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Teaching 3-Dimensional Modeling of 2 Concentrations of Substances with Diffusion Reaction System

Astrid Sovana Situmorang[a)], Desy Dwi Ariyanti[b)], Muhamad Syeha Nursidiq[c)]

Department of Physics Education, Faculty of Mathematics and Natural Science, Universitas Negeri Jakarta, Jl. Rawamangun Muka, Jakarta 13220, Indonesia

Email: [a)]astrid_1306622072@mhs.unj.ac.id, [b)]desy_1306622046@mhs.unj.ac.id, [c)]muhamad_1306622076@mhs.unj.ac.id

Abstract

This research models the concentration of two substances in three-dimensional space with a reactiondiffusion system. The underlying partial differential equations (PDEs) are solved numerically using the finite difference method. Simulation results show the spatial and temporal variation of the concentrations of the substances, influenced by the diffusion, reaction, and boundary constants. This study introduces an innovative 3-dimensional modeling tool specifically designed to enhance students' understanding of complex diffusion reaction systems. Through the interactive 3-dimensional modeling tool students can observe how these substances diffuse and react over time, offering a dynamic way to explore complex scientific concepts. The result of the research with this tool is that it can significantly improve the learning process by transforming theoretical knowledge into practical, real-world understanding.

Keywords: finite difference method, numerical methods, partial differential equations, reaction-diffusion, three-dimensional space

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INTRODUCTION

Understanding the principles of diffusion reaction systems is an important aspect of science education, as this process is the basis of many disciplines, including chemistry, biology and environmental science (Schmitt et al., 2022). Traditional teaching methods, while effective in conveying basic concepts, often fall short in providing students with a comprehensive understanding of concepts that are sometimes abstract and difficult for students to grasp (Lian et al., 2022). 3-Dimensional modeling provides a transformative approach to this challenge by offering a powerful and immersive way for students to visualize and interact with these systems. Through the use of 3D models, students can observe how substances move and react in a given space, explore and see the direct impact on the system (Alexander et al., 2024). This direct interaction not only makes the learning process more engaging, but also significantly improves students' understanding of complex scientific concepts, bridging the gap between theoretical knowledge and practical application.According to Kalogeris and Papadopoulos (2021), the diffusion equation is a partial differential equation that represents the movement of a substance in a solvent from a high concentration part to a low concentration part. Muñoz-Gil et al. (2019)states that, each diffusion particle moves randomly in the diffusion field. The diffusion equation can be used to describe the spread of mass transfer such as the spread of oxygen concentration in a body tissue, environmental pollution, and chemical fluids.

According to previous study (Pinar, 2021), Reaction-Diffusion Equations occur naturally in systems formed by the interaction of many components and are widely used to describe various biological, chemical and physical systems. (Li et al, 2020) stated that, reaction-diffusion systems have attracted considerable attention in recent years. They appear naturally in various chemical models to describe spatiotemporal concentration changes of one or more chemical species involving local chemical reactions and diffusion simultaneously. Chemical reactions transform substances from one form to another and diffusion processes cause substances to spread throughout the spatial domain. The reaction-diffusion system consists of a set of partial differential equations (PDEs) to represent the behavior of each chemical species individually.

According to previous study (Ishtiaq Ali & Malika Tehseen Saleem, 2023), Partial differential equations (PDEs) are used for the mathematical formulation of many real-world problems in various fields of science and engineering. The most common types are hyperbolic, parabolic, and elliptic. These types of partial differential equations are used to model several physical phenomena. Many natural situations, such as biological or human, mechanical, chemical, or financial systems, can be described by systems of partial differential equations. (Raviprakash et al. (2022) stated that, the implicit finite difference method is used to solve 2D and 3D second-order partial differential equation systems.

