

Modeling Convection-Diffusion
Utilizing the Finite Element Method and
Partial Differential Equation Solver FreeFEM++

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1 Abstract

This project is an introduction to solving the convection-diffusion equation by utilizing the Finite Element Method (FEM) and the partial differential equation solving software FreeFem++. Applications of the convection-diffusion model to simulating airborne and water-borne pollutant dispersal are the subject of ongoing research and are prevalent in the supporting literature. Pollutant dispersion models help environmental authorities properly employ regulations to stave off potential disasters, and provide real-time decision support when severe environmental impacts occur. This project examines the derivation of the convection-diffusion equation's weak formulation and incorporates the basics of the finite element method. This includes defining the spatial domain's mesh, defining the FEM space, and providing both the semi and fully discretized equations respectively. FreeFem++ is thereby utilized to numerically solve the convection-diffusion equation via its weak formulation and visually outputs the resulting dispersion behaviors of particle concentrations through processes of pure diffusion and low/moderate convection-diffusion.

2 Introduction

The convection-diffusion equation describes the physical processes of particle dispersion and is well known for its applications involving atmospheric, oceanic, and watershed/river system pollution modeling. There are multiple techniques used to obtain high-resolution solutions to these particular type of partial differential equation models including the finite difference, finite volume, and finite element methods. The finite element method is a relatively newer methodology in comparison to its counterparts, but it is often preferred for modeling more realistic pollution impact scenarios due to its ability to handle non-geometric, unstructured, and adaptive meshes. The adaptive techniques of the finite element method are often utilized in real-world applications because they often provide high resolution solutions while maintaining or lowering computational time/cost.

2.1 Problem Statement

This research will primarily focus on the basic convection-diffusion equation and its application to atmospheric pollution through the utilization of the finite element method (FEM) and the partial differential equation solving software FreeFEM++. The objective being to create a time-dependent model of the convection-diffusion equation with a concentration of pollutant specie (in the form of smoke) emitting from a singular source from which the pollutant is thereby dispersed within a finite space through the natural process of low/moderate convection-diffusion over a short duration.

2.2 Literature Review

Literature surrounding the topic of convection-diffusion based pollution models consists of increasingly complicated variations of partial differential equations characterizing specific attributes of mass transportation models that more realistically predict the physical process of pollution dispersion. In order to better grasp a more comprehensive understanding of the background information surrounding the applications of modeling the convection-diffusion equation to pollution modeling, parabolic equations such as the diffusion, convection-diffusion, and heat equations as presented in [Myint-U], [Betounes], and [Burnett] should be studied extensively. In addition, in [Johnson] and [Schwarz] by Johnson and Schwarz, the basic components of the finite element method including the construction of the mesh, finite element space, and the subdivision (partitioning/triangulation) of the domain can be quickly referenced.

Moreover, to use the variational formulation in conjunction with high-level programming languages, the derivation of said weak formulation should be examined in full detail to gain insight into the mathematical foundations of FEM. Photochemical models are considerably more involved than the basic convection-diffusion model and their concentration gradients take into account the chemical properties of particular pollutant species of interest as in [Kach], [Mont], [Pochai] and [Sanin]. However, many such as Pai [Pai] chose to simplify their model with the assumption of passive (non-reactive) contaminants, exemplifying the classic dispersion model. Ferragut [Ferragut] whom like Pai chose to assume non-reactivity, insisted that although he negates the chemical properties of reactive agents, models with these included chemical properties could promptly be generalized regardless.

The equations for vorticity and the stream-function present in Pochai's article [Pochai] create the basis for a mass transportation model that more accurately depicts the physical process of smoke plume distribution/dissipation in the (lower atmosphere) Troposphere and the application of wind fields are indispensable for accurately simulating the atmospheric turbulence characteristically dominating the convection-based transport of air pollutants. Realistic data for wind fields are crucial for achieving the level of accuracy required to lend

real-time decision making support to environmental regulators/authorities and this data is collected in a multitude of ways. For more information pertaining to the wind field approach refer to [Sanin]. Some of the ways in which naturalistic data is obtained include research from wind tunnel experiments and/or observational data obtained from multi-locational meteorological sites as in [Pai] where Pai confirms the occurrence of what is known as plume lift off, which transpires when emission sources are oriented closer to the ground.

