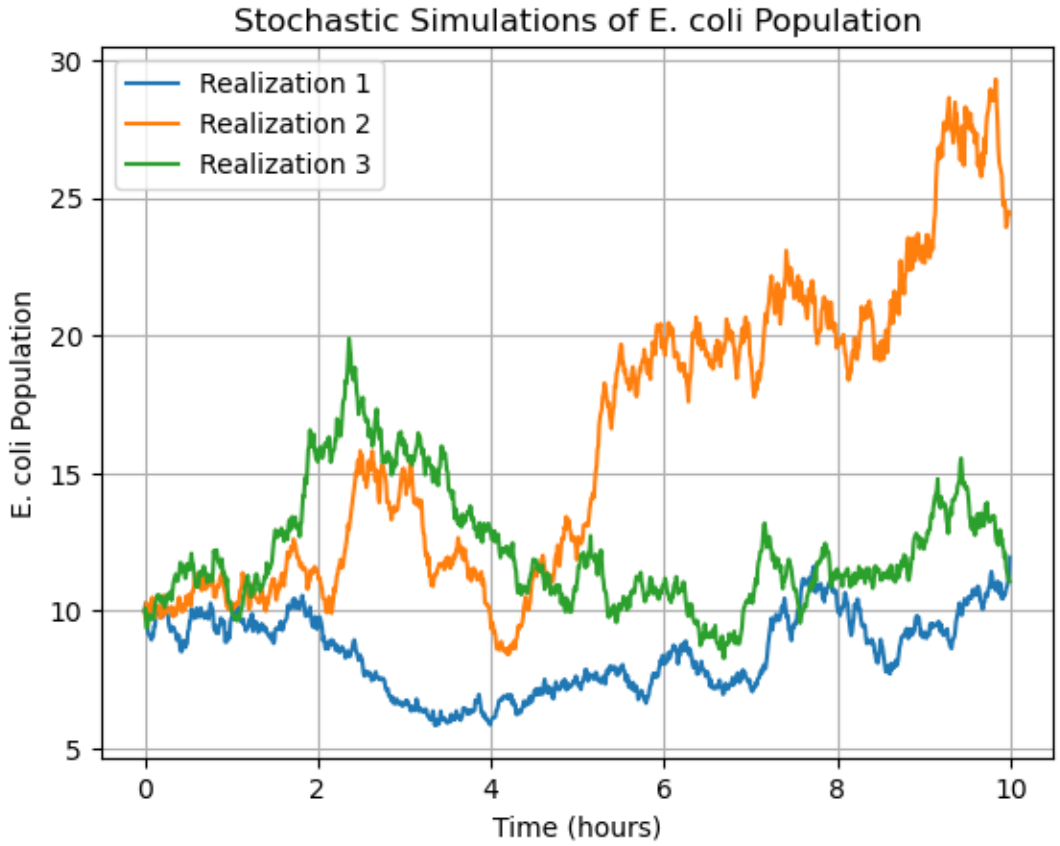

Figure 4: Impact of MoS2 Nanotubes on E. coli Population Dynamics

This plot revels that the SDE used to model the antibacterial activity of MoS2 nanotubes against Escherichia coli populations demonstrate significant fluctuations in bacterial counts over a period of ten hours. Three separate simulations, termed as 'Realizations', exhibit distinct trajectories, indicating the inherent randomness in biological interactions modeled by such equations. Despite this variability, all three realizations show an overall trend of increasing E. coli population size over time.

Table 1 presents the data generated from the numerical solution to the stochastic differential equations modeling the antibacterial activity of MoS2 nanotubes against E. coli. The table is structured to provide a detailed view of the system's state at various time points, with the position values representing the concentration of E. coli and the probability values indicating the likelihood of observing the system in that state.