Saylors and Trafimow (2020) also stated, along with complex facts, the ordinary differential equations formed are also increasingly complex, so that analytical solutions cannot be obtained. Therefore, many methods are formulated to obtain high accuracy approximation solutions for these differential equations or called numerical methods. The system represented by the Gray-Scott model is the autocatalytic Selkov variant of glycolysis developed by Gray and Scott. This model takes the form of the following equation: (Gray, P & Scott, S.K, 2012).

$$u_t = D_u \nabla^2{}_u - uv^2 - F(u-1),$$

$$v_t = D_u \nabla^2{}_u - (K+F)v + uv^2$$

Where U and V represent the concentrations of chemicals U and V. The rate of change of concentration with respect to time is determined by the chemical reaction rate which depends on the concentration of the other chemical and by diffusion which is modeled by the Laplacian of concentration with respect to space. Du and Dv are diffusion coefficients for concentration, F is the rate of entry, and K is a dimensionless rate constant (Olaye & Ojo, 2021).

According to Ahn et al. (2024), 3D programming is a broad field that covers a wide variety of topics, including 3D modeling, 3D animation, and 3D graphics. In the context of programming, 3D programming refers to the use of programming languages to create applications that can generate 3D graphics. Riggi et al. (2024) states that, 3D programming refers to the process of creating computer programs that can produce 3D graphics. 3D graphics are visual representations of objects and scenes created using mathematical models. These models are then rendered into images or videos that can be viewed on a computer screen.

Park et al. (2022) also stated that, 3D programming continues to evolve with the emergence of new technologies. For example, the rise of machine learning and artificial intelligence opens up new possibilities for creating realistic and interactive 3D graphics. As a result, 3D programming is likely to play an increasingly important role in our lives in the future.

METHOD

Partial Differential Equation (PDE) Method

John et al. (2019) states that, the two most commonly known types of differential equations are ordinary differential equations and partial differential equations. Ordinary differential equations consist of derivatives consisting of one variable, while partial differential equations consist of derivatives consisting of two or more independent variables. Heat, wave, and telegraph equations are some examples of cases that are usually found in the process of mathematical modeling in the form of partial differential equations (Mahmudah et al. 2024; Raya et al. 2024).

The classification of partial differential equations is also based on the same elements, namely order, linearity, and boundary conditions. The order of a partial differential equation is determined based on the order of the highest derivative in the partial differential equation. For example, the following differential equations are first, second, and third order equations:

PDE First order: $\frac{\partial c}{\partial x} - \alpha \frac{\partial c}{\partial y} = 0$

PDE Second order: $\frac{\partial^2 c}{\partial x^2} - D_e \frac{\partial c}{\partial y} = 0$

PDE Third order: $\left(\frac{\partial^3 u}{\partial x^3}\right)^2 + \frac{\partial^2 u}{\partial x \partial y} + \frac{\partial u}{\partial y} = 0$

The following partial differential equation is a form of second-order differential equation:

$$a(.)\frac{\partial^2 u}{\partial y^2} + 2b(.)\frac{\partial^2 u}{\partial x \partial y} + c(.)\frac{\partial^2 u}{\partial x^2} + d(.) = 0$$

The Finite Difference Method

According to Vargas (2022), the finite difference method is one of the basic tools for numerical solving of differential equations. In general, the process of solving this method begins by dividing the independent variables in the differential equation into count points or what is called a grid. In simple terms, this method is applied by replacing each derivative in the differential equation using a finite difference approximation formed by the Taylor series. In this method, the distance between points is defined as equal or uniform grid. The results of this approach depend on the distance between the points chosen, the smaller the distance chosen, the more accuracy is obtained. According to Ding et al. (2023), the finite difference method will be used to solve the differential equation that has been modeled by applying several predetermined boundary conditions. Because the solution of the numerical calculation results is an approximate or approximate solution, the error of the numerical calculation will be found.

