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Theoretical Study, Resolution, and Numerical Simulation of an Atmospheric Pollution Model: The Three-Dimensional Case

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Abstract. In this paper, a mathematical and numerical study is presented for a pollution model that describes the evolution of pollutant concentration within a cylindrical bounded domain of the atmosphere. The model represents a time-dependent problem in three-dimensional space, incorporating physical parameters relevant to atmospheric dynamics. The effectiveness of the proposed method is evaluated through analytical error estimates and numerical simulations.The results demonstrate not only the accuracy of the approximate solutions but also the stability and robustness of the method under various discretization settings.This confirms the finite element method as a reliable computational tool for modeling atmospheric pollution phenomena and sets the stage for future studies involving more intricate models or real-world environmental data.

Key Words and Phrases: partial differential equations; variational methods; atmospheric pollution; numerical methods

2010 Mathematics Subject Classifications: 35A15, 35Kxx, 65M06

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1. Introduction

Addressing atmospheric pollution has become increasingly critical in the context of global climate change and its far-reaching impacts on the environment, human health, and societal systems. Air pollution is widely recognized as a major contributor to ozone layer depletion and the rise in global temperatures, which lead to severe environmental consequences. Due to its profound impact, this topic has attracted widespread interest across various scientific disciplines, resulting in a substantial volume of research and publications.This type of pollution modeling has been extensively investigated by numerous researchers (see, for example, [4, 11, 14, 17, 18, 19, 20], reflecting its importance for both theoretical analysis

and practical environmental applications.
In this paper, we focus on the mathematical modeling and numerical simulation of atmospheric pollution in a three-dimensional bounded cylindrical domain. The following model problem, which is analyzed in this work, describes the evolution of the concentration of a pollutant in a bounded area of the atmosphere. It is given by:

$$\begin{cases} \frac{\partial u}{\partial t} + div(\alpha u) + \sigma u = \frac{\partial}{\partial x_3}(\eta \frac{\partial u}{\partial x_3}) + \mu \Delta_2 u + f, & \text{on } \Omega = [0,T] \times C, \\ u = u_S, & \text{on } S, \\ \frac{\partial u}{\partial x_3} = d \cdot\ u, & \text{if } x_3 = 0, \\ \frac{\partial u}{\partial x_3} = 0, & \text{if } x_3 = H, \\ u(r,0) = u_0 & \end{cases} \tag{1}$$

where

- $u(r,t)$ is the concentration of the pollutant at the time t and at the point $r(x_1, x_2, x_3)$;
- $u(r,0) = u_0$ is the initial condition;
- C is a cylindrical domain with lateral surface S;
- $\Delta_2 = \dfrac{\partial^2}{\partial x_1^2} + \dfrac{\partial^2}{\partial x_2^2}$ is the two-dimensional Laplace operator;
- α is the air velocity satisfying the continuity equation : div $\alpha = 0$;
- $\sigma = cte > 0$ is the specific rate of deterioration of the pollutant;
- $\mu > 0$ and $\eta > 0$ are the horizontal and vertical diffusion coefficients respectively;
- $d \geq 0$ is the sedimentation rate;
- $f(r,t)$ is the term source of pollution;

This model describes the transport and dispersion of pollutants under the influence of advection, diffusion, and, optionally, chemical reactions. To solve (1), we adopt the finite element method (FEM), [12] a well-established numerical technique based on subdomain discretization, which transforms the continuous problem into an equivalent discrete system suitable for computational analysis. The main objectives of this study are threefold: to establish a well-posed mathematical framework for the three-dimensional pollution model, to develop a reliable and efficient numerical scheme using Lagrange P1 finite elements, and to validate

the model through computational simulations implemented in MATLAB.
The paper is organized as follows. Sect. 2 presents the reformulation and variational formulation of the proposed model. This section is also dedicated to the theoretical analysis, where the existence and uniqueness of the solution are established using variational methods and appropriate functional spaces. Sect. 3 describes the numerical approximation of the model problem. Sect. 4 presents the numerical simulations, including error analysis and graphical results, to demonstrate the accuracy and effectiveness of the proposed approach.
Additionally, it should be noted that, a similar study was carried out in the authors' earlier work ([15, 21, 22]), addressing a specific case of the current problem in a two-dimensional bounded domain, using two numerical methods: the finite difference method and the finite element method.

2. Problem Modeling and Theoretical Analysis

2.1. New formulation of the problem

Now consider the new formulation of the problem (1). Let a_{ij} be positive real numbers and let $A = (a_{ij})$ be the 3×3 square matrix, with entries a_{ij}, given by:

$$A = \begin{pmatrix} \mu & 0 & 0 \\ 0 & \mu & 0 \\ 0 & 0 & \eta(x_3) \end{pmatrix}.$$

It's easy to see that:

$$\sum_{ij} \frac{\partial}{\partial x_j}\Big(a_{ij}\frac{\partial u}{\partial x_i}\Big) = \frac{\partial}{\partial x_3}\Big(\eta(x_3)\frac{\partial u}{\partial x_3}\Big) + \mu\Delta_2 u$$

