Finite Element and Finite Difference Numerical Simulation Comparison for Air Pollution Emission Control to Attain Cleaner Environment

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Today, the world major problem is the air pollution because of the rapid growth of industrial areas. The emission of pollutant by factories into the atmosphere is affecting human health and the environment, hence the need for accurate and efficient numerical schemes in modelling this problem is expedient. The purpose of this research is to compare the Finite Element methods (FEMs) and Finite Difference Methods (FDMs) for the simulation of air pollution problem and show the better numerical method out of the two methods. The C program and Matlab software were adopted for the efficient simulation, and result presentation of the two diffusion problem tested. The results show that both numerical models are efficient for solving the problem of diffusion and are suitable for air pollution emission control for a cleaner environment.

1. Introduction

The study of diffusion equation is of great importance since it represents many physical and chemical phenomena such as air pollution, water quality in rivers, oceans, water transfer in soils, thermal pollution in river systems and contaminant dispersion in shallow lakes (Fung et al., 2005). The air quality in lots of areas today is not conducive to a healthy environment for the people existing in those areas let alone upholding their societal and fiscal progression (Gabriela and Loan, 2012). The burden of health impacts associated with polluted air falls most severely on the poor. Air pollution carries a high social, economic and environmental cost that is seldom borne by the polluter. Atmospheric emissions of ozone-depleting substances, greenhouse gases and other substances have deleterious effects on the environment both locally and globally. Everyone has the constitutional right to an environment that is not harmful to his or her health or well-being. Also, every human being has the constitutional right to dwell in a protected environment. For the benefit of present and future generations, through reasonable legislative and other measures that are: (a) prevent pollution, and ecological degradation (b) promote conservation and (c) secure ecologically sustainable development and use of bioresources (Ogunbode et al., 2017). Minimisation of pollution through dynamic control, cleaner technologies and cleaner production practices is vital to make sure that air quality is improved (Ogunbode et al., 2017). The further statute is essential to fortify the Government's policies for the protection of the environment and, more precisely, the improvement of the quality of air, to secure an environment that is not harmful to the health or well-being of the public.

According to Daniela et al. (2012), the processes governing the transport and diffusion of pollutants in the air are numerous, and of such complexity that it would be impossible to describe them without the use of mathematical models. Such models, therefore, must have high numerical accuracy.

Numerical accuracy is one of those major areas of scientific computing that researchers are trying to enhance by using different numerical schemes. In general, more bits of precision are better and acknowledging when dealing with numerical computation and too low a precision can introduce non-physical objects into physical simulations, and this might cause significant criticality phenomena to be missed, or result in the application exhibiting other undesirable or unreasonable behaviour. Since both accuracy and time efficiency are highly required in the solution of differential equations hence the interest in searching for a numerical scheme that has

both accuracy and computational time efficiency is paramont. Researchers have done numerous work in the area of using numerical methods in solving physical problems (Benjamen et al., 2006). In the work of Mehra et al. (2010), a one-dimensional advection-diffusion equation was used in solving an adaptive-step algorithm for the analysis of pollutant dispersion. They also compare it with other recent work and obtained very similar results for two solute dispersion scenarios, one along steady flow through the inhomogeneous medium and another along uniform flow through a homogeneous medium. Their method was characterized by low computational time and simplicity of the code. Jaime and Maria (2011) presented a detailed study of a specific algorithm based on the moving finite element methods to solve Stefan problems in the one-dimensional space domain. The numerical test to demonstrate the accuracy and robustness of their formulation of Moving Finite Element Method (MFEM) to solve moving boundary problems with accurate results and acceptable computational time.

Wiele et al. (2016) compared Finite-difference and Finite-element Schemes on magnetisation dynamics simulation in 3-D particles, the convergence of these methods were studied by varying the time and space discretisation. They also found that both schemes are in accordance with each other. Benjamen et al. (2006) compared Extended Finite element Method (X-FEM) and the Immersed Interface Method (IIM). Inclusively, the X-FEM performed well compared to the IIM. This paper compares the accuracy and computational time efficiencies of two powerful numerical schemes, FEM and FDM.