Approximation of first-order differential terms with forward difference:

$$\frac{dC}{dx} \cong \frac{C_{i+1,j} - C_{i,j}}{h} \; and \; \frac{dC}{dy} \cong \frac{C_{i,j+1} - C_{i,j}}{k}$$

$$\frac{dC}{dy} \cong \frac{C_{i,j}^{m+1} - C_{i,j}^{m}}{\Delta t}$$

Approximation of 2nd order differential terms:

$$\frac{\partial^2 C}{\partial x^2} = \frac{C_{i+1,j} - 2C_{i,j} + C_{i-1,j}}{h^2} \; dan \; \frac{\partial^2 C}{\partial y^2} = \frac{C_{i,j+1} - 2C_{i,j} + C_{i,j-1}}{k^2}$$

(Oktavia, 2018)

Reaction-Diffusion System Algorithm

a. **Function Algorithm def animate(i):**
    1. Calls plt.clf() to clean up the current plot so that it does not overlap with the previous animation frame.
    2. Extracting and Reshaping Data D1 and D2 according to the grid shape.
    3. Creating Subplots for u1 and u2
        - Creating the first (ax1) and second (ax2) subplots with 3D projection.
        - Use 3-Dimensional scatter to create 3D plots of the u1 and u2 data, with flattened X and Y coordinates (flat_X and flat_Y).
        - Set the subplot title with the appropriate time (sol.t[i]), as well as labels for the X, Y, and Z axes.
    4. Save the current plot as a PNG image with a filename formatted by index i, in the output_dir directory.
    5. Returns a figure object (fig) in the form of a tuple, which is required by Matplotlib's animation functions.

b. **Function Algorithm def reaction_diffusion(t, u, D1, D2, shape):**
    1. Data Initialization and Reshaping:

- u is the combined vector of u1 and u2, which is decomposed into two separate 3-Dimensional arrays based on the shape.
- u1 is obtained from the initial part of the vector u and reshaped according to the shape.
- u2 is obtained from the end part of the vector u and reshaped according to the shape.

2. Calculating Laplacings:
   - The overlay of u1 is calculated using np.roll to sum the neighboring values in the three axes (x, y, z) and subtracted by 6 times the original value to get the overlay operator.
   - The laplation of u2 is calculated in the same way.
3. Calculating the Time Derivative:
   - du1_dt is calculated by the formula: $D1$*laplacian_u1+$u1$*(1−$u1$)−$u1$*$u2$
   - du2_dt is calculated by the formula: $D2$*laplacian_u2+$u1$*$u2$−$u2$

4. Combining and Returning Results:
   - Combines the flattened du1_dt and du2_dt into one vector.
   - Returns the merged vector as output.

c. Main Algorithm

1. Start
2. Import the required libraries
3. Define the 3-Dimensional domain by using meshgrid from NumPy to create a 3D grid of the specified points.
4. The meshgrid that has been created is then "flattened" to make data manipulation easier. This means that each x, y, and z coordinate is represented as a one-dimensional array.
5. Defined the `reaction_diffusion` function which represents the reactiondiffusion equation.
6. Defines the initial conditions `u1_0` and `u2_0` given in the form of the corresponding sine and cosine functions. These two initial conditions are then combined into one array that represents the initial conditions of the system.
7. Using `solve_ivp` from SciPy to solve partial differential equations (PDE) in the 3-dimensional domain using the `reaction_diffusion` function.
8. The numerical solution obtained is then reshaped to a suitable shape and then plotted.
9. Create animation by using `FuncAnimation` from `Matplotlib`. At each iteration, the numerical solution at a certain point in time is used to update the animation plot.
10. Display the animation that has been created
11. Finish

RESULTS AND DISCUSSION

Diffusion is the flow or movement of substance molecules from a high concentration to a low concentration. The difference in concentration that exists in two solutions is called a concentration gradient. The diffusion process involves at least two substances, one of which has a higher concentration than the other or is not in equilibrium. In diffusion, the diffusion coefficient is known. The diffusion coefficient is a parameter that expresses the magnitude of the charge carrier concentration gradient. This coefficient is not fixed like a constant in general. This happens because the value of the diffusion coefficient is influenced by particle size, membrane thickness, area, distance between two concentrations and temperature. The larger the diffusion coefficient, the faster the diffusion process will occur. The basic model used in diffusion research is usually Fick's law, but its form will vary according to the assumptions of the researcher. According to Fick's Law I, the rate of diffusion in the x-direction is proportional to the concentration gradient, while according to Fick's Law II, the change in concentration over time in a given region is proportional to the change in concentration difference at that point. Fick's Law has the advantage of clearly depicting mass transfer from higher to lower concentrations, but has the disadvantage that diffusion will stop if it is in an equilibrium state.

