ISSN XXXX XXXX © 2018 IJESC

Research Article Volume 8 Issue No.6

Three Dimensional Mathematical Models for Convective-Dispersive Flow of Pesticides in Porous Media

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Abstract:
The transport of solutes through porous media where chemicals undergo adsorption or change process on the surface of the porous materials has been a subject of research over years. Usage of pesticides has resulted in production of diverse quantity and quality for the market and disposal of excess material has also become an acute problem. The concept of adsorption is essential in determining the movement pattern of pesticides in soil in order to assess the effect of migrating chemical, from their disposal sites, on the quality of ground water. Most studies made of movement of pesticides in the ground environment, the mathematical models so far developed emphasis axial movement and in a few cases both axial and radial movements. Soil processes have a 3D character; modeling therefore in principle, should employ three dimensions. It should also be noted that the appropriate number of dimensions is closely related to the required accuracy of the research question. The 1D and 2D approaches are limited since they are not capable of giving dependable regional influence of pesticides movement in the porous media and ground water. They give us only theoretical results which are devoid of the reality in the field due to lumping of parameters. In this publication, three dimensional formulas are developed so that it can enhance our capacity to analyze the realistic regional impact of adsorption of pesticides in a porous media and the ground water in the field condition. The methodology will involve determining the comprehensive dispersion equation accounting for 3D movement of solutes in the porous media and finding the solution of the governing equation using Alternate Direction Implicit method (ADI) which is unconditionally stable for 3D equations of Douglas and Gunn approach.

Key Words: convective-dispersive, adsorption, pesticides, porous media, solutes

1.INTRODUCTION

Convective-Dispersive equations have been solved using implicit methods. This is due to their unconditional stability but the challenges associated with the matrices have become a concern and a limitation in obtaining solutions [1, 9]. Implicit finite difference methods obtain the solution for the next step from the state of both the current and the next steps, while explicit methods obtain the solution from the current step only. Implicit methods require computation per time step and can implement long time step intervals without suffering numerical instabilities. On the contrary explicit numerical methods suffer from instabilities. Implicit numerical methods are stable in one-dimension problems but they do not guarantee stability in multidimensional problems. Inversion of matrices produced by explicit numerical are easier to solve compared to those of implicit numerical methods, but require smaller time interval thus increasing computation time. In this paper we adopt ADI method. In numerical analysis, the Alternating Direction Implicit (ADI) method is a finite difference method for solving parabolic and elliptic partial differential equations. The advantage of the ADI method is that the equations that have to be solved in each step have a simpler structure and can be solved efficiently with the tridiagonal matrix algorithm., also called Thomas Alogarithm, whis is user friendly [6]Douglas and Gunn modified Crank and Nicolson Method developed a general ADI scheme that is unconditionally stable and retains second order accuracy when applied to 3D problems with varied implicit and explicit steps. This method gives a tridiagonal matrix algorithm (TDMA) which is a simplified Gaussian elimination. [3] These details are essential in analysis of many environmental studies related to irrigation and drainage strategies(efficient water use), transport of nutrients and pesticides movements towards ground water and surface water system (pollution), surface water management of agricultural areas and natural areas (agronomic and ecological interest). In this study, we derive a 3D convective dispersive equation describing movement of pesticides in underground porous media and solve the equation using an efficient alternating direction implicit method by Peaceman and Rachford [1], and Douglas and Gunn [3] developed from a variation on the Crank Nicolson approximation. Advantages of ADI method is that it prevents numerical problems encountered by the fully implicit schemes and it shortens computing time by a factor of 2 compared to the implicit method and does not encounter numerical problems such as negative distribution functions or crashes during matrix inversion [6] that are seen in implicit methods.

2. DERIVATION OF CONVECTIVE-DISPERSIVE SOLUTE TRANSPORT EQUATION WITH STEADY STATE WATER FLOW CONDITION

For a control volume

$$\sum M_{in} = \sum M_{out}$$

$$\frac{\partial M_{cv}}{\partial t} = 0$$

Where, M_{cv} is the mass of controlled volume=a constant (Steady state) The speed of water in porous media is determined by considering the,

Average pore water velocity $v(LT^{-1}) = \frac{q}{\theta}$

i.e. $q = -\ k\frac{\partial H}{\partial l}$, is the flux density, and $\theta = \frac{v_w}{v_s}$ in which V_w is the volume of water in the porous media and V_s is the volume of solids, k-is the permeability

∂H -the hydraulic head

∂l -distance travelled

In this study we use the concept of dispersion through a cubically packed soil vessel with internal dimensions x, y, and z to derive our equation.