We can reformulate the model problem (1) as follows:

$$\begin{cases} \frac{\partial u}{\partial t} + \sum_{i=1}^{3} \frac{\partial(\alpha_i u)}{\partial x_i} + \sigma u = \sum_{ij} \frac{\partial}{\partial x_j}(a_{ij}\frac{\partial u}{\partial x_i}) + f, & \text{on } [0,T]\times C \\ u = u_S, & \text{on } S \\ \frac{\partial u}{\partial x_3} = d \cdot u, & \text{if } x_3 = 0 \\ \frac{\partial u}{\partial x_3} = 0, & \text{if } x_3 = H \end{cases},$$

with $a_{ij} \in L^\infty(C \times [0,T])$ we have

$$\forall \xi \in R^3, \ \sum_{ij} a_{ij}\xi_i\xi_j = \mu\xi_1^2 + \mu\xi_2^2 + \eta\xi_3^2.$$

We show that these coefficients satisfy the ellipticity conditions. Knowing that the domain is bounded, we will first assume that η is also bounded, that is, $\exists m > 0$ such that $M > 0, x_3 \in [0, H], 0 < m \leq \eta(x_3) \leq M$. We trivially, show that,

- $$\forall \xi \in R^3, (A\xi, \xi) \leq \beta|\xi|^2$$
  A is uniformly bounded, for $\beta = max(\mu, M)$,
- $$\forall \xi \in R^3, (A\xi, \xi) \geq \theta|\xi|^2$$
  A is uniformly elliptic, for $\theta = min(\mu, m)$.

2.2. Variational formulation of the problem

Assume $f \in L^2(0, T; H^1(C)')$ and $u_0 \in L^2(C)$. Let $\Gamma_S = S$ and $\Gamma_B = \Gamma_0 \cup \Gamma_H$ so that $\partial C = \Gamma_S \cup \Gamma_B$. For test functions $v \in H^1(C)$, the weak form of (1) is

$$\int_C \frac{\partial u}{\partial t} v\, dr + \int_C \nabla \cdot (\alpha u)\, v\, dr + \sigma \int_C u\, v\, dr = \int_C \nabla \cdot (A \nabla u)\, v\, dr + \int_C f\, v\, dr.$$

Let $u = \overline{u} + R$, where R is a lift of the Dirichlet data on Γ_S (i.e., $R \in H^1(C)$ and $R|_{\Gamma_S} = u_S$). After integration by parts and using the boundary conditions, one obtains

$$\int_C \frac{\partial \overline{u}}{\partial t} v\, dr + \int_C (\alpha \cdot \nabla \overline{u})\, v\, dr + \sigma \int_C \overline{u}\, v\, dr + \int_C A \nabla \overline{u} \cdot \nabla v\, dr + d \int_{\Gamma_0} \eta\, \overline{u}\, v\, d\epsilon = \int_C \widetilde{f}\, v\, dr, \tag{2}$$

where $\widetilde{f}$ collects the contributions of f and the lifting R (details omitted for brevity; they follow the standard construction).

Define the bilinear form and linear functional

$$a(\overline{u}, v) := \int_C (\alpha \cdot \nabla \overline{u})\, v\, dr + \sigma \int_C \overline{u}\, v\, dr + \int_C A \nabla \overline{u} \cdot \nabla v\, dr + d \int_{\Gamma_0} \eta\, \overline{u}\, v\, d\epsilon,$$

$$L(v) := \int_C \widetilde{f}\, v\, dr.$$

Then (2) reads

$$\left\langle \frac{d\overline{u}}{dt}, v \right\rangle + a(\overline{u}, v) = L(v), \qquad \overline{u}(0) = \overline{u}_0. \tag{3}$$

Let us now introduce without proof the theorem of existence and uniqueness of the solution of the problem

Theorem 2.1. *Let* $f \in L^2(0, T, (H^2(C) \cap H^1(C))')$ *and* $u_0 \in L^2(C)$. *Assume that* α *satisfies*

$$\frac{\|\alpha\|_\infty}{2} < \delta,$$

where $\delta = \min(\min(\inf \eta, \mu), \sigma)$, *for bounded* η. *Then, there exists a unique solution* $u = u(r, t)$ *of the problem* (1) *such that:*

$$u \in L^2(0, T, H^2(C) \cap H^1(C)) \cap \mathcal{C}(0, T, L^2(C)),$$

and

$$\frac{\partial u}{\partial t} \in L^2(0, T, (H^2(C) \cap H^1(C))').$$

3. Numerical resolution of the problem

This section is devoted to the numerical approach to the model problem (1). The method employed is the P1 Lagrange finite element method ([6**? ?**]), an approximation technique based on subdomains, through which the continuous problem can be replaced by an equivalent discretized problem.

3.1. Preliminaries: Finite Element Method (Linear Lagrange Elements)

Firstly, we begin by defining the basis functions, which are the barycentric coordinates λ_i with $i = 1, .., 4$, given by:

$$\begin{cases} \widehat{\lambda_1}(\widehat{x}, \widehat{y}, \widehat{z}) = 1 - \widehat{x} - \widehat{y} - \widehat{z} \\ \widehat{\lambda_2}(\widehat{x}, \widehat{y}, \widehat{z}) = \widehat{x} \\ \widehat{\lambda_3}(\widehat{x}, \widehat{y}, \widehat{z}) = \widehat{y} \\ \widehat{\lambda_4}(\widehat{x}, \widehat{y}, \widehat{z}) = \widehat{z}. \end{cases}$$