3-Dimensional Visualization

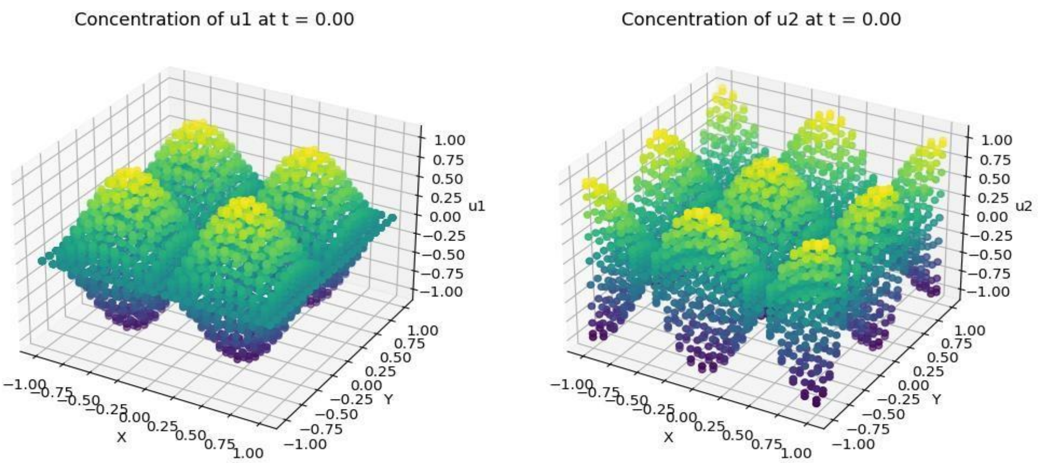

Figure 1. 3-Dimensional visualization of substance concentrations u1 and u2 at t=0.00 with python

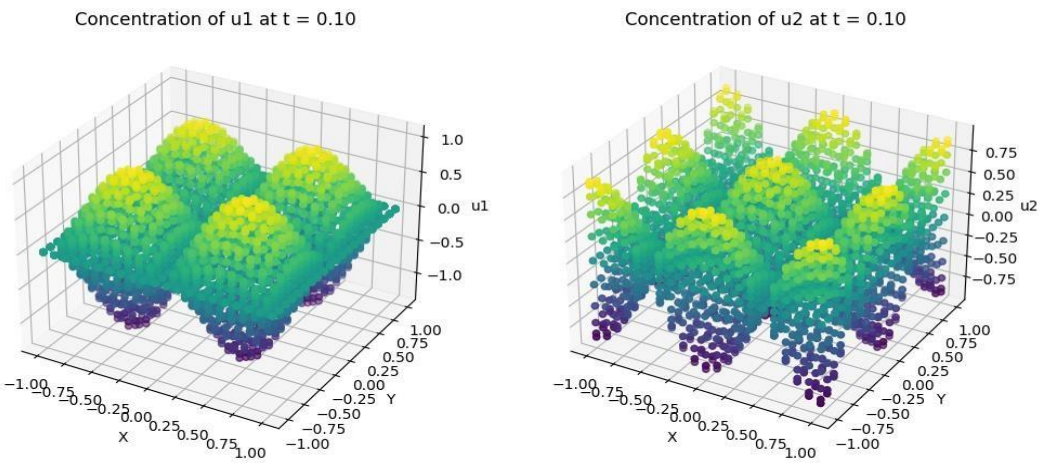

Figure 2. 3-Dimensional visualization of substance concentrations u1 and u2 at t=0.10 with python