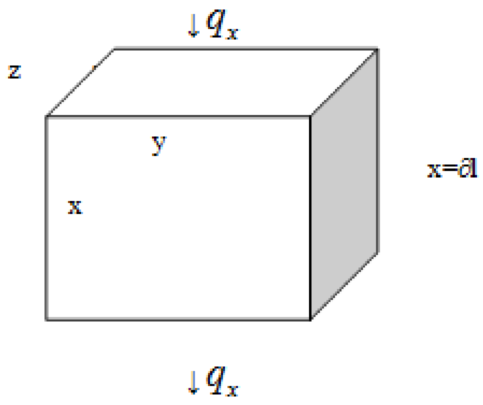

Figure 1

At very low flow rate, the dispersion is different in the three directions. The dispersion coefficients are denoted by D_x , D_y , and D_z for x, y and z directions respectively.

$$D(\theta, v) = D_m + D_d$$

where $D_m(L^2T^{-1})$ is molecular diffusion coefficient and $D_d(L^2T^{-1})$ is the hydrodynamic dispersion and is the mixing of spreading of the solute during transport due to differences in velocities within the pores and between the pores.

The volumetric water content denoted by θ can be assumed to be void ratio for saturated soils. The element height is denoted by ∂l . The measurements are denoted by x , y and z for x, y and z-axis of the cube respectively. C is the concentration of the material to be dispersed and is a function of axial position x, radial positions y and z, time t and dispersion coefficients D_R and D_L radial and axial respectively.

The rate of entry of reference adsorption material due to flow in axial direction,

$$q_x(y\partial y)C + q_x(z\partial z)C \qquad (1.1)$$

The corresponding efflux rate,

$$q_x y\partial y\left(C + \frac{\partial C}{\partial l}\partial l\right) + q_x z\partial z\left(C + \frac{\partial C}{\partial l}\partial l\right) \qquad (1.2)$$

The net accumulation rate in element due to axial flow,

$$-q_x y\partial y\frac{\partial C}{\partial l}\partial l - q_x z\partial z\frac{\partial C}{\partial l}\partial l \qquad (1.3)$$

Rate of diffusion in axial direction across inlet boundary,

$$-y\partial y\theta D_l\frac{\partial C}{\partial l} - z\partial z\theta D_l\frac{\partial C}{\partial l} \qquad (1.4)$$

Corresponding rate at outlet boundary,

$$-y\partial y\theta D_l\left[\frac{\partial C}{\partial l} + \frac{\partial^2 C}{\partial l^2}\partial l\right] - z\partial z\theta D_l\left[\frac{\partial C}{\partial l} + \frac{\partial^2 C}{\partial l^2}\partial l\right] \qquad (1.5)$$

The net accumulation due to diffusion from boundaries in axial direction is,

$$y\partial y\theta D_l\frac{\partial^2 C}{\partial l^2}\partial l + z\partial z\theta D_l\frac{\partial^2 C}{\partial l^2}\partial l \qquad (1.6)$$

Diffusion at inlet y and z direction

$$-z\theta\partial zD_y\frac{\partial C}{\partial y} - y\theta\partial yD_z\frac{\partial C}{\partial z} \qquad (1.7)$$

The corresponding rate at y and z outlet is,

$$-z\theta\partial zD_y\left[\frac{\partial C}{\partial y} + \frac{\partial^2 C}{\partial y^2}\partial y\right] - y\theta\partial yD_z\left[\frac{\partial C}{\partial z} + \frac{\partial^2 C}{\partial z^2}\partial z\right] \qquad (1.8)$$

The net accumulation rate due to diffusion from boundaries in axial directions y and z

$$y\partial y\theta D_z\frac{\partial^2 C}{\partial z^2}\partial z + z\partial z\theta D_y\frac{\partial^2 C}{\partial y^2}\partial y \qquad (1.9)$$

For a representative volume of soil, the total amount of a given chemical species $X(ML^{-2})$ is represented by the sum of the amount retained by the soil. When the adsorption isotherm obeys the Freundlich equation the Matrix and the amount present in the soil,

$$X = \rho_b S + \theta C \quad (1.10)$$

where, ρ_b is bulky density and S is the solute adsorbed, therefore,

θC is the solute in the solution

$$\frac{\partial X}{\partial t} = \rho_b\frac{\partial S}{\partial t} + \theta\frac{\partial C}{\partial t} \qquad (1.11)$$

Now the total accumulation rate,

$$\partial x\partial y\partial z\frac{\partial X}{\partial t} = \partial x\partial y\partial z\left(\rho_b\frac{\partial S}{\partial t} + \theta\frac{\partial C}{\partial t}\right)(1.12)$$