On an arbitrary tetrahedral element T with vertices (x_i, y_i, z_i), $i = 1, ..., 4$, any quantity within the element can be expressed through the following parameterization:

$$\begin{pmatrix} x(\widehat{x}, \widehat{y}, \widehat{z}) \\ y(\widehat{x}, \widehat{y}, \widehat{z}) \\ z(\widehat{x}, \widehat{y}, \widehat{z}) \end{pmatrix} = \begin{pmatrix} \widehat{\lambda}_i(\widehat{x}, \widehat{y}, \widehat{z}) x_i \\ \widehat{\lambda}_i(\widehat{x}, \widehat{y}, \widehat{z}) y_i \\ \widehat{\lambda}_i(\widehat{x}, \widehat{y}, \widehat{z}) z_i \end{pmatrix} = \Lambda(\widehat{x}, \widehat{y}, \widehat{z}).$$

Let J_Λ be the Jacobian matrix of Λ,

$$\overline{x} = \begin{pmatrix} x_1 \\ x_2 \\ x_3 \\ x_4 \end{pmatrix}, \overline{y} = \begin{pmatrix} y_1 \\ y_2 \\ y_3 \\ y_4 \end{pmatrix}, \overline{z} = \begin{pmatrix} z_1 \\ z_2 \\ z_3 \\ z_4 \end{pmatrix},$$

$$J_\Lambda = \begin{pmatrix} {}^t\overline{x} \\ {}^t\overline{y} \\ {}^t\overline{z} \end{pmatrix} \begin{pmatrix} \frac{\partial \lambda_i}{\partial \widehat{x}} & \frac{\partial \lambda_i}{\partial \widehat{y}} & \frac{\partial \lambda_i}{\partial \widehat{z}} \end{pmatrix},$$

then we have

$$J_\Lambda = \begin{pmatrix} x_2 - x_1 & x_3 - x_1 & x_4 - x_1 \\ y_2 - y_1 & y_3 - y_1 & y_4 - y_1 \\ z_2 - z_1 & z_3 - z_1 & z_4 - z_1 \end{pmatrix} = (\theta_{i,j}).$$

For any function f, we obtain

$$\nabla_{\widehat{x},\widehat{y},\widehat{z}} f = ({}^t J_\Lambda)\, \nabla_{x,y,z} f, \qquad \nabla_{x,y,z} f = ({}^t J_\Lambda)^{-1} \nabla_{\widehat{x},\widehat{y},\widehat{z}} f,$$

or equivalently,

$$({}^t J_\Lambda)^{-1} = \frac{1}{\det J_\Lambda} ({}^t C_{i,j}) \quad \text{with} \quad C_{i,j} = (-1)^{i+j} c_{i,j} \quad \text{and} \quad \det J_\Lambda = 6V(T),$$

where $(C_{i,j})$ is the cofactor matrix. After calculations, we deduce that,

$$({}^t J_\Lambda)^{-1} = \frac{1}{6V(T)} \begin{pmatrix} \theta_{22}\theta_{33} - \theta_{32}\theta_{23} & \theta_{23}\theta_{31} - \theta_{21}\theta_{33} & \theta_{21}\theta_{32} - \theta_{22}\theta_{31} \\ \theta_{13}\theta_{32} - \theta_{12}\theta_{33} & \theta_{11}\theta_{33} - \theta_{13}\theta_{31} & \theta_{12}\theta_{31} - \theta_{11}\theta_{32} \\ \theta_{12}\theta_{23} - \theta_{13}\theta_{22} & \theta_{13}\theta_{21} - \theta_{11}\theta_{23} & \theta_{11}\theta_{22} - \theta_{12}\theta_{21} \end{pmatrix},$$

$$\nabla_{x,y,z} \widehat{x} = ({}^t J_\Lambda)^{-1} \nabla_{\widehat{x},\widehat{y},\widehat{z}} \widehat{x}.$$

Consequently, the gradients of the reference coordinates can be expressed as:

$$\nabla \widehat{x} = \frac{1}{6V(T)} \begin{pmatrix} \theta_{22}\theta_{33} - \theta_{32}\theta_{23} \\ \theta_{13}\theta_{32} - \theta_{12}\theta_{33} \\ \theta_{12}\theta_{23} - \theta_{13}\theta_{22} \end{pmatrix} = \frac{1}{6V(T)} \overrightarrow{S_1S_3} \wedge \overrightarrow{S_1S_4}, \tag{4}$$

$$\nabla \widehat{y} = \frac{1}{6V(T)} \begin{pmatrix} \theta_{23}\theta_{31} - \theta_{21}\theta_{33} \\ \theta_{11}\theta_{33} - \theta_{13}\theta_{31} \\ \theta_{13}\theta_{21} - \theta_{11}\theta_{23} \end{pmatrix} = \frac{1}{6V(T)} \overrightarrow{S_1S_4} \wedge \overrightarrow{S_1S_2}, \tag{5}$$

$$\nabla \widehat{z} = \frac{1}{6V(T)} \begin{pmatrix} \theta_{21}\theta_{32} - \theta_{22}\theta_{31} \\ \theta_{12}\theta_{31} - \theta_{11}\theta_{32} \\ \theta_{11}\theta_{22} - \theta_{12}\theta_{21} \end{pmatrix} = \frac{1}{6V(T)} \overrightarrow{S_1S_2} \wedge \overrightarrow{S_1S_3}. \tag{6}$$

