IMPLEMENTATION OF FINITE ELEMENTS METHOD ON A DIFFUSION-ADVECTION PROBLEM
Research practise 1 project presentation

Obed Ríos-Ruiz
oriosru@eafit.edu.co

Advisor: Jairo Alberto Villegas-Gutiérrez
javille@eafit.edu.co

EAFIT University

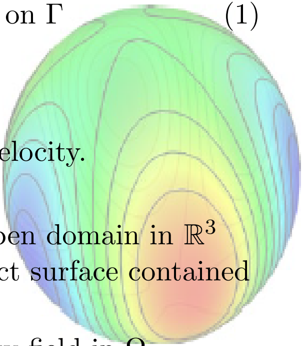
November 23, 2015

Introduction

Main equations describing the phenomena

Time dependent equation on steady surfaces

$$c_t + \mathbf{w} \cdot \nabla_\Gamma c - D \triangle_\Gamma c = 0 \quad \text{on } \Gamma \tag{1}$$



- $c \Rightarrow$ chemical species concentration.
- $\mathbf{u} \Rightarrow$ the *Darcy* or chemical crossflow velocity.
- $\mathbf{D} \Rightarrow$ the diffusion coefficient.
- $\Omega \Rightarrow$ the physical domain seen as an open domain in $\mathbb{R}^3$ and therefore Γ a connected C^2 compact surface contained in Ω.
- $\mathbf{w} : \Omega \to \mathbb{R}^3 \Rightarrow$ a divergence-free velocity field in Ω.
- $\triangle_\Gamma \Rightarrow$ *Laplace-Beltrami* operator on Γ.

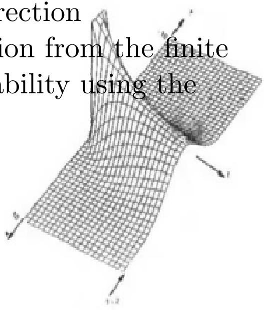
Introduction

Main equations describing the phenomena

Time dependent equation in space

$$\frac{\partial C}{\partial t} + \nabla \cdot (\mathbf{u}C) = D\nabla^2 C \qquad (2)$$

In this case **u** can be considered as the wind velocity and it is usually taken as constant in any horizontal direction $\vec{\mathbf{u}} = (U, V, 0)$. So it is possible to build a solution from the finite difference method as well as a study of the stability using the *von Neumann* stability criterion. Example



Von Neumann criterion

The difference method for an initial value problem (for a differential equation with constant coefficients) with a bounded solution is stable if every solution to the finite difference equation having the form $c_j^n = \xi^n e^{i\beta j}$, ($\beta$ real, $\xi = \xi(\beta)$ complex) has the property $| \xi | \leq 1$. Example

Finite elements method first criterion idea

In the study of the elastic theory where three kinds of magnitudes, stresses, strains and displacements determine the solution by using the finite elements method, if certain conditions concerning completeness and the good behavior of the approximate solution are satisfied then convergence is insured. Continuation

Developments

Example proposition

Solve the advection diffusion problem [1] governed by (2) subject to:

Problem conditions

$$\vec{u} = (U, V, 0) = (-\sin\theta, \cos\theta, 0)$$

$$c_0(x, y) = \begin{cases} 50(1 + \cos\frac{\pi R}{4}) & \text{, if } R < 4 \\ 0 & \text{, if } R > 4 \end{cases}$$

$$\text{where} \begin{cases} \theta & = \arctan\frac{y}{x} \\ R^2 & = (x - x_0)^2 + (y - y_0)^2 \\ (x_0, y_0) & = (5, -10) \end{cases}$$