2. Finite difference method.

FDM is the oldest and most direct approach to discretising partial differential equations; it is also the most commonly used method to solve Ordinary Differential Equations (ODEs) and PDEs in a bounded domain (Olaiju et al., 2017). The basic idea of finite difference methods is simply to write derivatives in differential equations regarding discrete quantities of dependent and independent variables, resulting in simultaneous algebraic equations with all unknowns prescribed at discrete nodal points for the entire domain. Their values define the different unknowns on a discrete grid, and differential operators are replaced by different operators using neighbouring points (Mehra et al., 2010). The Finite-difference method is typically defined on a regular grid, and this fact can be used for very efficient solution methods (Sjodin, 2016). The abilities of the FE and FD numerical methods will be tested on one-dimension diffusion problems given as;

$$\left.\begin{array}{c} \dfrac{\partial u}{\partial t} = \alpha \dfrac{\partial^2 u}{\partial x^2} \\ \text{Boundary Conditions: } u(t,0) = u(t,L) = 0 \\ \text{Initial condition: } u(0,x) = f(x) \end{array}\right\} \tag{1}$$

By considering Eq(2) and Eq(3), the discretization of Eq(1) is as follows;

Forward difference in time

$$\frac{\partial u(x_i, t_j)}{\partial t} = \frac{u(x_i, t_j + \Delta t) - u(x_i, t_j)}{\Delta t} + O(\Delta t) \tag{2}$$

Central difference in space

$$\frac{\partial^2 u(x_i, t_j)}{\partial x^2} = \frac{u(x_i + \Delta x, t_j)u_{i+1,j} - 2u(x_i, t_j) + u(x_i - \Delta x, t_j)}{\Delta x^2} + O(\Delta x^2) \tag{3}$$

Letting $u(x_i, t_j) = u_{i,j}$ equation 1 changes to;

$$\frac{u_{i,j+1} - u_{i,j}}{\Delta t} = D\frac{u_{i+1,j} - 2u_{i,j} + u_{i-1,j}}{\Delta x^2} \tag{4}$$

$$u_{i,j+1} = (1 - 2\alpha)u_{i,j} - \alpha(u_{i+1,j} + u_{i-1,j}) \tag{5}$$

Where:

$$\alpha = \frac{D\Delta t}{\Delta x^2} \tag{6}$$

Considering the Initial condition together with the boundary conditions in Eq(1) we have the following system of equations in matrix form; Eq(7) can be solved using C codes or Matlab codes.

$$U_{j+1} = AU_j \tag{7}$$

3. Finite element method

The quest for the solution of complicated problems especially elasticity and structural mechanics modelling in engineering brought about the development of FE method. Today the FEM is considered as one of the well-established and convenient technique for the computer solution of complex problems in different fields of engineering: civil engineering, mechanical engineering, nuclear engineering, biomedical engineering, hydrodynamics, heat conduction, geo-mechanics (Kiritsis et al., 2010). FEM can be examined as a powerful tool for the approximate solution of differential equations describing different physical processes. The success of FEM is based largely on the basic finite element procedures used: the formulation of the problem in variational form, the finite element discretization of this formulation and the effective solution of the resulting finite element equations. These basic steps are the same whichever problem is considered and together with the use of the digital computer present a quite natural approach to engineering analysis.

The Finite Element Analysis (FEA) is a numerical method for solving problems of engineering and mathematical physics. FEA is useful for problems with complicated geometries, loadings, and material properties where analytical solutions cannot be obtained. Design geometry is a lot more complex, and the accuracy requirement is a lot higher. We need to understand the physical behaviours of a complex object (strength, heat transfer capability, fluid flow, etc). To predict the performance and behaviour of the design, and to calculate the safety margin; and to identify the weakness of the design accurately and to identify the optimal design with confidence (Ferreira, 2014). FEMs model body by dividing it into an equivalent system of many smaller bodies or units (finite elements) interconnected at points common to two or more elements (nodes or nodal points) and boundary lines and surfaces.

Considering the 1D model problem 1; Eq(1) is termed the robust form of the original problem and to solve this problem using the FEM, the strong form must be reduced to weak form equivalent. The weak formulation is then a reformulation of the original PDE (strong form). The final FE approach is thereby established from it. A strong form of any partial differential equation is one which usually deals with the original governing equation of the physical problem, with no mathematical manipulation as such. That being said, sometimes, such problems are difficult to handle and at times, may even be infeasible, hence the construction of weak form. It should be noted that Weak form certainly doesn't imply that the solution is weak or the results we get would not comply with the actual ones. It simply is a technique to ease our task and works as good as the strong form would. It is a characteristic feature of the FE approach that the PDE in question is first reformulated into an equivalent form, and this form has the weak form. FEM takes the following steps:

Construction of a weak form: One of the first steps in FEM is to essentially identify the PDE associated with the physical phenomenon. The PDE, which is also known as the differential form is the strong variant, while the integral form is the weak form. Both interpretations are mathematically comparable, but allow for diverse numerical methods for finding approximate solutions. One uses FDM for resolving differential equations and FEM as one of its particular forms for minimizing the total energy. A weak form does not imply inaccuracy or inferiority. The strong form imposes continuity and differentiability requirements on the potential solutions to the equation. The weak form relaxes these requirements on solutions to a certain extent. This means that a larger set of functions are solutions of the weak form.

$$\int_0^L \frac{\partial u}{\partial t} \psi dx = -\alpha \int_0^L \frac{\partial u}{\partial x} \frac{d\psi}{dx} dx \tag{8}$$

$$\emptyset \in H_0^1(0.L) \tag{9}$$

$$\psi_j(x) = \begin{cases} \frac{x - x_{j-1}}{h} & if \ x_{i-1} \leq x \leq x_j \\ \frac{x_{j+1} - x}{h} & if \ x_j \leq x \leq x_{j+1} \\ 0 & otherwise \end{cases} \tag{10}$$
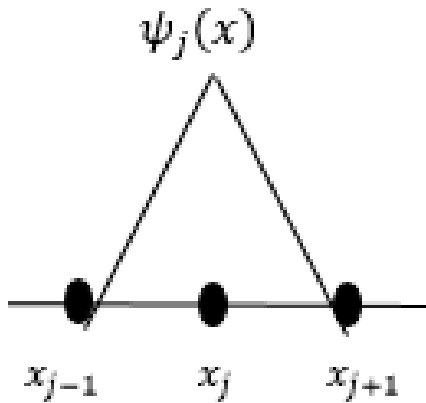
$$\psi_j(x)$$

Figure 1: Hat function

Where H^N span $\{\psi_j\}$.

An approximation of the equations is constructed, typically based on discretizations. These discretization methods approximate the PDEs with numerical model equations, which can be solved using numerical methods. The finite element method (FEM) is used to compute such approximations

Approximation framework: The approximate solution takes the form of

$$u^N(t,x) = \Sigma_{j=1}^{N-1} u_j(t)\psi_j(x) \tag{11}$$

Approximate System: For $i = 1,...N-1$

$$\int_0^L \sum_{j=1}^{N-1} \dot{u}_j(t)\psi_j(x)\psi_i(x)\,dx = -\alpha \int_0^L \sum_{j=1}^{N-1} u_i(t)\psi_j'(x)\,\psi_i'(x)\,dx \tag{12}$$

That is,

$$\sum_{j=1}^{N-1} \dot{u}_j(t)\int_0^L \psi_j(x)\psi_i(x)\,dx = -\alpha \sum_{j=1}^{N-1} u_j(t)\int_0^L \psi_j'(x)\,\psi_i'(x)\,dx \tag{13}$$

Matrix System:

$$\begin{pmatrix} a(\psi_1,\psi_1) & \cdots & a(\psi_1,\psi_{N-1}) \\ a(\psi_2,\psi_1) & \ddots & a(\psi_2,\psi_{N-1}) \\ \vdots & & \vdots \\ a(\psi_{N-1},\psi_{N-1}) & \cdots & a(\psi_{N-1},\psi_{N-1}) \end{pmatrix} \begin{pmatrix} \dot{u}_1(t) \\ \dot{u}_2(t) \\ \vdots \\ \dot{u}_{N-1}(t) \end{pmatrix} = -\alpha \begin{pmatrix} b(\psi_j',\psi_i') & \cdots & b(\psi_1',\psi_{N-1}') \\ b(\psi_2',\psi_{N-1}') & \ddots & b(\psi_2',\psi_{N-1}') \\ \vdots & & \vdots \\ b(\psi_{N-1}',\psi_{N-1}') & \cdots & b(\psi_{N-1}',\psi_{N-1}') \end{pmatrix} \begin{pmatrix} u_1(t) \\ u_2(t) \\ \vdots \\ u_{N-1}(t) \end{pmatrix} \tag{14}$$

Where

$$a(\psi_j^1\psi_i^1) = \int_0^L \psi_j^1\psi_i^1 dx \text{ and } b(\psi_i\psi_j) = \int_0^L \psi_j,\psi_i dx$$

Resulting in a semi-discrete system:

$$M\dot{r}(t) = -Kr(t) \tag{15}$$

Thus by using the forward difference scheme, we have temporal discretization, which is presented in Eq(16).