Transformation F^T:
We construct an affine bijection that transforms the reference tetrahedron T_0 into another tetrahedron T in the mesh, then we get

$$F^T(S_i^{T_0}) = S_i^T, \qquad i = 1, ..., 4,$$

where $S_i^{T_0}$ are the vertices of the reference tetrahedron and $S_i^T = \begin{pmatrix} x_i \\ y_i \\ z_i \end{pmatrix}$ are the corresponding vertices of the tetrahedron T. Since F^T is an affine mapping from $\mathbb{R}^3 \to \mathbb{R}^3$, it can be written in the form:

$$F^T(\widehat{x}, \widehat{y}, \widehat{z}) = (\alpha_1 + \beta_1\widehat{x} + \gamma_1\widehat{y} + \kappa_1\widehat{z}, \alpha_2 + \beta_2\widehat{x} + \gamma_2\widehat{y} + \kappa_2\widehat{z}, \alpha_3 + \beta_3\widehat{x} + \gamma_3\widehat{y} + \kappa_3\widehat{z}),$$

$$\begin{cases} F^T(0,0,0) = (x_1, y_1, z_1) \\ F^T(1,0,0) = (x_2, y_2, z_2) \\ F^T(0,1,0) = (x_3, y_3, z_3) \\ F^T(0,0,1) = (x_4, y_4, z_4) \end{cases},$$

which allows us to deduce the following relation:

$$F^T(\widehat{x}, \widehat{y}, \widehat{z}) = \begin{pmatrix} x_2 - x_1 & x_3 - x_1 & x_4 - x_1 \\ y_2 - y_1 & y_3 - y_1 & y_4 - y_1 \\ z_2 - z_1 & z_3 - z_1 & z_4 - z_1 \end{pmatrix} \cdot \begin{pmatrix} \widehat{x} \\ \widehat{y} \\ \widehat{z} \end{pmatrix} + \begin{pmatrix} x_1 \\ y_1 \\ z_1 \end{pmatrix},$$

hence

$$F^T(\widehat{x}, \widehat{y}, \widehat{z}) = J_\Lambda \begin{pmatrix} \widehat{x} \\ \widehat{y} \\ \widehat{z} \end{pmatrix} + \begin{pmatrix} x_1 \\ y_1 \\ z_1 \end{pmatrix}. \tag{7}$$

Since two finite elements are affine equivalents and the basis functions are affine, it follows that:

$$\lambda_i^T = \widehat{\lambda}_i \circ (F^T)^{-1} \Leftrightarrow \widehat{\lambda}_i = \lambda_i^T \circ F^T,$$

and therefore,

$$\lambda_i^T(x, y, z) = \widehat{\lambda}_i(\widehat{x}, \widehat{y}, \widehat{z}).$$

From (7) we also obtain:

$$(F^T)^{-1}(x, y, z) = (J_\Lambda)^{-1} \begin{pmatrix} x \\ y \\ z \end{pmatrix} - (J_\Lambda)^{-1} \begin{pmatrix} x_1 \\ y_1 \\ z_1 \end{pmatrix}.$$

3.2. Spatial semi-discretization of the problem

We now present the spatial semi-discretization of problem (1). In this approach, the spatial domain is discretized using finite elements, while time remains continuous. On the space $L^2\Big(0,T,H^2(C)\Big)\cap C\Big(0,T,L^2(C))\Big)$, consider the subspace $V_h \subset V$ with $\dim V_h = N_h$. Let $u = u_h + u_S$ and $u_h = \sum u_i\phi_i$, $u_S = \sum u_S^i\phi_i$, and let $v_i = \phi_j$ be the test functions. Then, the variational formulation of our problem gives:

$$\begin{aligned}
&\sum_{i\in I} u_i'(t)\int \phi_i\phi_j dr + \sum_{i\in I}\Big(\alpha\int \nabla\phi_i\phi_j dr + \sigma\int \phi_i\phi_j dr + \\
&+ \textstyle\int A\nabla\phi_i\nabla\phi_j dr\Big)u_i(t) + \sum_{i\in K} d\eta_0\Big(\int \phi_i\phi_j d\epsilon\Big)u_i(t) = \\
&= \sum_{i\in I}\int f_i\phi_j dr - \Big[\sum_{i\in J}\Big(\alpha\int \nabla\phi_i\phi_j dr + \sigma\int \phi_i\phi_j dr + \\
&- \textstyle\int A\nabla\phi_i\nabla\phi_j dr\Big) + \sum_{i\in J\cap K} d\eta_0\Big(\int \phi_i\phi_j d\epsilon\Big)\Big]u_S^i
\end{aligned}, \tag{8}$$

where I is the set of indices of the nodes of the mesh, J the set of indices of the nodes belonging to Γ_S and K the set of indices of the nodes belonging to Γ_0. We then obtain the following system:

$$\begin{cases} Mu'(t) + Ru(t) + Du(t) = B(t) \\ u(0) = u_0 \end{cases}, \tag{9}$$

with $M_{ij} = \displaystyle\int_C \phi_i\phi_j dr$, $R_{ij} = \displaystyle\int_C \alpha\nabla\phi_i\phi_j dr + \sigma M_{ij} + \int_C (A\nabla\phi_i)\nabla\phi_j dr$, $D_{ij} = d\eta_0 \displaystyle\int_{\Gamma_0} \phi_i\phi_j d\epsilon$,

$B_i = \displaystyle\int_C f\phi_j dr - \sum_{i\in J} R_{ij}u_S^i - d\eta_0 \sum_{i\in J\cap K} M_{ij}u_S^i$ and $\eta_0 = \eta(0)$.