From equations 1.3, 1.6, 1.9, and 1.12, we have the following combined equation,

$$\partial x\partial y\partial z\left(\rho_b\frac{\partial S}{\partial t} + \theta\frac{\partial C}{\partial t}\right) = y\partial y\partial x\theta D_x\frac{\partial^2 C}{\partial x^2} - q_x y\partial y\partial x\frac{\partial C}{\partial x} - q_x z\partial z\partial x\frac{\partial C}{\partial x}\,(1.13)$$
$$+ z\partial z\partial x\theta D_x\frac{\partial^2 C}{\partial x^2} + y\partial y\partial zD_z\frac{\partial^2 C}{\partial z^2} + z\partial z\partial y\theta D_y\frac{\partial^2 C}{\partial y^2}$$

For a cube x=y=z and $x = \partial l = \partial x = \partial y = \partial z$ for cube

Therefore the above equation gives us,

$$\rho_b\frac{\partial S}{\partial t} + \theta\frac{\partial C}{\partial t} = 2D_x\theta\frac{\partial^2 C}{\partial x^2} - 2q_x\frac{\partial C}{\partial x} + D_y\theta\frac{\partial^2 C}{\partial y^2} + D_z\theta\frac{\partial^2 C}{\partial z^2} \qquad (1.14)$$

The presentation of the amount of solute adsorbate per unit adsorbent as a function of the equilibrium concentration in bulky solution at a constant temperature is termed as the adsorption isotherm. One of the most popular adsorption isotherm equations that is used for liquids was described as

$$S = KC_e^{\,N}\ ,(1.15)$$

where $S = {}^{x}/_{m}$, is adsorbed solid and C_e is the solute equilibrium constant.

$$\frac{\partial S}{\partial t} = \frac{\partial S}{\partial C}\frac{\partial C}{\partial t} = NKC^{N-1}\frac{\partial C}{\partial t}\ .(1.16)$$

From equation (1.11) and (1.16) we get,

Where

$$R\,(C) = (1 + \frac{\rho NK_d C^{N-1}}{\theta})\ (1.17)$$

Taking $\partial l = x$, $v(LT^{-1}) = \frac{q}{\theta}$ and $\partial y = \partial z$ given that the width of the element in question is equal, therefore,

$$R(C)\frac{\partial C}{\partial t} = 2D_x\frac{\partial^2 C}{\partial x^2} - 2v_x\frac{\partial C}{\partial x} + D_y\frac{\partial^2 C}{\partial y^2} + D_z\frac{\partial^2 C}{\partial z^2}\,(1.18)$$

Therefore equation (1.18) is our model equation.

2.2 Problem formulation by finite difference

For uniform porous media, the adsorption of solute is give by our derive equation,

$$R(C)\frac{\partial C}{\partial t} = 2D_x \frac{\partial^2 C}{\partial x^2} - 2v_x \frac{\partial C}{\partial x} + D_y \frac{\partial^2 C}{\partial y^2} + D_z \frac{\partial^2 C}{\partial z^2} \quad (1.18)$$

This equation is the second order equation quasilinear partial differential equation. The first step is to establish a finite difference method solution of the partial differential equation is to discretize the continuous domain of its grids with finite number of grid points. At time step n, the concentration of the solute $C(x, y, z, t)$ at grid point (i, j, k) can be placed by $C(i\Delta x, j\Delta y, k\Delta z, n\Delta t)$ which is denoted by $C^n_{i,j,k}$. The initial conditions for solving the model equations are;

The partial derivatives of C with respect to x, implies y, z and t are kept constant and vice versa

$$\frac{\partial C}{\partial x}\bigg| i, j, k, n \equiv \frac{dC}{dx}\bigg|_{i,j,k,n}$$

$$\frac{\partial C}{\partial y}\bigg| i, j, k, n \equiv \frac{dC}{dy}\bigg|_{i,j,k,n}$$

$$\frac{\partial C}{\partial z}\bigg| i, j, k, n \equiv \frac{dC}{dz}\bigg|_{i,j,k,n}$$

and $\frac{\partial C}{\partial t}\bigg| i, j, k, n \equiv \frac{dC}{dt}\bigg|_{i,j,k,n}$

The initial condition; the concentration of pesticides at positions in the porous media at time zero is constant, and equal to $C_{i,j,k}$,

i.e. $C(x, y, z, 0) = C_{i,j,k}$ for $x, y, z > 0$

Boundary conditions: -Two conditions are necessary; 1, in the first case the concentration of pesticides at position x=o, y=0 and z=0 is specified for a period of time. Following that time, the concentration at the surface is zero

$$C(0,0,0,t) = C_0$$

For $0 < t \le t_0$ and $C(0,0,0,t) = 0$ for t>0

2. in the second case, the concentration of pesticides in the solution entering the soil system at point x=0, y=0 and z=0, is specified for a period of time. Following that time, the concentration at the surface is zero

Assumptions;

- The pore water velocity is constant in time and space. This condition can be met for a uniform medium if the flux density of water velocity and volumetric water content are constant for all positions all the time.
- The spread of solute is dominated by hydraulic dispersion rather than diffusion
- The hydraulic dispersion can be approximated as a product of dispersivity and pore water velocity
- The adsorption process is instantaneous and reversible. The concentration of the pesticides adsorbed on the soil solid is proportional to the concentration in the solution.