Developments

Example results

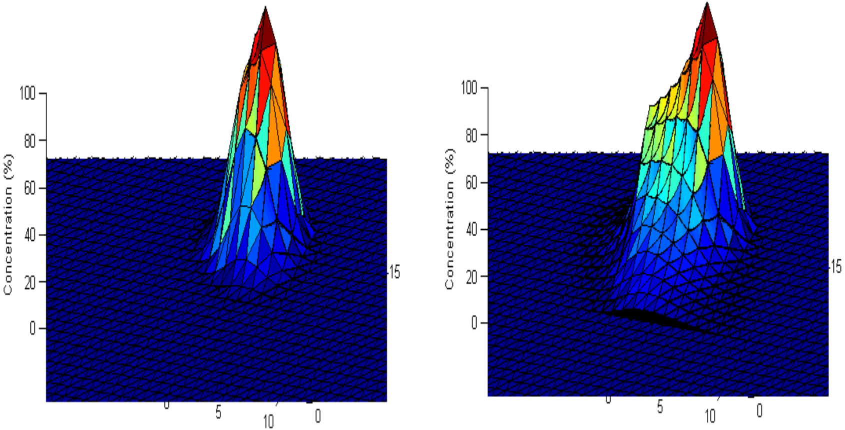


Figure 1: Concentration percentage evolution for 5 and 25 segs

Developments

Example results

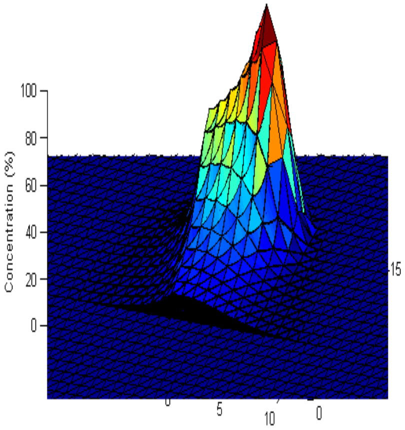


Figure 2: Concentration percentage evolution for 60 and 150 segs

Developments

Example results

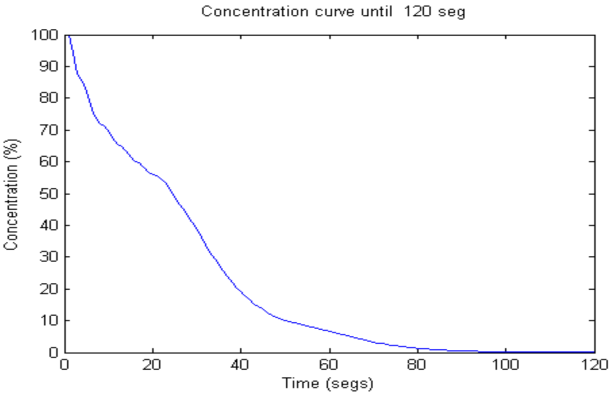


Figure 3: Concentration percentage curve until 120 segs

Continuation

Developments

Example results

Taking $\vec{u}$ as $\vec{u} = (U, 0, 0)$ the Equation(2) takes the following form.

$$C_j^{n+1} = C_j^n - U\frac{\Delta t}{\Delta x}(C_j^n - C_{j-1}^n) + D\tfrac{\Delta t}{(\Delta x)^2}(C_{j+1}^n - 2C_j^n + C_{j-1}^n) \tag{3}$$

Letting $C_j^n = \xi^n e^{i\beta j}$ and $r = \frac{\Delta t}{(\Delta x)^2}$ the *von Neumann* criterion is applied.

$$\begin{aligned}
\Rightarrow \xi^{n+1}e^{i\beta j} &= \xi^n e^{i\beta j} - U.r\Delta x(\xi^n e^{i\beta j} - \xi^n e^{i\beta(j-1)}) \\
&\quad + D.r(\xi^n e^{i\beta(j+1)} - 2\xi^n e^{i\beta j} + \xi^n e^{i\beta(j-1)}) \\
\Rightarrow \xi &= 1 - U.r\Delta x(1 - e^{-i\beta}) + D.r(e^{i\beta} - 2 + e^{-i\beta}) \\
&= 1 - U.r\Delta x(1 - cos\beta) - iU.r\Delta x sin\beta + 2D.r(cos\beta - 1) \\
&= \big(1 - (2D.r + U.r\Delta x)(1 - cos\beta)\big) - iU.r\Delta x sin\beta
\end{aligned} \tag{4}$$

Developments

Example results

$$\Rightarrow \mid \xi \mid^2 = 1 - 2(2D.r + U.r\Delta x)(1 - cos\beta) + (2D.r + U.r\Delta x)^2 (1 - cos\beta)^2 + U^2 r^2 (\Delta x)^2 sin^2\beta$$

$$\begin{aligned} \Rightarrow \mid \xi \mid^2 - 1 = & -2(2D.r + U.r\Delta x)(1 - cos\beta) \\ & + 4D^2 r^2 (1 - cos\beta)^2 + 4D.U.r^2 \Delta x (1 - cos\beta)^2 \\ & + U^2 r^2 (\Delta x)^2 (1 - 2cos\beta + 1) \end{aligned} \quad (5)$$