3.3. Application of the Semi-Discrete Model

In this part, we apply the semi-discrete model based on formulation (8) to the problem (1) and denote $\phi_i^T = \lambda_i^T = \lambda_i$. Then we obtain:

$$M_{ij}^T = \int_T \lambda_i\lambda_j dr,$$

$$R_{ij}^T = N_{ij}^T + \sigma M_{ij}^T + A_{i,j}^T,$$

$$D_{ij}^T = d\eta_0 \int_{\Gamma_0} \lambda_i\lambda_j d\epsilon,$$

$$\text{with} \quad N_{ij}^T = \int_T \alpha \nabla\lambda_i \lambda_j dr \quad \text{and } A_{ij}^T = \int_T (A\nabla\lambda_i)\nabla\lambda_j dr,$$

$$B_i^T = \int_T f\lambda_j dr - \sum_{i\in J} \Big(\alpha \int \nabla\lambda_i\lambda_j dr + \sigma \int \lambda_i\lambda_j dr + \int A\nabla\lambda_i\nabla\lambda_j dr\Big) u_S^i -$$

$$-d\eta_0 \sum_{i\in J\cap K} \Big(\int_T \lambda_i\lambda_j dr\Big) u_S^i,$$

$$\Leftrightarrow B_i^T = \int_T f\lambda_j dr - \sum_{i\in J} R_{ij}^T u_S^i - d\eta_0 \sum_{i\in J\cap K} M_{ij} u_S^i.$$

Recall the exact integration formula we get the following relation:

$$\int_T (\lambda_1^T)^{\alpha_1} ... (\lambda_{n+1}^T)^{\alpha_{n+1}} dr = n! V(T) \frac{\alpha_1! ... \alpha_{n+1}!}{(n + \alpha_1 + ... + +\alpha_{n+1})!}.$$

Now compute the previously defined matrices:

- The mass matrix (M_{ij}^T);

$$\int_T \lambda_i^2 dr = \frac{V}{10} \quad \text{and} \quad \int_T \lambda_i\lambda_j dr = \frac{V}{20}, \ \text{(with V(T)=V)},$$

  then we deduce:

$$M_{ij}^T = \frac{V}{20} \begin{pmatrix} 2 & 1 & 1 & 1 \\ 1 & 2 & 1 & 1 \\ 1 & 1 & 2 & 1 \\ 1 & 1 & 1 & 2 \end{pmatrix},$$

- Calculation of the elements of A_{ij}^T:

$$A\nabla\lambda_i = \begin{pmatrix} \mu & 0 & 0 \\ 0 & \mu & 0 \\ 0 & 0 & \eta \end{pmatrix} \cdot \begin{pmatrix} \frac{\partial\lambda_i}{\partial x} \\ \frac{\partial\lambda_i}{\partial y} \\ \frac{\partial\lambda_i}{\partial z} \end{pmatrix} = \begin{pmatrix} \mu\frac{\partial\widehat{\lambda}_i}{\partial x} \\ \mu\frac{\partial\widehat{\lambda}_i}{\partial y} \\ \eta\frac{\partial\widehat{\lambda}_i}{\partial z} \end{pmatrix} = \begin{pmatrix} \mu\frac{\partial\widehat{\lambda}_i}{\partial\widehat{x}}\frac{\partial\widehat{x}}{\partial x} + \mu\frac{\partial\widehat{\lambda}_i}{\partial\widehat{y}}\frac{\partial\widehat{y}}{\partial x} + \mu\frac{\partial\widehat{\lambda}_i}{\partial\widehat{z}}\frac{\partial\widehat{z}}{\partial x} \\ \mu\frac{\partial\widehat{\lambda}_i}{\partial\widehat{x}}\frac{\partial\widehat{x}}{\partial y} + \mu\frac{\partial\widehat{\lambda}_i}{\partial\widehat{y}}\frac{\partial\widehat{y}}{\partial y} + \mu\frac{\partial\widehat{\lambda}_i}{\partial\widehat{z}}\frac{\partial\widehat{z}}{\partial y} \\ \mu\frac{\partial\widehat{\lambda}_i}{\partial\widehat{x}}\frac{\partial\widehat{x}}{\partial z} + \mu\frac{\partial\widehat{\lambda}_i}{\partial\widehat{y}}\frac{\partial\widehat{y}}{\partial z} + \mu\frac{\partial\widehat{\lambda}_i}{\partial\widehat{z}}\frac{\partial\widehat{z}}{\partial z} \end{pmatrix} =$$

$$= \mu\frac{\partial\widehat{\lambda}_i}{\partial\widehat{x}}\nabla\widehat{x} + \mu\frac{\partial\widehat{\lambda}_i}{\partial\widehat{y}}\nabla\widehat{y} + \eta\frac{\partial\widehat{\lambda}_i}{\partial\widehat{z}}\nabla\widehat{z},$$

  equivalently, we get

$$A\nabla\lambda_i\nabla_j = \Big(\mu\frac{\partial\widehat{\lambda}_i}{\partial\widehat{x}}\nabla\widehat{x} + \mu\frac{\partial\widehat{\lambda}_i}{\partial\widehat{y}}\nabla\widehat{y} + \eta\frac{\partial\widehat{\lambda}_i}{\partial\widehat{z}}\nabla\widehat{z}\Big)\Big(\frac{\partial\lambda_i}{\partial\widehat{x}}\nabla\widehat{x} + \frac{\partial\widehat{\lambda}_i}{\partial\widehat{y}}\nabla\widehat{y} + \frac{\partial\widehat{\lambda}_i}{\partial\widehat{z}}\nabla\widehat{z}\Big).$$