S/n	Time	Position	Probability
1	0.0	-2.0000	0.05400
2	0.0	-1.8974	0.0659
3	0.0	-1.7949	0.0797
4	0.0	-1.6923	0.0953
5	0.0	-1.5897	0.1128
6	0.0	-1.4872	0.1320
7	0.0	-1.3846	0.1530

8	0.0	-1.2821	0.1754
9	0.0	-1.1795	0.1990
10	0.0	-1.0769	0.2234
195	0.95	-0.9744	0.0000
196	0.95	-0.6667	0.0000
197	0.95	-0.4615	0.0001
198	0.95	-0.1538	0.0001
199	0.95	0.0512	0.0002
395	0.95	1.0769	0.0031
396	0.95	1.2820	0.0050
397	0.95	1.5897	0.0094
398	0.95	1.7948	0.0135
399	0.95	2.00	0.0176

Tabe 1 - Temporal Distribution of E. coli Concentration Probabilities in the Presence of MoS2 Nanotubes

The data is organized into intervals that reflect the concentration ranges of E. coli, with five values between -2 and -1, five between -1 and 0, another five between 0 and 1, and the last five between 1 and 2. These intervals are chosen to capture the significant changes in the bacterial population due to the interaction with MoS2 nanotubes. The 'Time' column corresponds to discrete time steps in the simulation, while the 'Position' column represents the discretized state space of E. coli concentration, and the 'Probability' column provides the computed probability density for each state.

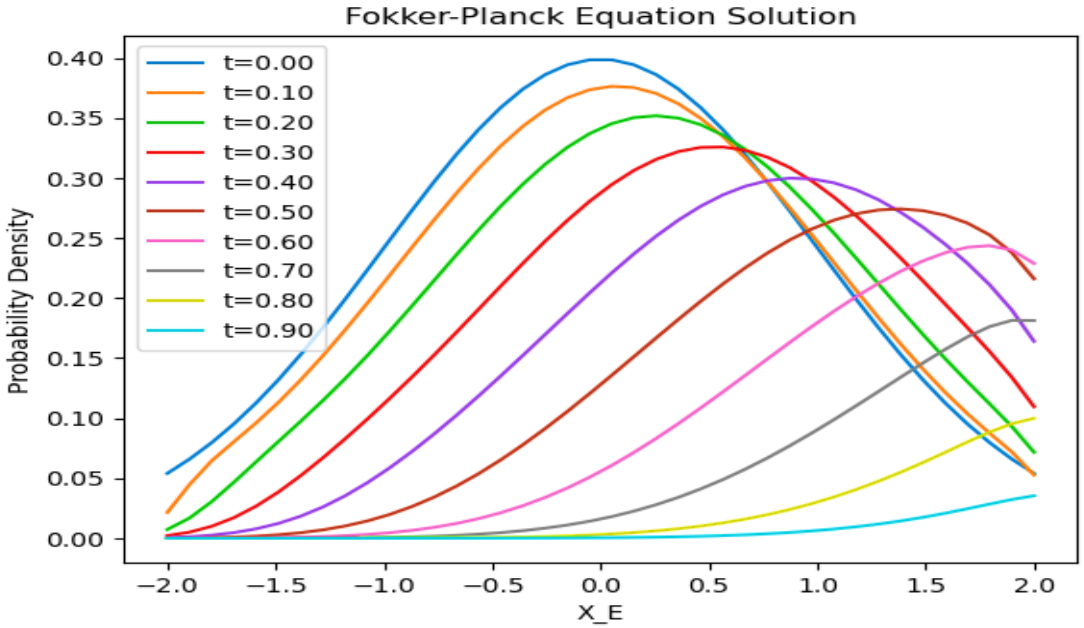

Figure 5 - Dynamic Evolution of E. coli Probability Density Under MoS2 Nanotube Influence

Figure 5 illustrates the dynamic evolution of the probability density function (PDF) for the concentration of E. coli when exposed to MoS2 nanotubes, as predicted by stochastic differential equations. Each curve represents the PDF at a specific time interval, starting $from\, t = 0.00$

(initial state) and ending at $t = 0.90$. Initially, the PDF is narrowly peaked, indicating a high probability of E. coli concentration around a particular value. As time progresses, the curves become broader and flatter, reflecting the diffusion of the bacterial population and the impact of the antibacterial activity of MoS2 nanotubes. This spread signifies a decrease in the likelihood of finding E. coli at high concentrations, suggesting that MoS2 nanotubes are effective in dispersing and reducing the bacterial population, thereby offering a potential method to combat antibiotic resistance. Figure 1 provides a visual representation of the antibacterial efficacy over time, supporting the use of MoS2 TMDs as a novel antibacterial agent.