For $(1 - cos\beta) > 0$ the condition $\mid \xi \mid^2 \leq 1$ is equivalent to

$$-(2k + U\Delta x) + 2D^2 r(1 - cos\beta) + 2D.U.r\Delta x(1 - cos\beta) + U^2 r(\Delta x)^2 \leq 0$$

$$\Rightarrow \quad r(U^2(\Delta x)^2 + (2D^2 + 2D.U\Delta x)(1 - cos\beta)) \leq 2D + U\Delta x$$

$$\Rightarrow \quad r(U^2(\Delta x)^2 + 4D.U\Delta X + 4D^2) = r(U\Delta x + 2D)^2 \leq 2D + U\Delta x$$

$$\Rightarrow \quad r(2D + U\Delta x) \leq 1$$

Continuation

Developments

Example results

As long as $r(2D + U\Delta x) \leq 1 = \frac{\Delta t}{\Delta x^2}(2D + U\Delta x) \leq 1$ is hold then (3) and therefore (2) are convergent.

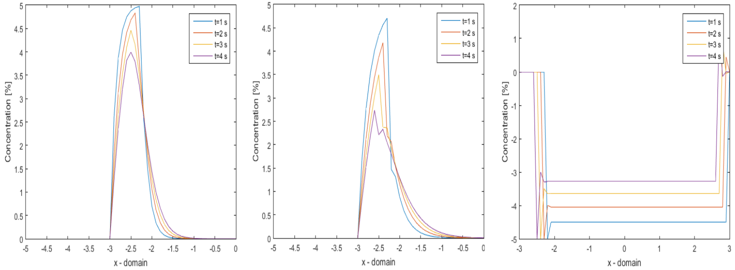


Figure 4: Solution to particular problem with $\Delta x = \frac{1}{10}$ and Δt equal to $\frac{1}{211}$ (stable), $\frac{1}{210}$ (semi-stable) and $\frac{1}{209}$ (unstable) respectively [1].

Consider the reduced equation from (2):

$$\frac{\partial C}{\partial t} + u\frac{\partial C}{\partial x} = D\frac{\partial^2 C}{\partial x^2}, \quad -1 < x < 1, \quad t \in [0, T], \tag{6}$$

The global finite elements approximation is sought in terms of linear *Lagrange* polynomials making up hat functions such that the numerical discretization is

$$C_h(x) = \sum_{i=1}^{\epsilon+1} C_i(t)\varphi_i(x), \quad -1 \leq x \leq 1, \tag{7}$$

where h refers to the finite element grid size. i denotes the index of the finite element grid nodes and ϵ the number of elements covering the spacial domain and therefore $N = \epsilon + 1$ is the number of grid points. C_i are the time dependent nodal values [3].

Replacing the finite elements into the equation below, where v is a test function:

$$\int_{-1}^{1} \left((\frac{\partial C}{\partial t} + u \frac{\partial C}{\partial x}) v + D \frac{\partial C}{\partial x} \frac{\partial v}{\partial x} \right) dx = 0 \tag{8}$$

we get the following linear system of algebraic equations of order $N-2$, where the end points are given boundary values, i.e., $k=1$ and $k=N$ correspond to $C(-1,t)$ and to $C(1,t)$ correspondingly.

Developments

Finite Element Method

$$\sum_{k=2}^{N-1} \left(M_{i,k} \frac{dC_k}{dt} + \left(u R_{i,k} + D K_{i,k} \right) C_k \right) = 0$$

where the mass matrix $[M]$, weak derivative matrix $[R]$ and stiffness matrix $[K]$ corresponds respectively to

$$M_{i,k} = \int_{-1}^{1} \varphi_i \varphi_k dx, \quad 2 \leq i \leq N-1,$$

$$R_{i,k} = \int_{-1}^{1} \frac{d\varphi_i}{dx} \varphi_k dx, \quad 2 \leq i \leq N-1,$$

$$K_{i,k} = \int_{-1}^{1} \frac{d\varphi_i}{dx} \frac{d\varphi_k}{dx} dx, \quad 2 \leq i, k \leq N-1.$$