Therefore,

$$A\nabla\lambda_i\nabla\lambda_j = \mu\frac{\partial\widehat{\lambda}_i}{\partial\widehat{x}}\frac{\partial\widehat{\lambda}_j}{\partial\widehat{x}}|\nabla\widehat{x}|^2 + \mu\frac{\partial\widehat{\lambda}_i}{\partial\widehat{y}}\frac{\partial\widehat{\lambda}_j}{\partial\widehat{y}}|\nabla\widehat{y}|^2 + \eta\frac{\partial\widehat{\lambda}_i}{\partial\widehat{z}}\frac{\partial\widehat{\lambda}_j}{\partial\widehat{z}}|\nabla\widehat{z}|^2 +$$
$$\mu\Big(\tfrac{\partial\widehat{\lambda}_i}{\partial\widehat{x}}\tfrac{\partial\widehat{\lambda}_j}{\partial\widehat{y}} + \tfrac{\partial\widehat{\lambda}_i}{\partial\widehat{y}}\tfrac{\partial\widehat{\lambda}_j}{\partial\widehat{x}}\Big)\nabla\widehat{x}\nabla\widehat{y} +$$
$$+\Big(\mu\frac{\partial\widehat{\lambda}_i}{\partial\widehat{x}}\frac{\partial\widehat{\lambda}_j}{\partial\widehat{z}} + \eta\frac{\partial\widehat{\lambda}_i}{\partial\widehat{z}}\frac{\partial\widehat{\lambda}_j}{\partial\widehat{x}}\Big)\nabla\widehat{x}\nabla\widehat{z} + \Big(\mu\frac{\partial\widehat{\lambda}_i}{\partial\widehat{y}}\frac{\partial\widehat{\lambda}_j}{\partial\widehat{z}} + \eta\frac{\partial\widehat{\lambda}_i}{\partial\widehat{z}}\frac{\partial\widehat{\lambda}_j}{\partial\widehat{y}}\Big)\nabla\widehat{y}\nabla\widehat{z}.$$

Using the relations (4), (5) and (6), we obtain:

$$36V^2A\nabla\widehat{\lambda}_i\nabla_j = \mu\frac{\partial\widehat{\lambda}_i}{\partial\widehat{x}}\frac{\partial\widehat{\lambda}_j}{\partial\widehat{x}}|\overrightarrow{S_1S_3}\wedge\overrightarrow{S_1S_4}|^2 +$$
$$\mu\tfrac{\partial\widehat{\lambda}_i}{\partial\widehat{y}}\tfrac{\partial\widehat{\lambda}_j}{\partial\widehat{y}}|\overrightarrow{S_1S_4}\wedge\overrightarrow{S_1S_2}|^2 + \eta\tfrac{\partial\widehat{\lambda}_i}{\partial\widehat{z}}\tfrac{\partial\widehat{\lambda}_j}{\partial\widehat{z}}|\overrightarrow{S_1S_2}\wedge\overrightarrow{S_1S_3}|^2 +$$
$$+$$
$$\mu\Big(\tfrac{\partial\widehat{\lambda}_i}{\partial\widehat{x}}\tfrac{\partial\widehat{\lambda}_j}{\partial\widehat{y}} + \tfrac{\partial\widehat{\lambda}_i}{\partial\widehat{y}}\tfrac{\partial\widehat{\lambda}_j}{\partial\widehat{x}}\Big)(\overrightarrow{S_1S_3}\wedge\overrightarrow{S_1S_4})(\overrightarrow{S_1S_4}\wedge\overrightarrow{S_1S_2}) +$$
$$\Big(\mu\tfrac{\partial\widehat{\lambda}_i}{\partial\widehat{x}}\tfrac{\partial\widehat{\lambda}_j}{\partial\widehat{z}} + \eta\tfrac{\partial\widehat{\lambda}_i}{\partial\widehat{z}}\tfrac{\partial\widehat{\lambda}_j}{\partial\widehat{x}}\Big)(\overrightarrow{S_1S_3}\wedge\overrightarrow{S_1S_4})(\overrightarrow{S_1S_2}\wedge\overrightarrow{S_1S_3}) +$$
$$+\Big(\mu\frac{\partial\widehat{\lambda}_i}{\partial\widehat{y}}\frac{\partial\widehat{\lambda}_j}{\partial\widehat{z}} + \eta\frac{\partial\widehat{\lambda}_i}{\partial\widehat{z}}\frac{\partial\widehat{\lambda}_j}{\partial\widehat{y}}\Big)(\overrightarrow{S_1S_4}\wedge\overrightarrow{S_1S_2})(\overrightarrow{S_1S_2}\wedge\overrightarrow{S_1S_3}).$$