2.3 Alternate Direct Implicit Method (ADI)

The implicit method is also known as the Backward in Time Central in Space (BTCS) scheme, and is unconditionally stable. Although it has this great advantage, the drawback is that a tridiagonal system must be solved for each time step. Alternate Direct Implicit Method (ADI) is a Difference Method for solving Parabolic and Partial difference equations.

In this study we will deal with two methods

- Crank &Nicolson Method,
- Douglas & Gunn Method

2.3.1 Crank and Nicolson Method

Implicit numerical methods are stable in one dimension problem but do not guarantee stability in multidimensional. Alternate Direct implicit (ADI) Method is a numerical method developed by Crank and Nicolson and is unconditionally stable, accurate and deal with time matching problems by taking simple explicit and implicit methods. It prevents numerical problems encountered by fully implicit schemes and shortens computing times by a factor of 2. It also does not encounter numerical problems such as negative distribution function or crash during matrix inversion that are seen in other implicit numerical methods. However its matrix is complicated to solve. Crank and Nicolson [3] dealt with the time marching problem by taking the average of simple explicit and implicit methods. For our equation (1.18),

$$R(C)\frac{\left(C^{n+1} - C^n\right)}{\Delta t} = 2D_x \frac{\partial_x^2\left(C^{n+1} + C^n\right)}{2(\Delta x)^2} - 2v_x \frac{\partial_x\left(C^{n+1} + C^n\right)}{4(\Delta x)} + D_y \frac{\partial_y^2\left(C^{n+1} + C^n\right)}{2(\Delta y)^2} + D_z \frac{\partial_z^2\left(C^{n+1} + C^n\right)}{2(\Delta z)^2}$$

Rearranging the Crank Nicolson equation;

$$\begin{aligned} R\left(C_{i,j,k}\right)\frac{\left(C^{n+1}_{i,j,k} - C^n_{i,j,k}\right)}{\Delta t} &= D_x\left(\frac{\left(C^{n+1}_{i+1,j,k} - 2C^{n+1}_{i,j,k} + C^{n+1}_{i-1,j,k}\right)}{(\Delta x)^2}\right) + D_x\left(\frac{\left(C^{n}_{i+1,j,k} - 2C^{n}_{i,j,k} + C^{n}_{i-1,j,k}\right)}{(\Delta x)^2}\right) \\ &- v_x \frac{\left(C^{n+1}_{i+1,j,k} - C^{n+1}_{i-1,j,k}\right)}{2\Delta x} - v_x\left(\frac{C^{n}_{i+1,j,k} - C^{n}_{i-1,j,k}}{2\Delta x}\right) \\ &+ D_y\left(\frac{\left(C^{n+1}_{i,j+1,k} - 2C^{n+1}_{i,j,k} + C^{n+1}_{i,j-1,k}\right)}{2(\Delta y)^2}\right) + D_y\left(\frac{\left(C^{n}_{i,j+1,k} - 2C^{n}_{i,j,k} + C^{n}_{i,j-1,k}\right)}{2(\Delta y)^2}\right) \\ &+ D_z \frac{\left(C^{n+1}_{i,j,k+1} - 2C^{n+1}_{i,j,k} + C^{n+1}_{i,j,k-1}\right)}{(\Delta z)^2} + 2D_z\left(\frac{\left(C^{n}_{i,j,k+1} - 2C^{n}_{i,j,k} + C^{n}_{i,j,k-1}\right)}{(\Delta z)^2}\right) \end{aligned} \quad (1.20)$$

The equation above gives us;

where $r_x = \frac{\Delta t}{(\Delta x)^2}$, $r_y = \frac{\Delta t}{(\Delta y)^2}$, $r_z = \frac{\Delta t}{(\Delta z)^2}$, $m_x = \frac{\Delta t}{\Delta x}$, and $i = 1,2............I - 1$, $j = 1,2...............J - 1$, and $k = 1,2...................K - 1$.