$$\frac{1}{k}(r_{j+1} - r_j) = -M^{-1}Kr_j \tag{16}$$

Hence,

$$r_{j+1} = (I - kM^{-1}K)r_j \tag{17}$$

The following test problems will be solved using both the Finite element and FDMs via C code and Matlab. From Eq(1). Test problem 1 is formed by letting *L=1, BC*: $u(t,0) = u(t,L) = 0$. Figure 2 illustrates the solution of both FEM and FDM on test problem 1.

$$u(x,t) = 12\,sin\left(\frac{9\pi x}{L}\right)e^{-k\left(\frac{9\pi}{L}\right)^2 t} - 7\,sin\left(\frac{4\pi x}{L}\right)e^{-k\left(\frac{4\pi}{L}\right)^2 t} \tag{19}$$

$$u(0,x) = 12\,sin\left(\frac{9\pi x}{L}\right) - 7\,sin\left(\frac{4\pi x}{L}\right) \tag{18}$$
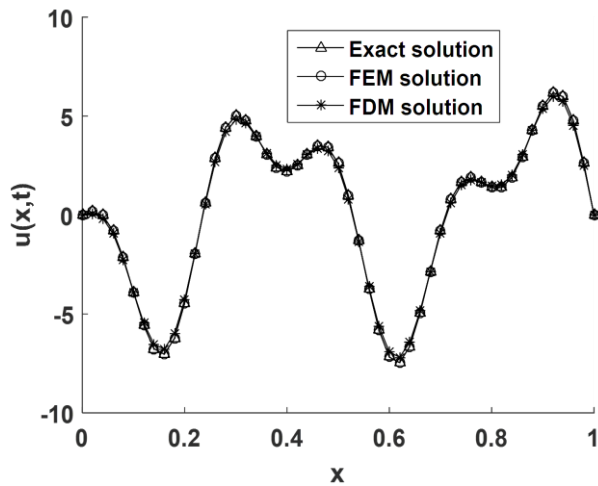
The exact solution is given as:

Figure 2: Solution of both FEM and FDM on test problem 1

Test problem 2 is form also by letting *L=1, BC;* $u(t,0) = u(t,L) = 0.$ Figure 3 presents the solution of both the FEM and FDM on test problem 2.

$$u(0,x) = 6\,sin\left(\frac{\pi x}{L}\right) \tag{20}$$

The exact solution is given by Eq(21): $\quad u(x,t) = 6\,sin\left(\frac{9\pi x}{L}\right)e^{-k\left(\frac{9\pi}{L}\right)^2 t} \tag{21}$
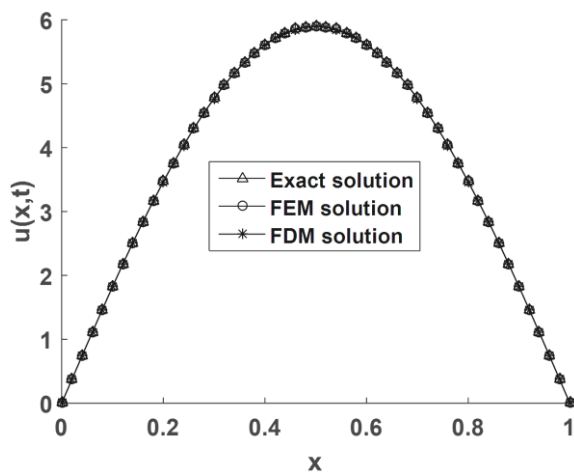

Figure 3: Solution of both FEM and FDM on test problem 2

4. Conclusions

The results showed that both numerical models are efficient for solving the problem of diffusion and are suitable for air pollution emission control for a cleaner environment. It is essential to use numerical methods to find solutions to partial differential equations. It was seen that Matlab and C program are powerful and indispensable in solving diffusion equation problem. These types of tools simplify the solution process of complex equations which result from the application of the FDM and FEM and allow us to obtain reliable results in a relatively quick and efficient way. The results also showed how the discretising process of the meshes can influence the numerical results, and how the refinement of those meshes can enhance the accuracy of the numerical solutions. Thus, having an infinite number of nodes can result in higher accuracy in which all the numerical results by FDM and FEM and the physical reality will be coincidental. However, this will have a negative effect on computational time of the software, which is one of the limitations of the numerical approach to solving these problems. In conclusion, it is essential to know accurate and reliable numerical schemes to give us an improved capacity to evaluate, compare, and discuss the physical problems around us.

Acknowledgments

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