This enables us to compute the entries of the matrix $A(i,j)$. For example:

$$A_{11}^T = \frac{1}{36V^2}\Big[\mu|\overrightarrow{S_2S_3}\wedge\overrightarrow{S_1S_4}|^2 + \eta|\overrightarrow{S_1S_2}\wedge\overrightarrow{S_1S_3}|^2 + (\mu+\eta)(\overrightarrow{S_2S_3}\wedge\overrightarrow{S_1S_4})(\overrightarrow{S_1S_2}\wedge\overrightarrow{S_1S_3})\Big]$$

All rest entries can be found analogously

- Determination of $N_{i,j}^T$;

$$N_{i,j}^T = \int_T \alpha\nabla\lambda_i\lambda_j dr,$$

we get

$$\alpha\nabla\lambda_i = \alpha\cdot\Big(\frac{\partial\widehat{\lambda}_i}{\partial\widehat{x}}\nabla\widehat{x} + \frac{\partial\widehat{\lambda}_i}{\partial\widehat{y}}\nabla\widehat{y} + \frac{\partial\widehat{\lambda}_i}{\partial\widehat{z}}\nabla\widehat{z}\Big) = \tau_i,$$

$$\int_T \alpha\nabla\lambda_i\cdot\lambda_j dr = \tau_i\int_T\widehat{\lambda}_j dr = \tau_i\frac{V}{4}.$$

Now calculate the elements τ_i in the preceding formulas. Let $x_{ij} = x_i - x_j$, $y_{ij} = y_i - y_j$ and $z_{ij} = z_i - z_j$. Then, it follows that:

$$\begin{aligned}\tau_1 = -\frac{1}{6V}\Big[&\alpha_1\big(z_4y_{32} + z_3y_{21} + z_2y_{43}\big)\\ &- \alpha_2\big(z_4x_{32} + z_3x_{24} + z_2x_{43}\big)\\ &+ \alpha_3\big(y_4x_{32} + y_3x_{24} + y_2x_{43}\big)\Big].\end{aligned} \tag{10}$$

$$\tau_2 = \frac{1}{6V}\Big[\alpha_1(y_{31}z_{41} - z_{31}y_{41}) + \alpha_2(x_{31}z_{41} - z_{31}x_{41}) + \alpha_3(x_{31}y_{41} - y_{31}x_{41})\Big],$$

$$\tau_3 = \frac{1}{6V}\Big[\alpha_1(y_{41}z_{21} - z_{41}y_{21}) + \alpha_2(z_{41}x_{21} - x_{41}z_{21}) + \alpha_3(x_{41}y_{21} - y_{41}x_{21})\Big],$$

$$\tau_4 = \frac{1}{6V}\Big[\alpha_1(y_{21}z_{31} - z_{21}y_{31}) + \alpha_2(z_{21}x_{31} - x_{21}z_{31}) + \alpha_3(x_{21}y_{31} - y_{21}x_{31})\Big].$$

As a result, the matrix (N_{ij}^T) takes the following form:

$$(N_{ij}^T) = \frac{V}{4}\begin{pmatrix} \tau_1 & \tau_1 & \tau_1 & \tau_1 \\ \tau_2 & \tau_2 & \tau_2 & \tau_2 \\ \tau_3 & \tau_3 & \tau_3 & \tau_3 \\ \tau_4 & \tau_4 & \tau_4 & \tau_4 \end{pmatrix}.$$

Note that terms (B_i^T), and $(D_{i,j}^T)$ also can be determined effectivly.

3.4. Full Discretization: Time and Space Integration

In the full discretization of time and space for our problem (1), using the system (9), and letting $S = R + D$, we obtain:

$$\begin{cases} Mu'(t) + Su(t) = B(t) \\ u(0) = u_0 \end{cases}.$$

To derive a fully discrete formulation, we employ a time-implicit finite difference scheme, which ensures numerical stability even for relatively large time steps. Applying this scheme to the above system, we obtain:

$$M\frac{U^{n+1} - U^n}{\Delta t} + SU^{n+1} = B(t),$$

hence,

$$\Big(M + \Delta t S\Big)U^{n+1} = MU^n + \Delta t B.$$

4. Numerical simulations

Since the source term is not explicitly given, we will assume that the source of pollution does not have a fixed position in the domain. Therefore, for the rest of this document, we will use a synthetic solution (analytical solution) that will allow us to generate the source term, the boundary conditions and the initial condition, while taking care to respect the rules of regularity and the working space established during the mathematical analysis of the problem. Using the method

of separation of variables, we determine the eigenmodes of diffusion ([10]).The simulations were implemented in MATLAB to perform finite element simulations, implementing the spatial discretization of the domain and the temporal integration of the systeThe simulations were implemented in MATLAB to perform finite element simulations, implementing the spatial discretization of the domain and the temporal integration of the systemm.
In a particular case, the synthetic solution we will use, which satisfies the boundary conditions, is given by:

$$u(t,x,y,z) = \sin\left(\frac{\pi x}{2H}\right)\sin\left(\frac{\pi y}{2H}\right)\sin\left(\frac{\pi(z+3-H)}{2H}\right)e^{-\frac{3(\mu+\eta_0+\sigma)\pi^2 t}{4H^2}},$$

$$\begin{aligned}
&\frac{\partial u}{\partial z} = \frac{\pi}{2}\cot\left(\frac{\pi}{2}(-H+3)\right)\cdot u = d\cdot u, && \text{if } z=0,\\
&\frac{\partial u}{\partial z} = 0, && \text{if } z=H,\\
&u(0,x,y,z) = u_0.
\end{aligned}$$