Developments

Finite Element Method

Using an implicit *Crank-Nicolson* and a second-order *Adams-Bashforth* explicit integration on the set of ordinary differential equations $[M]\frac{d\underline{C}(t)}{dt} + ([K] + [R])\underline{C}(t) = 0$, where $\underline{C}$ is the vector collecting all the problem unknowns, then the full discrete equations read as:

$$\left([M] + \frac{\Delta t}{2}[K]\right)\underline{C}^{n+1} = \left([M] - \frac{\Delta t}{2}[K]\right)\underline{C}^{n} + \frac{\Delta t}{2}[R]\big(3\underline{C}^{n} - \underline{C}^{n-1}\big) \quad (9)$$

Developments

Finite Element Method

Let D and u as 1 and $\frac{1}{10\pi}$ respectively. Corresponding to the method Δt is set as $\frac{1}{100}$ with $\epsilon = 1000$ elements. Applying the scheme (9) we get the following curves for equally spaced domain with $\Delta x = 0.2$.

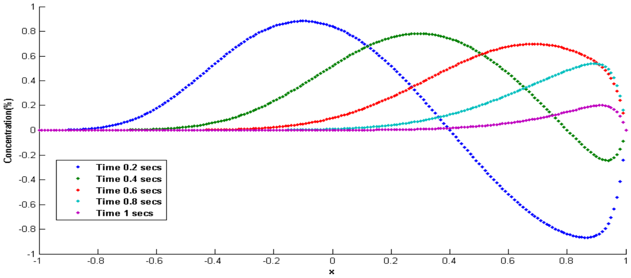


Figure 5: Concentration percentage curves for different times using finite element method.

Current work

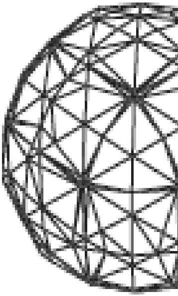
Towards a general formulation

Given the following variation [2] from (1), bilinear form and the functional respectively:

$$\mathbf{w} \cdot \nabla_\Gamma u + c(\mathbf{x})u = f + \epsilon \Delta_\Gamma u \quad \text{on } \Gamma$$

$$a(u,v) := \epsilon \int_\Gamma \nabla_\Gamma u \cdot \nabla_\Gamma v \, \mathrm{d}s + \int_\Gamma (\mathbf{w} \cdot \nabla_\Gamma u) v \, \mathrm{d}s + \int_\Gamma uv \, \mathrm{d}s$$

$$f(v) := \int_\Gamma fv \, \mathrm{d}s$$



where $f \in L^2\Gamma$, $c(\mathbf{x}) \geq 0$ and Δ_Γ and ∇_Γ defined as before, find $u \in V$ such that

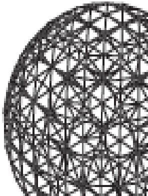
Actual work

$$\boxed{a(u,v) = f(v) \quad \text{, for all } v \in V}$$

with

$$V = \begin{cases} \left\{ v \in H^1(\Gamma) \mid \int_\Gamma v \, \mathrm{d}s = 0 \right\} & \text{, if } c = 0 \\ H^1(\Gamma) & \text{, if } c > 0 \end{cases}$$

where $H^1(\Gamma)$ denotes the Sobolev spaces with $p = 2$ and owing to the *Lax-Milgramm* lemma, there exist a unique solution of this last equation.



Acknowledgment

THANK YOU FOR YOUR ATTENTION!

QUESTIONS?

Bibliography

[1] Friedman, A. and Littman, W., Industrial Mathematics:*A Course in Solving Real-World Problems*. SIAM: Society for Industrial and Applied Mathematics (1994).

[2] Olshanskii, Maxim A., Reusken, Arnold and Xu, Xianmin, *A stabilized finite element method for advection–diffusion equations on surfaces*. IMA Journal of Numerical Analysis (2013).

[3] Abdelkader Mojtabi and Michel O. Deville, *One-dimensional linear advection–diffusion equation: Analytical and finite element solutions*. Computers & Fluids (2015).