$$-\left(\frac{V_x m_x}{2R(C_{i,j,k})}+\frac{D_x r_x}{R(C_{i,j,k})}\right)C^{n+1}_{i-1,j,k}-\frac{D_y r_y}{2R(C_{i,j,k})}C^{n+1}_{i,j-1,k}-\frac{D_z r_z}{2R(C_{i,j,k})}C^{n+1}_{i,j,k-1}$$

$$+\left(1+\frac{2D_x r_x}{R(C_{i,j,k})}+\frac{D_y r_y}{R(C_{i,j,k})}+\frac{D_z r_z}{R(C_{i,j,k})}\right)C^{n+1}_{i,j,k}$$

$$-\left(\frac{D_x r_x}{R(C_{i,j,k})}+\frac{D_x m_x}{2R(C_{i,j,k})}\right)C^{n+1}_{i+1,j,k}-\frac{D_y r_y}{2R(C_{i,j,k})}C^{n+1}_{i,j+1,k}-\frac{D_z r_z}{2R(C_{i,j,k})}C^{n+1}_{i,j,k+1}$$

$$=\left(\frac{D_x r_x}{R(C_{i,j,k})}-\frac{V_x m_x}{2R(C_{i,j,k})}\right)C^{n}_{i-1,j,k}+\frac{D_y r_y}{2R(C_{i,j,k})}C^{n}_{i,j-1,k}+\frac{D_z r_z}{2R(C_{i,j,k})}C^{n}_{i,j,k-1}$$

$$-\left(1+\frac{D_x r_x}{R(C_{i,j,k})}-\frac{D_y r_y}{2R(C_{i,j,k})}-\frac{D_z r_z}{2R(C_{i,j,k})}\right)C^{n}_{i,j,k}+\left(\frac{D_x r_x}{R(C_{i,j,k})}-\frac{V_x m_x}{2R(C_{i,j,k})}\right)C^{n}_{i+1,j,k}$$

$$+\frac{D_y r_y}{2R(C_{i,j,k})}C^{n}_{i,j+1,k}+\frac{D_z r_z}{2R(C_{i,j,k})}C^{n}_{i,j,k+1} \quad (1.21)$$

$$TR=0\left[(\Delta t)^2,(\Delta x)^2,(\Delta y)^2,(\Delta z)^2\right]$$

The matrix generated by Crank & Nicolson Method has the best accuracy and unconditionally stable but its main disadvantage is the matrix generated is expensive (or Complicated) to solve.

Model Equation Solution
ADI Method

Peaceman and Rachford [1] and Douglas and Gunn[3] developed a variation on the Crank & Nicolson approximation which is known as ADI Method. Douglas & Gunn scheme is more relevant for our calculation.

2.3.2 Douglas & Gunn Method

This numerical method is an alternative solution method which instead of solving 3D problem solves a succession of three one dimensional problems. The breakdown of the method is explained diagrammatically as shown below.

STEP: X Implicit

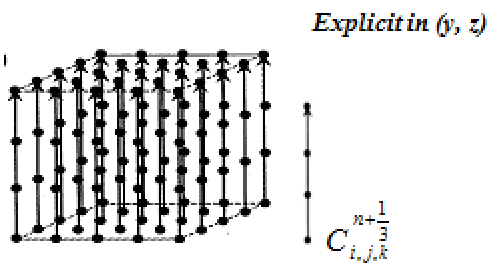

Figure.2.

STEP: Y Implicit

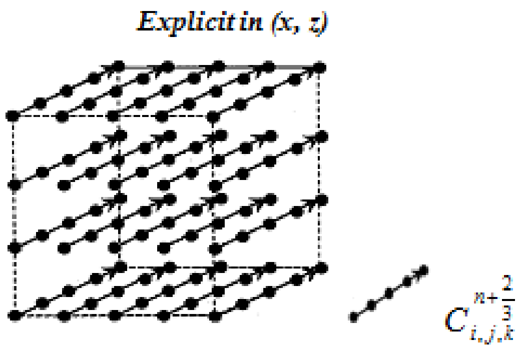

Figure.3.

STEP3: Z Implicit

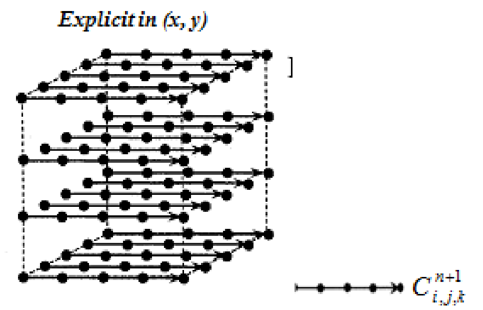

Figure.4.

Douglas and Gunn [3] modified the Crank Nicolson method and developed a general ADI scheme that is unconditionally stable and retains second order accuracy when applied to 3D problems. This approach exploits the understanding that Implicit numerical methods are stable in one-dimension problem but do not guarantee stability in multi-dimensional problems. The incorporation of Thomas algorithm is based on the fact that the inversions of matrices produced by explicit numerical methods are easier to solve compared to those of implicit numerical methods but require smaller time intervals

Based on Douglas and Gunn approach we rewrite our equation as follows;

$$R(C)\left(C^{n+1}-C^{n}\right)=D_x r_x\left(\partial_x^2\left(C^{n+1}+C^{n}\right)-\frac{v_x m_x}{2}\left(\partial_x\left(C^{n+1}+C^{n}\right)\right)\right)$$

$$+\frac{D_y r_y}{2}\partial_y^2\left(C^{n+1}+C^{n}\right)+\frac{D_z r_z}{2}\partial_z^2\left(C^{n+1}+C^{n}\right) \quad (1.23)$$