4.1. Error Analysis and Convergence Study

This section presents quantitative error evaluations and convergence analysis.Tabulated results demonstrate how the numerical solution behaves with mesh refinement and time step variation, verifying the expected order of accuracy. The observed trends highlight the consistent performance of the proposed method across varying discretization levels. These results underscore the robustness and accuracy of the numerical approach for practical applications.
In each of the following cases, with parameters $\alpha_1 = 2$, $\alpha_2 = 1$, $\alpha_3 = 1$, $\mu = 3$, $\sigma = 3$, and $\eta = -\max_{M_i \in T_k} z_i + H$, the error estimation table summarizes the differences between the approximate solution and the synthetic solution, measured in the infinity norm, L^2 and H^1 norm.
If the following tables are analyzed separately and in detail, it can be observed that:

- **Table 1** reports the L_2, L_∞, and H^1 error norms for a coarse mesh of 64 points, providing a baseline for assessing the accuracy of the method. The results indicate that even at this coarse resolution, the numerical solution closely approximates the exact solution, demonstrating the method's reliability.

- **Table 2** shows the corresponding estimates for a mesh of 189 points, demonstrating a noticeable reduction in errors with mesh refinement. This confirms that increasing the number of points improves the accuracy of the numerical solution, highlighting the convergence of the method.

- **Table 3** presents the error norms for a mesh of 315 points, further illustrating the convergence behavior of the method as the discretization becomes finer. The results clearly show a continued decrease in all error norms, confirming the method's robustness and consistency with theoretical expectations.

- **Table 4** summarizes the results for a highly refined mesh of 625 points, confirming the accuracy of the method, stability, and convergence trends. The error norms reach their minimal values at this level of refinement, demonstrating the effectiveness and reliability of the numerical scheme for practical computations.

N	20	70	120	170	220	270	320	370
$L^2\mathbf{E}$	6.0196e-14	2.7993e-14	2.4353e-14	2.2971e-14	2.2244e-14	2.1796e-14	2.1492e-14	2.1273e-14
$L^\infty\mathbf{E}$	6.0706e-06	4.0474e-06	3.7622e-06	3.6488e-06	3.5880e-06	3.5500e-06	3.5241e-06	3.5053e-06
$H^1\mathbf{E}$	3.0451e-05	2.0312e-05	1.8883e-05	1.8315e-05	1.8010e-05	1.7820e-05	1.7690e-05	1.7595e-05

Table 1: Table of error estimates for 64 points

N	20	70	120	170	220	270	320	370
$L^2\mathbf{E}$	1.2692e-12	5.6330e-13	5.2141e-13	4.8683e-13	4.4289e-13	4.3359e-13	4.2730e-13	4.2276e-13
$L^\infty\mathbf{E}$	1.2053e-05	1.0168e-05	8.4365e-06	7.9030e-06	7.5739e-06	7.5018e-06	7.4525e-06	7.4166e-06
$H^1\mathbf{E}$	6.7869e-05	4.4545e-05	4.1299e-05	3.9322e-05	3.8892e-05	3.8598e-05	3.8385e-05	3.8223e-05

Table 2: Table of error estimates for 189 points

N	20	70	120	170	220	270	320	370
$L^2\mathbf{E}$	9.4542e-12	5.4646e-12	4.9640e-12	4.7694e-12	4.6660e-12	4.6019e-12	4.5583e-12	4.5267e-12
$L^\infty\mathbf{E}$	3.3858e-05	2.7846e-05	2.6876e-05	2.6481e-05	2.6265e-05	2.6130e-05	2.6037e-05	2.5970e-05
$H^1\mathbf{E}$	1.4829e-04	1.1044e-04	1.0490e-04	1.0268e-04	1.0148e-04	1.0073e-04	1.0022e-04	9.9847e-05

Table 3: Table of error estimates for 315 points

The error behavior is analyzed in the above tables from two perspectives: varying the time step and varying the number of points:

- When these tables are read horizontally, i.e., by fixing the number of points and varying the time step, it can be observed that as the time step increases,

N	20	70	120	170	220	270	320	370
$L^2\mathbf{E}$	2.0912e-10	1.6509 e-10	1.5853e-10	1.5589e-10	1.5446e-10	1.5357e-10	1.5295e-10	1.5251e-10
$L^\infty\mathbf{E}$	1.0843e-04	1.0292 e-04	1.0193e-04	1.0152e-04	1.0129e-04	1.0115e-04	1.0105e-04	1.0098e-04
$H^1\mathbf{E}$	5.9528e-04	5.2721 e-04	5.1635e-04	5.1192e-04	5.0951e-04	5.0800e-04	5.0696e-04	5.0620e-04

Table 4: Table of error estimates for 625 points

the errors decrease progressively. The values remain very small, whether in the L^2 norm, the L^∞ norm, or the H^1 norm, indicating the high accuracy of the method across different time steps.

- Conversely, when the tables are read vertically, i.e., by fixing the time step and increasing the number of points, we notice a slight increase in the L^2 errors. This is due to the larger number of points, which introduces additional computational approximations when evaluating the solution at each point. However, this increase becomes negligible for meshes with 189 points or more. A similar behavior is observed for the L^∞ and H^1 error norms.

- Additionally, comparing the horizontal and vertical trends highlights the method's stability: while increasing the time step reduces errors and the method maintains consistent convergence and accuracy.

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