The Eulerian model employed in [Ferragut] utilizes meteorological wind fields rather than simulating the trajectory of individual particles to describe convection-diffusion. However, the limitations of Eulerian models are acknowledged due to there problems with resolving steep gradients over fixed meshes. Deterministic models, namely of the Eulerian, Gaussian, and Lagrangian type can be used in concurrence with one another, for example, the Eulerian model presented in [Ferragut] applies a Gaussian model to empirically determine the spatial distribution of pollutants through finding the coefficient matrix values of turbulent diffusion.

Furthermore, the utilization of splitting techniques found in [Ferragut], [Mont], and [Pai] vary in their specific uses. For instance, the article by Monforte uses splitting techniques to separate the processes by which the pollutants are transported from the reactivity of the pollutant species of interest in order compartmentalize the problem, whereas it is also observed in [Ferragut] being used to split the transport equation into horizontal and vertical directions with the vertical direction treated with the finite difference method and the horizontal with adaptive finite element, the ultimate goal being to create simpler systems from those that are more complicated and handle the variable time as an ordinary differential equation.

Mesh adaptivity is essential to the process of applying finite difference, finite volume, and finite element methods to modeling air pollution while meeting constraints particular to the specific conditions of the problem. Conditions vary in Although, Sanin and Montero [Sanin] utilize the finite difference method due to its suitability for cubes, they recognize that (FEM) is essential for meshes that are unstructured or require mesh adaptivity. Adaptivity is essential to the process of applying these methods to air pollution modeling while meeting constraints particular to the specific problems. Adaptive methods reveal features

that can remain undetected with the use of coarse meshes, and they are computationally less intensive than applying a fine mesh over the entire domain. These adaptive techniques allow for finer meshes to be used in conjunction with the coarse mesh and when the coarse mesh and fine mesh overlap the coarse mesh is replaced by the finer one in order to obtain a higher resolution solution while maintaining relative computational cost. The r-adaptive and h-adaptive methods are well known adaptive techniques and are presented in Monforte's article [Mont]. The r-adaptive method changes the position of the nodal points that create the basis for the mesh, whereas the h-adaptive method introduces new nodes where the error is found to be higher than a given tolerance. The introduction of new nodal points in these areas reduce the error, providing a higher resolution solution but at increased computational time/cost.

(Fill out literature review with more references and background)

2.3 Relevance

Mankind's ability to model, predict and understand changes in our environment is essential to the continuation and well-being of our respective societies. The applications of pollution modeling are far-reaching, from modeling pollution concentrations in various river systems and identifying their significant sources as in [Kach], [Klaychang], and [Meyer], to modeling air quality and the atmospheric transport of pollutants from emission sources such as for example the industrial smokestacks illustrated in [Pochai]. Organizations such as the Environmental Protection Agency (EPA) use variations of the convection-diffusion model to help predict the environmental impact of industrial emissions to pollution sensitive regions such as national and state parks. These pollutant dispersion models help environmental authorities employ regulations to stave off potential disasters, and provide real-time decision support when severe environmental impacts occur. Many scholarly articles contain applications of the finite element method to solving complicated pollution dispersion models and may be researched in order to gain a more robust comprehension of how to accurately illustrate the physical processes/phenomena that dominate the convection-diffusion equation, as well as other mass-transportation models used by environmental authorities and other scientific organizations.

Moreover, software packages are constantly being created and redeveloped for tackling the computational challenges of air pollution modeling, some specific packages include ADAM, ASPEN, CALPUFF, and AERMOD, etc. These packages are often utilized to predict how both meteorological phenomena and industrial emissions effect the dispersal of different pollutant species over varying topography. As further advances in computer systems are made, the methodologies for simulating pollutant distribution for photochemical/dispersion models and applying them in real-world situations will drastically improve on both a micro (local/regional/urban) and global (troposphere/atmospheric) scale.