CONCLUSION

The mathematical model developed in this study using stochastic differential equations has provided valuable insights into the antibacterial activity of MoS2 nanotubes against Escherichia coli populations. The results demonstrate that varying levels of efficacy (β) and volatility (η) of MoS2 significantly impact the antibacterial activity, with higher values of volatility leading to more effective suppression of E. coli populations. Additionally, the model reveals that controlling the growth rate parameter (r) is crucial for optimizing antibacterial activity. This novel approach highlights the potential of MoS2 TMDs as effective antibacterial materials and emphasizes their controllable aspects via mathematical parameters. The approach also provides insights into optimizing dosages of TMDs nanotubes for combating antibiotic-resistant bacteria through precise mathematical models. The variability observed in the phase plane plots underscores the need for a probabilistic approach to understanding and predicting the outcomes of antibacterial interventions. Future work should focus on refining these models to account for more biological factors and experimental validation of the predicted behaviors. This research paves the way for developing more effective antibacterial strategies that are robust to the inherent uncertainties of complex biological systems, providing a promising solution to combat antibiotic resistance. The findings of this study demonstrate the potential of mathematical modeling using stochastic differential equations to optimize the design and application of TMDs nanotubes as antibacterial agents, highlighting the importance of interdisciplinary approaches in addressing the pressing issue of antibiotic resistance.

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SIMULATION ALGORITHMS IN PYTHON Modeling of Antibacterial Activity of MoS2 (MX2) Transition Metal Dichalcogenides (TMDs) Nanotubes against Escherichia coli (E. coli)

```
import numpy as np

import matplotlib.pyplot as plt

import pandas as pd

# Parameters

r_E = 0.2  # E. coli growth rate
```

```
K_E = 100  # Carrying capacity for E. coli

alpha_EM = 0.03  # Efficacy of MoS2

beta_M = 0.03  # Degradation rate of MoS2

sigma_XE = 0.2  # Volatility of E. coli population

sigma_MM = 0.2  # Volatility of MoS2 concentration

dt = 0.01  # Time step

T = 10  # Total simulation time (in hours)

N_paths = 10  # Number of sample paths


# Initialize arrays for E. coli and MoS2

X_E = np.zeros((N_paths, int(T / dt)))

M_M = np.zeros((N_paths, int(T / dt)))

time_steps = np.arange(0, T, dt)


# Generate sample paths

for path in range(N_paths):

   X_E[path, 0] = 10  # Initial E. coli population

   M_M[path, 0] = 5  # Initial MoS2 concentration

   for t in range(1, int(T / dt)):

      dW_XE = np.random.normal(0, np.sqrt(dt))

      dW_MM = np.random.normal(0, np.sqrt(dt))

      X_E[path, t] = X_E[path, t - 1] + (r_E * X_E[path, t - 1] * (1 - X_E[path, t - 1] / K_E) - alpha_EM *
X_E[path, t - 1] * M_M[path, t - 1]) * dt + sigma_XE * X_E[path, t - 1] * dW_XE

      M_M[path, t] = M_M[path, t - 1] + (-beta_M * M_M[path, t - 1]) * dt + sigma_MM * dW_MM


# Plotting sample paths

plt.figure(figsize=(18, 12))


# Time series plots

plt.subplot(3, 2, 1)

plt.plot(time_steps, X_E[0], label="E. coli population")
```

```
plt.xlabel("Time (hours)")
plt.ylabel("Population")
plt.title("E. coli Population Over Time")
plt.legend()
plt.grid(True)

plt.subplot(3, 2, 2)
plt.plot(time_steps, M_M[0], label="MoS2 concentration", color='orange')
plt.xlabel("Time (hours)")
plt.ylabel("Concentration")
plt.title("MoS2 Concentration Over Time")
plt.legend()
plt.grid(True)

# Phase plane plot
plt.subplot(3, 2, 3)
plt.plot(X_E[0], M_M[0], label="Phase Plane")
plt.xlabel("E. coli Population")
plt.ylabel("MoS2 Concentration")
plt.title("Phase Plane Plot")
plt.legend()
plt.grid(True)

# Parameter sensitivity plots (showing only one example for brevity)
plt.subplot(3, 2, 4)
for r in [0.1, 0.2, 0.3]:
    X_E_sensitivity = np.zeros(int(T / dt))
    X_E_sensitivity[0] = 10
    for t in range(1, int(T / dt)):
        X_E_sensitivity[t] = X_E_sensitivity[t - 1] + (r * X_E_sensitivity[t - 1] * (1 - X_E_sensitivity[t - 1] / K_E))
* dt
```

```
    plt.plot(time_steps, X_E_sensitivity, label=f"r_E={r}")
plt.xlabel("Time (hours)")
plt.ylabel("E. coli Population")
plt.title("Parameter Sensitivity: E. coli Population for Different Growth Rates")
plt.legend()
plt.grid(True)

# Stochastic simulations (showing only one example for brevity)
plt.subplot(3, 2, 5)
for path in range(3):  # Plotting only 3 paths for clarity
    plt.plot(time_steps, X_E[path], label=f"Realization {path+1}")
plt.xlabel("Time (hours)")
plt.ylabel("E. coli Population")
plt.title("Stochastic Simulations of E. coli Population")
plt.legend()
plt.grid(True)

# Bifurcation diagram (simplified example)
plt.subplot(3, 2, 6)
for alpha in [0.01, 0.02, 0.03]:
    plt.scatter(alpha, X_E[0][-1], label=f"α_EM={alpha}")  # Plotting final population size
plt.xlabel("α_EM")
plt.ylabel("Final E. coli Population")
plt.title("Bifurcation Diagram (Simplified)")
plt.legend()
plt.grid(True)

plt.tight_layout()
plt.show()

# Creating data tables for each plot using Pandas
```

```
time_series_data_ecoli = pd.DataFrame({'Time (hours)': time_steps, 'E. coli Population': X_E[0]})

time_series_data_mos2 = pd.DataFrame({'Time (hours)': time_steps, 'MoS2 Concentration': M_M[0]})

phase_plane_data = pd.DataFrame({'E. coli Population': X_E[0], 'MoS2 Concentration': M_M[0]})

sensitivity_data = pd.DataFrame({'Time (hours)': time_steps, 'E. coli Population (r_E=0.1)': X_E_sensitivity})


# Displaying one example data table

print("Time Series Data for E. coli Population:")

print(time_series_data_ecoli.head())
```