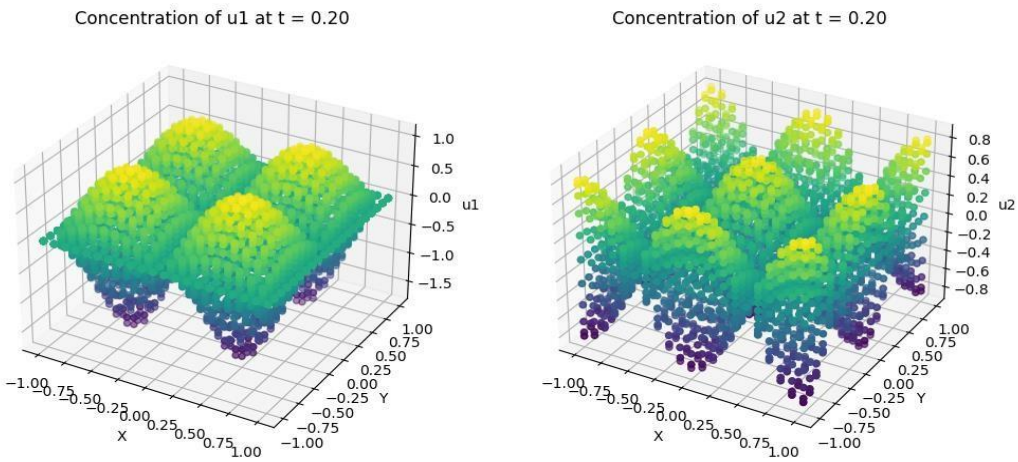

Figure 3. 3-Dimensional visualization of substance concentrations u1 and u2 at t=0.20 with python

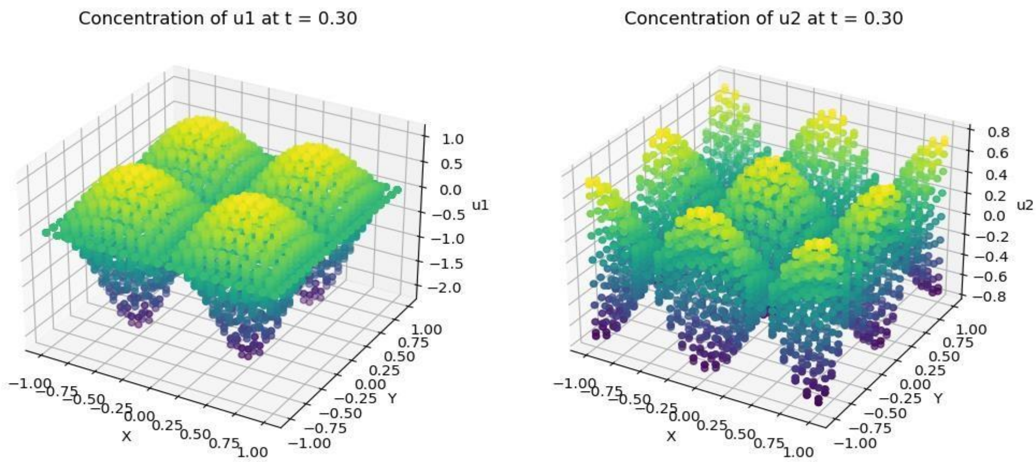

Figure 4. 3-Dimensional visualization of substance concentrations u1 and u2 at t=0.30 with python