3 Modeling Convection-Diffusion

The main portion of this research consists of three subsections, the first of which covers the definition of basic convection-diffusion, the diffusive coefficient, convection vector, source emission, as well as different types of boundary conditions and their applications to various topographies. The weak/variational formulation is defined in the second subsection, with its derivation as well as existence and uniqueness shown. This segment also contains the basics of the Finite Element Method in addition to the semi/fully-discrete formula. The final subsection is composed of the basic elements of FreeFem++ and presents the simulations modeling both pure diffusion, and convection-diffusion within a square finite space.

3.1 Basic Convection-Diffusion

The natural processes conveying the dispersion of particles and energy from areas of high concentration to areas of low concentration are represented by the convection-diffusion equation

$$U_t - \nabla \cdot (D \nabla u) - \nabla \cdot (\vec{b}u) = f \text{ on } \Omega \times [0, T] \quad (1)$$

where the coefficient of diffusion D is a constant whose concentration gradient is assumed to be proportional to the rate of diffusion, and the vector \vec{b} represents the convection term determining the trajectory of the concentrated particles emitted from the source f on the generalized domain Ω with boundary $\partial\Omega$. This particular convection-diffusion model is limited in its ability to accurately depict smoke plume dispersal due to the omission of other variables and equations that are heavily relied upon in more renowned mass transportation models. These omissions include voracity (the swirling phenomena observed in smoke plumes), the stream function, and the reactionary properties of the particular chemical/pollutant species being measured. However, this model still provides the basis for more technical convection-diffusion dominated mass transportation equations often used in real-world applications.

3.1.1 Boundary Conditions

Different types of boundary conditions are often used in conjunction with one another when modeling partial differential equations such as the convection-diffusion equation for a variety of reasons, one being to apply the properties of the topography specific to the problem. The Neumann boundary condition, also referred to as the natural boundary condition, is often used for problems related to convection-diffusion such as the heat equation. The physical mechanics behind the Neumann boundary condition are associated with the freedom of movement, so particles are allowed to pass through the boundary. Hence, the boundary exerts no force specifying the flux or flow of particles in and out of the defined space. The Neumann boundary condition is denoted as follows:

$$\frac{\partial u}{\partial n} = g \text{ on } \partial\Omega \quad (2)$$

Furthermore, the Dirichlet boundary condition or fixed boundary condition is often used to force the particles near the boundary to go to zero, illustrating the reaction of a particle distribution within a finite space that faces obstruction by a solid surface. The Dirichlet boundary condition is denoted:

$$u = 0 \text{ on } \partial\Omega \quad (3)$$

Applied air pollution models often use a combination of the previously mentioned boundary conditions in the form of Robin boundary conditions or (mixed boundary conditions) denoted as:

$$\frac{\partial u}{\partial n} = g - au \text{ on } \partial\Omega \quad (4)$$

This type of boundary makes physical sense when formulating applied convection-diffusion models due to the flow of particles through a medium such as air (Neumann) and no flow through obtrusive surfaces such as the ground, buildings or mountains (Dirichlet). Thus, Robin boundary conditions provide the most precise representation for modeling the physical environment of applied pollution dispersal problems due to its flexibility with regards to the flux adhering to the topography of a given problem space.

3.2 Weak Formulation

The weak formulation of a partial differential equation is an essential component to the successful utilization of the finite element method and consists of an integral function containing more conveniently solvable ordinary differential equations implicitly. In essence, before its transformation into the weak form, the differential function has many conditions/constraints that its solution must strictly adhere too, whereas, when the weak formulation is implemented the conditions are less restrictive allowing for a more achievable solution that still approximates the stronger differential function. The weak formulation for the basic convection-diffusion equation employed in the simulation is represented by:

$$\int_{\Omega} \frac{\partial u}{\partial t} \cdot v \, dx = a(u, v) \quad \forall u, v \in L^2(0, T; H^1(\Omega)) \quad (5)$$

where all u and v belong to L^2 from 0 to T and both L^2 and $H^1(\Omega)$ are multi-dimensional Hilbert spaces defined as:

$$H^1(\Omega) = \{v \in L^2 : \frac{\partial v}{\partial x_i} \in L^2(\Omega)\}$$

and

$$L^2(\Omega) = \{v : v \text{ is defined on } \Omega \text{ and } \int_{\Omega} v^2 \, dx < \infty\}$$