THE FORKK EQUATION SIMULATION CODE

```
import numpy as np

import matplotlib.pyplot as plt

import pandas as pd


# Parameters

alpha = 0.5  # Drift coefficient

beta = 0.1   # Diffusion coefficient

t_max = 1.0  # Maximum time

dt = 0.05    # Time step size

dx = 0.1     # Space step size

x_min, x_max = -2.0, 2.0  # Spatial domain limits

n_t = int(t_max / dt)    # Number of time steps

n_x = int((x_max - x_min) / dx)  # Number of spatial steps


# Initial condition (Gaussian distribution centered at 0 with standard deviation 1)

def P_0(x):

   return (1/np.sqrt(2*np.pi)) * np.exp(-0.5*x**2)


# Discretize the spatial domain

x_values = np.linspace(x_min, x_max, n_x)
```

```
# Initialize the solution matrix
P = np.zeros((n_x, n_t))

# Set the initial condition
P[:, 0] = P_0(x_values)

# Time evolution
for i in range(1, n_t):
    t = i * dt
    for j in range(n_x):
        X_E = x_values[j]
        integral_sum = 0
        for k in range(n_x):
            xi = x_values[k]
            integral_sum += dx * (1/np.sqrt(2*np.pi*beta*t)) * np.exp(-((X_E - xi - alpha*t)**2)/(2*beta*t)) *
P[k, i-1]
        P[j, i] = integral_sum

# Generate a table for at least 20 values
table_data = []
for i in range(0, n_t, max(1, n_t//20)):  # Select 20 time steps
    for j in range(n_x):
        table_data.append({'Time': i*dt, 'Position': x_values[j], 'Probability': P[j, i]})

# Convert to DataFrame and display
df = pd.DataFrame(table_data)
print(df.head(20))  # Display first 20 rows

# Plotting the results
for i in range(0, n_t, n_t//10):  # Plot every 10th time step
```

```
    plt.plot(x_values, P[:, i], label=f't={i*dt:.2f}')


plt.xlabel('X_E')
plt.ylabel('Probability Density')
plt.title('Fokker-Planck Equation Solution')
plt.legend()
plt.show()
```