Instead of directly solving the equation at time step n, we solve the same equation at three sub-time steps;

Step 1:-

$$R(C)\left(C^{n+\frac{1}{3}}-C^{n}\right)=D_x r_x\partial_x^2\left(C^{n+\frac{1}{3}}+C^{n}\right)-\frac{v_x m_x}{2}\partial_x\left(C^{n+\frac{1}{3}}+C^{n}\right)$$

$$+D_y r_y\partial_y^2 C^{n}+D_z r_z\partial_z^2 C^{n} \quad (1.24)$$

Step 2:-

$$R(C)\left(C^{n+\frac{2}{3}}-C^{n}\right)=D_x r_x\partial_x^2\left(C^{n+\frac{1}{3}}+C^{n}\right)-\frac{v_x m_x}{2}\partial_x\left(C^{n+\frac{1}{3}}+C^{n}\right)$$

$$+\frac{D_y r_y}{2}\partial_y^2\left(C^{n+\frac{2}{3}}+C^{n}\right)+D_z r_z\partial_z^2\left(C^{n}\right) \quad (1.25)$$

Step 3:- $R(C)\left(C^{n+1}-C^{n}\right)=D_x r_x \partial_x^2\left(C^{n+\frac{1}{3}}+C^{n}\right)-\frac{v_x m_x}{2}\partial_x\left(C^{n+\frac{1}{3}}+C^{n}\right)$

$$+\frac{D_y r_y}{2}\partial_y^2\left(C^{n+\frac{2}{3}}+C^{n}\right)+\frac{D_z r_z}{2}\partial_z^2\left(C^{n+1}+C^{n}\right) \quad (1.26)$$

Expanding the equation in the steps above

Step 1

$$R\left(C_{i,j,k}\right)\left(C_{i,j,k}^{n+1}-C_{i,j,k}^{n}\right)=D_x r_x\left[\left(C_{i+1,j,k}^{n+\frac{1}{3}}-2C_{i,j,k}^{n+\frac{1}{3}}+C_{i-1,j,k}^{n+\frac{1}{3}}\right)+\left(C_{i+1,j,k}^{n}-2C_{i,j,k}^{n}+C_{i-1,j,k}^{n}\right)\right]$$

$$-\frac{V_x m_x}{2}\left[\left(C_{i+1,j,k}^{n+\frac{1}{3}}-C_{i-1,j,k}^{n+\frac{1}{3}}\right)+\left(C_{i+1,j,k}^{n}-C_{i-1,j,k}^{n}\right)\right]$$

$$+D_y r_y\left[\left(C_{i,j+1,k}^{n}-2C_{i,j,k}^{n}+C_{i,j-1,k}^{n}\right)+D_z r_z\left(C_{i,j,k+1}^{n}-2C_{i,j,k}^{n}+C_{i,j,k-1}^{n}\right)\right] \quad (1.27)$$

Step 2

$$R\left(C_{i,j,k}\right)\left(C_{i,j,k}^{n+\frac{2}{3}}-C_{i,j,k}^{n}\right)=D_x r_x\left[\left(C_{i+1,j,k}^{n+\frac{1}{3}}-2C_{i,j,k}^{n+\frac{1}{3}}+C_{i-1,j,k}^{n+\frac{1}{3}}\right)+\left(C_{i+1,j,k}^{n}-2C_{i,j,k}^{n}+C_{i-1,j,k}^{n}\right)\right]$$

$$-\frac{V_x m_x}{2}\left[\left(C_{i+1,j,k}^{n+\frac{1}{3}}-C_{i-1,j,k}^{n+\frac{1}{3}}\right)+\left(C_{i+1,j,k}^{n}-C_{i-1,j,k}^{n}\right)\right]$$

$$+\frac{D_y r_y}{2}\left[\left(C_{i,j+1,k}^{n+\frac{2}{3}}-2C_{i,j,k}^{n+\frac{2}{3}}+C_{i,j-1,k}^{n+\frac{2}{3}}\right)+\left(C_{i,j+1,k}^{n}-2C_{i,jk}^{n}+C_{i,j-1,k}^{n}\right)\right]$$

$$+D_z r_z\left[C_{i,j,k+1}^{n}-2C_{i,j,k}^{n}+C_{i,j,k-1}^{n}\right] \quad (1.28)$$