Johnson claims in his book, “the formulation (V) is said to be a weak formulation of (D) and the solution of (V) is said to be a weak solution of (D).” Where (V) and (D) are defined as:

$$(D) \quad -\Delta u = f \text{ in } \Omega$$

$$u = 0 \text{ on } \partial\Omega$$

and

$$(V) \quad \text{Find } u \in H_0^1(\Omega) \text{ such that } a(u, v) = (f, v) \quad \forall v \in H_0^1(\Omega)$$

Additionally, Johnson explains the mathematical advantage to the weak formulation (V) is in its ability to prove the existence of its solutions with less difficulty than that of the

differential function (D), furthermore noting that with regards to non-linear functions, a classical solution can be nearly unattainable when on the contrary there is higher likelihood of finding a “sufficiently regular” weak solution that can approximate/model the same behavior.

3.2.1 Derivation of Weak Formulation

The derivation of the weak formula for the convection diffusion equation starts with

$$\frac{\partial u}{\partial t} - \text{div}(D \nabla u) + \text{div}(\vec{b}u) = f \quad \forall x \in \Omega, t \in [0, T]$$

where $v=v(x)$ is a smooth function and is multiplied throughout the equation in order to obtain

$$\int_{\Omega} (u_t v + D \nabla u \cdot \nabla v - \nabla \cdot (\vec{b}u) v) dx - \int_{\Omega} f v dx = 0 \quad \forall v \in H_0^1(\Omega, [0, T]) \text{ on } (c, u = 0)$$

and by Green’s first formula $-\int_{\Omega} D \nabla u \cdot \nabla v dx = \int_{\Omega} (D \nabla u) \cdot \nabla v dx - \int_{\partial\Omega} \frac{\partial u}{\partial n} v ds$ so that through utilizing Neumann boundary conditions the equation is represented by:

$$\text{If } \frac{\partial u}{\partial n} = g \text{ on } \partial\Omega, \text{ then } u \in H'(\Omega, [0, T]) \text{ s.t}$$

$$\int_{\Omega} (u_t v - D \nabla u \cdot \nabla v - \nabla \cdot (\vec{b}u) v) dx - \int_{\Omega} f v dx - D \int_{\partial\Omega} g v ds$$

likewise, Robin boundary conditions produce the equation:

$$\text{If } au + \frac{\partial u}{\partial n} = g \text{ on } \partial\Omega, \text{ then } \frac{\partial u}{\partial n} = g - au \text{ s.t}$$

$$\int_{\Omega} (u_t v + D \nabla u \cdot \nabla v + \nabla \cdot (\vec{b}u) v) dx + D \int_{\partial\Omega} (au) v ds - \int_{\Omega} f v dx - D \int_{\partial\Omega} g v ds$$

where $u, v \in H_0^1(\Omega, [0, T])$, the first derivatives of the Hilbert space H^1 are integrable, $H^1([0, T])$ and $H^1(\Omega)$ are the weak time and spacial derivatives respectively.

Finally, employing $u_t \approx \frac{u - u_{old}}{dt}$ yields the following weak formulation:

$$\int_{\Omega} (uv + D \nabla u \cdot \nabla v + \nabla \cdot (\vec{b}u) v) dx + D \int_{\partial\Omega} (au) v ds - \int_{\Omega} f v dx - D \int_{\partial\Omega} g v ds - \int_{\Omega} u_{old} \cdot v dx$$

The resulting formulation is thereby translated into FreeFem++ programming language and used to solve the convection-diffusion equation.