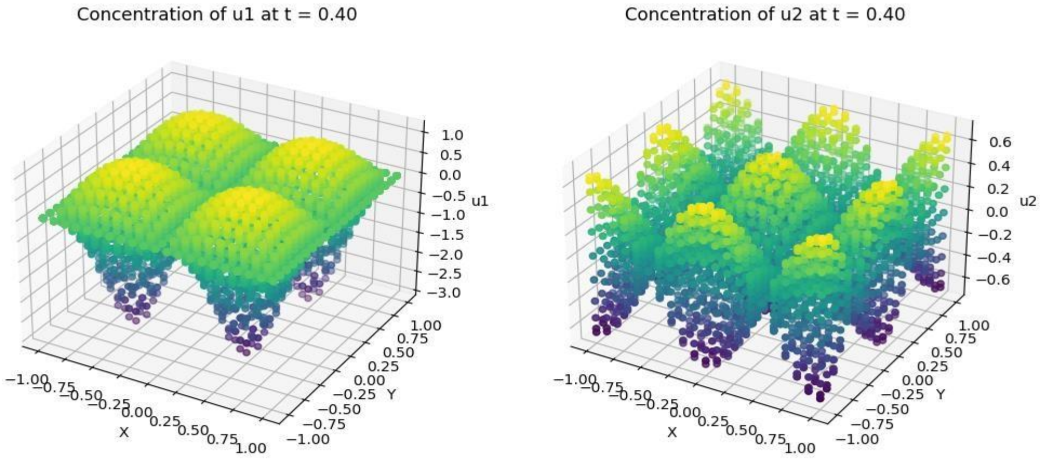

Figure 5. 3-Dimensional visualization of substance concentrations u1 and u2 at t=0.40 with python

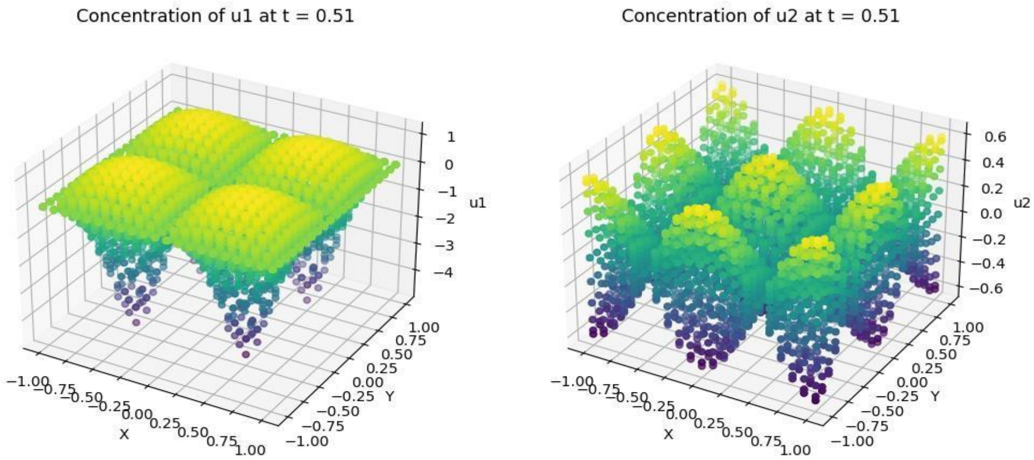

Figure 6. 3-Dimensional visualization of substance concentrations u1 and u2 at t=0.51 with python

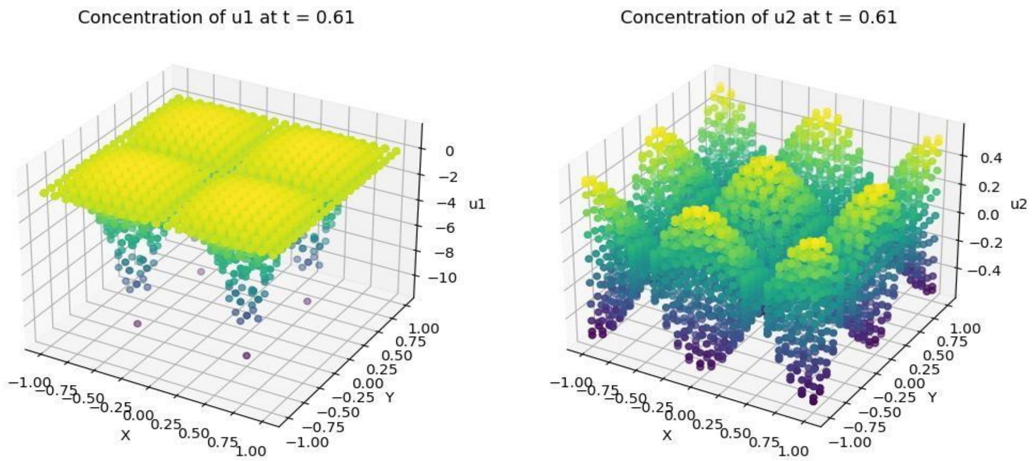

Figure 7. 3-Dimensional visualization of substance concentrations u1 and u2 at t=0.61 with python