Step 3

$$R\left(C_{i,j,k}\right)\left(C_{i,j,k}^{n+1}-C_{i,j,k}^{n}\right)=D_x r_x\left[\left(C_{i+1,j,k}^{n+\frac{1}{3}}-2C_{i,j,k}^{n+\frac{1}{3}}+C_{i-1,j,k}^{n+\frac{1}{3}}\right)+\left(C_{i+1,j,k}^{n}-2C_{i,j,k}^{n}+C_{i-1,j,k}^{n}\right)\right]$$

$$-\frac{V_x m_x}{2}\left[\left(C_{i+1,j,k}^{n+\frac{1}{3}}-C_{i-1,j,k}^{n+\frac{1}{3}}\right)+\left(C_{i+1,j,k}^{n}-C_{i-1,j,k}^{n}\right)\right]$$

$$+\frac{D_y r_y}{2}\left[\left(C_{i,j+1,k}^{n+\frac{2}{3}}-2C_{i,j,k}^{n+\frac{2}{3}}+C_{i,j-1,k}^{n+\frac{2}{3}}\right)+\left(C_{i,j+1,k}^{n}-2C_{i,jk}^{n}+C_{i,j-1,k}^{n}\right)\right]$$

$$+\frac{D_z r_z}{2}\left[\left(C_{i,j,k+1}^{n+1}-2C_{i,j,k}^{n+1}+C_{i,j,k-1}^{n+1}\right)+\left(C_{i,j,k+1}^{n}-2C_{i,j,k}^{n}+C_{i,j,k-1}^{n}\right)\right] \quad 1.29)$$

Rearranging Douglas & Gunn equation gives us the equation which provides the matrix of solving the model equation;

Stage 1; Implicit in x direction, explicit in (y, z) directions

$$-\left(\frac{V_x m_x}{2R\left(C^{n}{}_{i,j,k}\right)}+\frac{D_x r_x}{R\left(C^{n}{}_{i,j,k}\right)}\right)C_{i-1,j,k}^{n+\frac{1}{3}}+\left(1+\frac{2D_x r_x}{R\left(C^{n}{}_{i,j,k}\right)}\right)C_{i,j,k}^{n+\frac{1}{3}}+\left(\frac{V_x m_x}{2R\left(C^{n}{}_{i,j,k}\right)}-\frac{D_{x_i} r_x}{R\left(C^{n}{}_{i,j,k}\right)}\right)C_{i+1,j,k}^{n+\frac{1}{3}}$$

$$=\left(\frac{D_x r_x}{R\left(C^{n}{}_{i,j,k}\right)}-\frac{V_x m_x}{2R\left(C^{n}{}_{i,j,k}\right)}\right)C_{i-1,j,k}^{n}+\frac{D_y r_y}{R\left(C^{n}{}_{i,j,k}\right)}C_{i,j-1,k}^{n}+\frac{D_z r_z}{R\left(C^{n}{}_{i,j,k}\right)}C_{i,j,k-1}^{n}$$

$$+\left(1-\frac{2D_x r_x}{R\left(C^{n}{}_{i,j,k}\right)}-\frac{2D_y r_y}{R\left(C^{n}{}_{i,j,k}\right)}-\frac{2D_z r_z}{R\left(C^{n}{}_{i,jk}\right)}\right)C_{i,j,k}^{n}+\left(\frac{D_x r_x}{R\left(C^{n}{}_{i,j,k}\right)}+\frac{V_x m_x}{2R\left(C^{n}{}_{i,j,k}\right)}\right)C_{i+1,j,k}^{n}$$

$$+\frac{D_y r_y}{R\left(C^{n}{}_{i,j,k}\right)}C_{i,j+1,k}^{n}+\frac{D_z r_z}{R\left(C^{n}{}_{i,j,k}\right)}C_{i,j,k+1}^{n} \quad (1.30)$$

Stage 2; Implicit in y direction, explicit in (x, z) directions

$$-\frac{D_y r_y}{2R\left(C_{i,j,k}^{n}\right)}C_{i,j-1,k}^{n+\frac{2}{3}}+\left(1+\frac{D_y r_y}{R\left(C_{i,j,k}^{n}\right)}\right)C_{i,j,k}^{n+\frac{2}{3}}-\frac{D_y r_y}{2R\left(C_{i,j,k}^{n}\right)}C_{i,j+1,k}^{n+\frac{2}{3}}=\frac{D_x r_x}{R\left(C_{i,j,k}^{n}\right)}C_{i-1,j,k}^{n+\frac{1}{3}}+\frac{V_x m_x}{2R\left(C_{i,j,k}^{n}\right)}C_{i-1,j,k}^{n+\frac{1}{3}}$$

$$
+\frac{D_x r_x}{R\left(C^n_{i,j,}\right)}C^n_{i-1,j,k}+\frac{V_x m_x}{2R\left(C^n_{i,j,k}\right)}C^n_{i-1,j,k}+\frac{D_y r_y}{2R\left(C^n_{i,j,k}\right)}C^n_{i,j-1,k}+\frac{D_z r_z}{R\left(C^n_{i,j,k}\right)}C^n_{i,j,k-1}
$$