3.2.2 Basics of Finite Element Method

One of the most prominent methods for approximating partial differential equation solutions involving variable coefficients and irregular/adaptive meshes is the finite element method. Finite element analysis is a relatively newer field in modern mathematics in comparison to its classically based counterpart, the finite difference method. The finite element methods first introduction to the mathematical community transpired through engineers for the structural engineering of frames/beams, the applications of FEM grew exponentially with the emergence of computers during the 1960's and 1970's. Mathematicians began to explore the use of these new variational methods to solve strenuous differentiable and integrable functions common in both science and engineering, and they quickly discovered preexisting roots of FEM from early twentieth century variational methods. Today, FEM is utilized extensively in conjunction with computer aided systems for design and engineering, known as (CAD or CAE) systems. Applications of FEM for convection-diffusion/reaction-diffusion based pollution models is now standard practice for those in the field, and examples of the FEM's application to solving problems real-world data and scenarios are prevalent in the literature mentioned in the previous chapter. The supporting substructure of FEM relies on the construction of the spatial domain's mesh and the FEM space V_h .

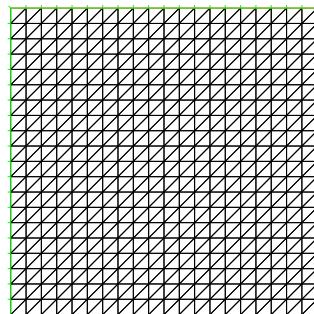
3.2.3 Mesh of Spatial Domain

The mesh of the spatial domain consists of connected nodal points that subdivide the partial differential equation into smaller components through which partitioning/triangulation creates a finite number of more manageable “elements”. The model and simulations presented in this paper utilize a square mesh which is subdivided through the introduction of triangular elements. Mesh adaptivity can provide more accurate approximations for solutions containing higher spatial errors. Introducing new nodal points or modifying the location of existing ones are two types of adaptive mesh methodologies, known as the h-adaptive and r-adaptive methods respectively.

+(Triangulation/Partitioning with two added figures)

+(Details about mesh construction)

Figure 1: Simulation Mesh



3.2.4 Finite Element Method Space

In order to construct a finite element space, the domain Ω is subdivided into a finite number of geometric representations/elements, namely triangles or rectangles, the finite element space is inevitably a subspace of the Hilbert space H^1 . Moreover, the property of smoothness (infinite continuity over the domain Ω) is required for a function to have the proper suitability for finite elements to subdivide the domain.

3.2.5 Semi-Discrete Form

Semi-discrete formulations are the middle step for obtaining an equations fully discrete form. We seek to find:

$$u(t, x) \in L^2(0, T; H^1(\Omega)) \text{ s.t. } \int_{\Omega} u_t(t, x) v(x) dx = a(u, v) \quad \forall v \in H^1(\Omega) \text{ and } \forall t \in [0, T]$$

$$\text{where } u(0, x) = u_0(x)$$

Since $V \subseteq H^1(\Omega)$, we can then construct a semi-discrete problem with a discretized spatial coordinate. We would like:

$$u(t, x) \in L^2(0, T; V) \text{ s.t. } \int_{\Omega} u_t(t, x) v dx = a(u, v) \quad \forall v \in V \text{ and } \forall t \in [0, T]$$

$$\text{where } u(0, x) = \tilde{u}_0(x) \text{ and } \tilde{u}_0 \text{ is an interpolant of } u_0 \in V$$

Therefore, the semi-discrete formulation for the basic convection-diffusion equation is denoted:

$$\int_{\Omega} \frac{\partial u}{\partial t} v dx = a(u, v) \quad \forall u, v \in L^2(0, T; V) \quad (6)$$

3.2.6 Fully-Discrete Form

The fully-discrete form utilizes the semi-discrete form in order to discretize the time component by replacing $\frac{\partial u}{\partial t}$ with the difference $\frac{u^{n+1}-u^n}{h}$. Hence, the fully-discrete formulation is denoted:

$$\int_{\Omega} \left(\frac{u^{n+1} - u^n}{h} \cdot v \right) dx = a(u^n, v) \text{ where } \{u^n\}_{n=1}^{\infty}, v \in V \text{ and } u^0 = \tilde{u}_0(x) \quad \forall n = 0, 1, 2, \dots, N \quad (7)$$