Analysis of Results

The model used in this analysis is a three-dimensional reaction-diffusion system involving two variables u1 and u2. The system is described by a partial differential equation (PDE) that includes a laplacian component to capture the diffusion phenomenon as well as several reaction terms that describe the interaction between the two variables. The diffusion coefficients D1 and D2 were each set at 0.1. The diffusion equations for both variables include laplacian components that calculate the changes in u1 and u2 due to diffusion, while the reaction equations capture the dynamics of the interaction between u1 and u2. The initial conditions for u1 and u2 were set using sine and cosine functions to provide spatial variation in the three-dimensional domain.

We use the `solve_ivp` method of SciPy to solve these partial differential equations in the time range from 0 to 10, with 100 evaluation points. This solution gives the values of u1 and u2 at various time points in the specified spatial domain. The visualization is done in the form of a 3-Dimensional animation showing the evolution of u1 and u2 concentrations over time. In the left subplot, we see the three-dimensional distribution of u1, while in the right subplot, we see the three-dimensional distribution of u2. Both graphs show how u1 and u2 are distributed in space and how their concentrations change.

Dynamic analysis shows that initially the concentration distribution is determined by the initial conditions (sine and cosine functions). Over time, a more complex pattern emerges due to the interaction between u1 and u2 and diffusion in the domain. The laplation term indicates that both variables undergo diffusion, which tends to smooth out the concentration difference in space. Meanwhile, the reaction term introduces a new pattern that varies depending on the nature of the interaction between u1 and u2. The interaction between u1 and u2 indicates that changes in the concentration of one variable affect the other, with variations in u1 often followed by variations in u2, reflecting their complex interactions.

This animation helps us understand how two substances interacting through the process of reacidiffusion can change over time in a three-dimensional domain. The patterns and concentration distributions of u1 and u2 show the combined effects of diffusion and reaction, resulting in complex phenomena such as non-linear spatial and temporal patterns. This approach can be applied in a variety of fields, including chemistry, biology, and materials physics, where reaction and diffusion processes often occur simultaneously. Understanding the dynamics of these systems can help in designing experiments, predicting system behavior, and further developing models for more complex studies.

CONCLUSION

The conclusion of this analysis shows that a three-dimensional reaction-diffusion system with two variables, u1 and u2, describes a complex phenomenon where diffusion and reaction interactions together create dynamic patterns in the spatial domain. Initial conditions defined by sine and cosine functions evolve into more complex concentration distributions over time, influenced by diffusion processes that smooth out concentration differences and reactions that introduce new variations.

The 3-Dimensional animation provides a deep visual insight into the evolution of u1 and u2 concentrations, highlighting their interactions and changes in spatial patterns. This understanding is important in the context of various disciplines, such as chemistry, biology and materials physics, where reaction and diffusion processes occur simultaneously, and can be used to design experiments, predict system behavior and develop more complex models for follow-up studies.

Based on the analysis, it is recommended to extend the study to include variations in the diffusion coefficient and reaction parameters to better understand how changes in these parameters affect the system dynamics. Additional experiments with different initial conditions may also provide insight into the stability and sensitivity of the patterns formed.

In addition, using higher spatial and temporal resolution can improve the accuracy of the results and help in capturing more subtle phenomena. The application of more advanced numerical methods or computational parallelization can speed up the simulation and allow exploration of a larger domain. Finally, integrating real experimental data can validate these models and make them more relevant for practical applications in fields such as biology, chemistry, and materials physics.Based on the results of research and data analysis on classroom action research (CAR) which has been carried out for 3 cycles, it is seen that there is an increase in learning outcomes, teacher and student activities, the ability of teachers to manage learning, and good student responses to the application of the PBL model.

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