3.2.7 Matrix Equations

$$\int u^{n+1} \cdot v \, dx = \int u^n \cdot v \, dx + ha(u^n, v) \, dx$$

$$u^n = \sum_{i=1}^N c_{i,n} \phi_i(x)$$

$$c_{n+1}^{\vec{}} = c_n^{\vec{}} + hA c_n^{\vec{}}$$

$$a_{ij} = a(\phi_j, \phi_i)$$

3.3 Testing and Analysis

The final section of the main body of research presents the foundational basis of the software program FreeFem++ and the process/methodologies employed in order to achieve the simulations subsequently illustrated while also providing a physical description of the simulation results.

3.3.1 FreeFem++

The development of FreeFem++ hinged on its initial development as MacFem and PCFem through the programming language Pascal, and later recompilations in C and C++ that resulted in both FreeFem and FreeFem+ respectively. Eventually yet another recompilation in C++ created the current maintained/working version of the program FreeFem++. FreeFem++ is a high-level programming language which condenses the amount of source code for solving a partial differential equation numerically via the finite element methods from several hundreds of lines to a more manageable code length. The language for the input of the partial differential equations is similar to that of their defined mathematical representations. FreeFem++ has a basic infrastructure consisting of an elliptic partial differential equation solver "solve", a module for convection appropriately named "convect", and likewise has the ability to refine solutions through various types of mesh adaptivity.

Moreover, FreeFem++ utilizes the weak formulations previously described in the aforementioned subsection titled Weak Formulations, in order to remove the constraints surrounding the required twice differentiability of the integrand as well as the infinite continuity obligatory of the function.

Source code to solve the convection-diffusion equation through FreeFem++ is first created by introducing the parameters, defining the mesh and finite element space for the proposed problem, and then the equation is subsequently defined using the specified boundary conditions and FreeFem++'s input language. Finally, the re-iteration process is created to display particle movement with respect to time through the use of time-stepping techniques and for my simulation postscript files are produced to capture the images at each individual time-step and appropriately name and store the respective files.

3.3.2 Simulations

Dirichlet boundary conditions are used in the first depicted simulation. The concentration of pollutant/particle specie is constantly emitted from a singular source near the upper-right center of the square mesh and disperses through the processes of both diffusion and circular convection. The simulation begins with a relatively small concentration of particles from the emission source and as time progresses the concentration rapidly increases due to the constant discharge of particles from the emission source. Furthermore, the area of this particle concentration expands due to its constant diffusion rate throughout the square finite space. The convection process rotates the area of concentration in a circular clockwise direction around the space while through the diffusive term D , the area of high particle concentrations spreads to that of the lower concentration levels and can be visually observed by the increased green coloring (low concentration) representing the plume's gradient. Towards the end of the simulation the area of the highest particle concentration is near the center of the mesh and the plume's low concentration gradient nearly fills up the entire space over the mesh. Hence, the simulation represents the dispersion of particles continually emitted from a singular source over a finite space through the processes of both circular convection and

constant diffusion.

Figure 2: Initial time-step

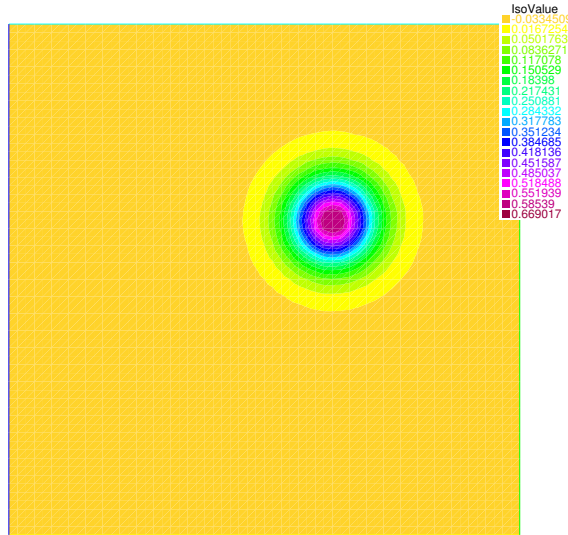


Figure 3: Time-step 5 of 79

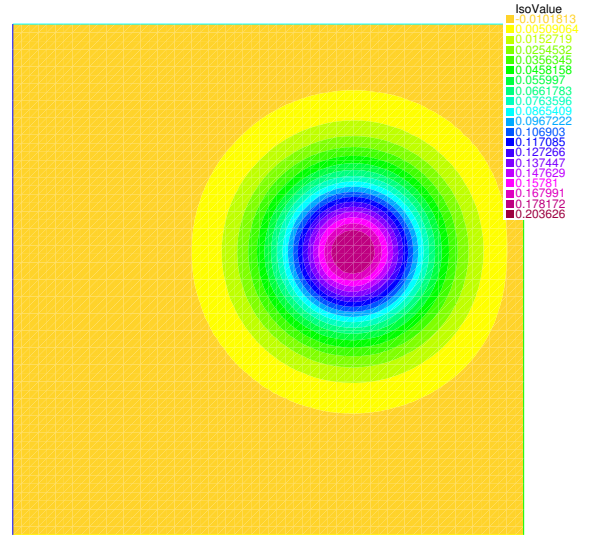


Figure 4: Time-step 15 of 79

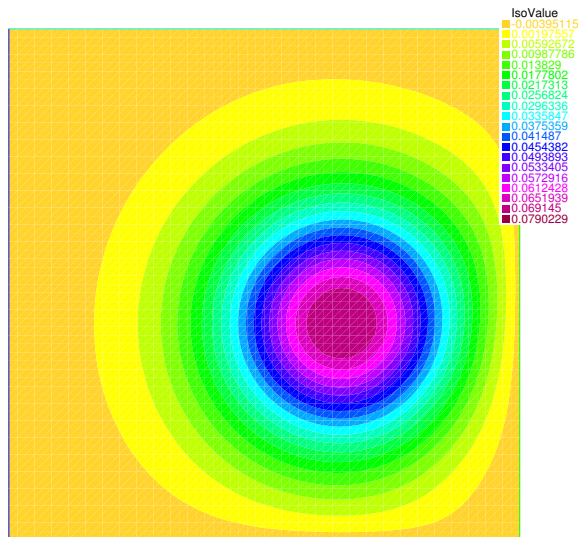


Figure 5: Time-step 25 of 79



Figure 6: Time-step 35 of 79

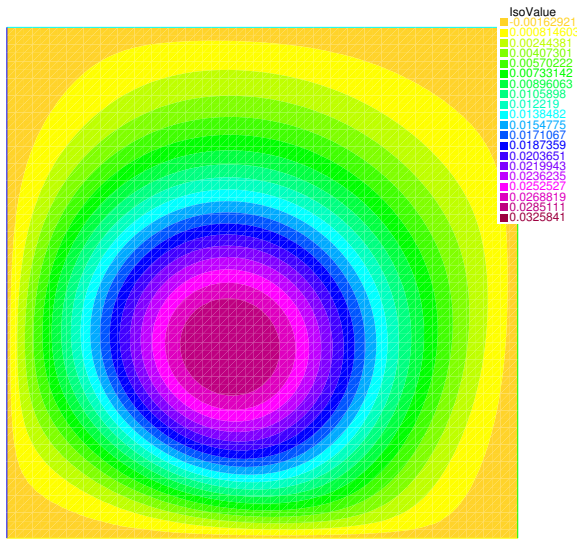


Figure 7: Time-step 45 of 79

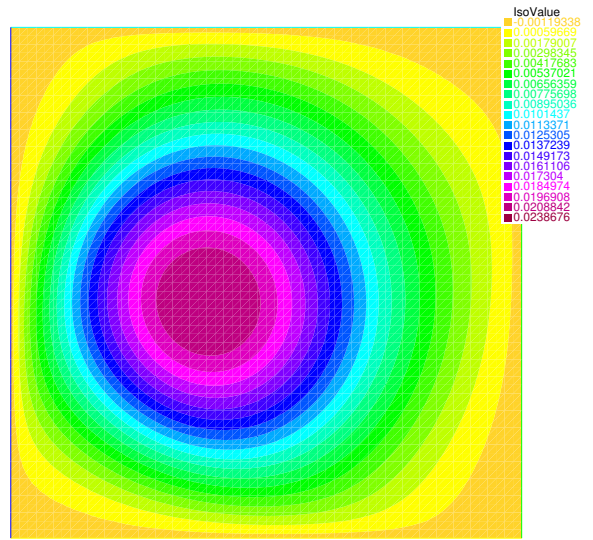


Figure 8: Time-step 55 of 79

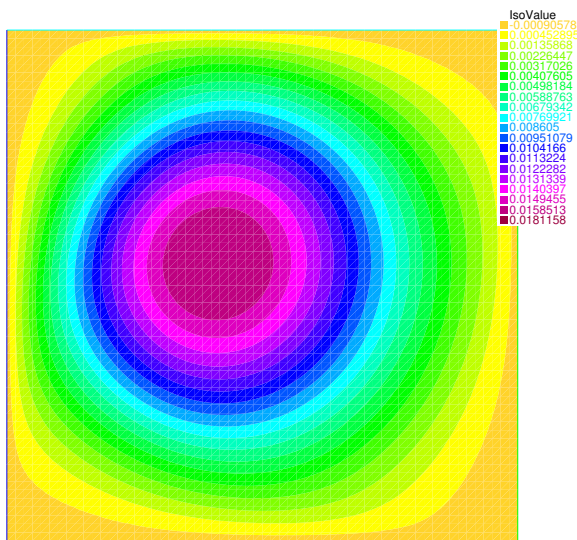
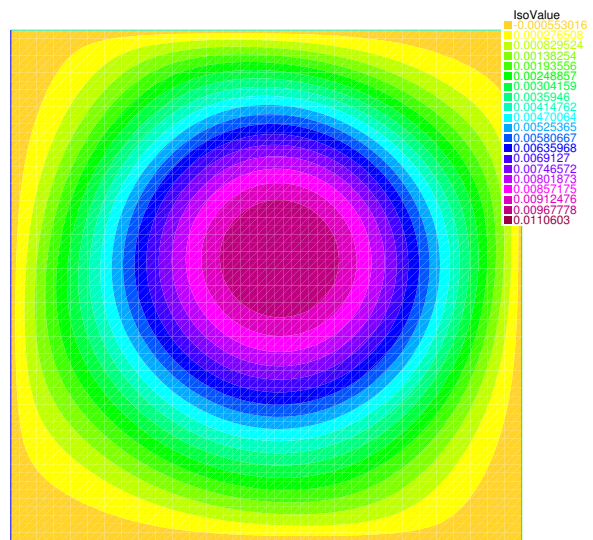


Figure 9: Time-step 75 of 79



4 Suggestions for Future Study

Suggestions for future study on this topic include improving upon the model by compounding the models basic foundation with variables such as voracity, stream-functions, and reactionary properties to create more realistic models of mass-transportation and complex advection phenomena. To create better models more accurately portraying the physical movement of air particles, the study of fluid dynamics is essential and should be researched extensively. Furthermore, the potential inclusion of stochasticity (random behavior) to the convection-diffusion equation greatly expands its capabilities for applied usage in the field of pollution modeling due to the atmospheric conditions often unpredictable behavior. Finally, new numerical methods could be employed in order to test for better quality solutions, and included mesh adaptively can play an important role for finding higher resolution solutions to more complicated convection-diffusion based models with lower computational intensity, thus reducing the overall time/cost of the methods operations.

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- +(Add few more sources)