$$
+\left(C^n_{i,j,k}-\frac{2D_x r_x}{R\left(C^n_{i,j,k}\right)}C^{n+\frac{1}{3}}_{i,j,k}-\frac{2D_x r_x}{R\left(C^n_{i,j,k}\right)}C^n_{i,j,k}-\frac{D_y r_y}{R\left(C^n_{i,j,k}\right)}C^n_{i,j,k}-\frac{2D_z r_z}{R\left(C^n_{i,j,k}\right)}C^n_{i,j,k}\right)
$$

$$
+\left(\begin{array}{l}\frac{D_x r_x}{R\left(C^n_{i,j,k}\right)}C^{n+\frac{1}{3}}_{i+1,j,k}+\frac{D_x r_x}{R\left(C^n_{i,j,k}\right)}C^n_{i+1,j,k}-\frac{V_x m_x}{2R\left(C^n_{i,j,k}\right)}C^{n+\frac{1}{3}}_{i+1,j,k}-\frac{V_x m_x}{2R\left(C^n_{i,j,k}\right)}C^n_{i+1,j,k}+\frac{D_y r_y}{2R\left(C^n_{i,j,k}\right)}C^n_{i,j+1,k}\\+\frac{D_Z r_z}{R\left(C^n_{i,j,k}\right)}C^n_{i,j,k+1}\end{array}\right) \quad (1.31)
$$

Step 3; Implicit in z direction, explicit in (x, y) direction

$$
-\frac{D_z r_z}{2R\left(C^n_{i,j,k}\right)}C^{n+1}_{i,j,k-1}+\left(1+\frac{D_z r_z}{R\left(C_{i,j,k}\right)}\right)C^{n+1}_{i,j,k}-\frac{D_z r_z}{2R\left(C^n_{i,j,k}\right)}C^{n+1}_{i,j,k+1}
$$

$$
=\left(\begin{array}{l}\frac{D_x r_x}{R\left(C^n_{i,j,k}\right)}C^{n+\frac{1}{3}}_{i-1,j,k}+\frac{V_x m_x}{2R\left(C^n_{i,j,k}\right)}C^n_{i-1,j,k}+\frac{V_x m_x}{2R\left(C^n_{i,j,k}\right)}C^{n+\frac{1}{3}}_{i-1,j,k}+\frac{D_x r_x}{2R\left(C^n_{i,j,k}\right)}C^n_{i-1,j,k}+\frac{D_y r_y}{2R\left(C^n_{i,j,k}\right)}C^{n+\frac{2}{3}}_{i,j-1,k}\\+\frac{D_y r_y}{2R\left(C^n_{i,j,k}\right)}C^n_{i,j-1,k}+\frac{D_z r_z}{2R\left(C^n_{i,j,k}\right)}C^n_{i,j,k-1}\end{array}\right)
$$

$$
+\left(C^n_{i,j,k}-\frac{2D_x r_x}{R\left(C^n_{i,j,k}\right)}C^{n+\frac{1}{3}}_{i,j,k}-\frac{2D_x r_x}{R\left(C^n_{i,j,k}\right)}C^n_{i,j,k}-\frac{D_y r_y}{R\left(C^n_{i,j,k}\right)}C^{n+\frac{2}{3}}_{i,j,k}-\frac{D_y r_y}{R\left(C^n_{i,j,k}\right)}C^n_{i,j,k}-\frac{D_z r_z}{R\left(C^n_{i,j,k}\right)}C^n_{i,j,k}\right)
$$

$$
+\left(\begin{array}{l}\frac{D_x r_x}{R\left(C^n_{i,j,k}\right)}C^{n+\frac{1}{3}}_{i+1,j,k}+\frac{D_x r_x}{R\left(C^n_{i,j,k}\right)}C^n_{i+1,j,k}-\frac{V_x m_x}{2R\left(C^n_{i,j,k}\right)}C^{n+\frac{1}{3}}_{i+1,j,k}-\frac{V_x m_x}{2R\left(C_{i,j,k}\right)}C^n_{i+1,j,k}+\frac{D_y r_y}{2R\left(C^n_{i,j,k}\right)}C^{n+\frac{2}{3}}_{i,j+1,k}\\+\frac{D_y r_y}{2R\left(C^n_{i,j,k}\right)}C^n_{i,j+1,k}+\frac{D_z r_z}{2R\left(C^n_{i,j,k}\right)}C^n_{i,j,k+1}\end{array}\right) \quad (1.32)
$$

The above is the solution to the model equation, which are equations (1.30), (1.31) and (.32).

Let $A'_i=\frac{D_{x_i} r_x}{R\left(C^n_{i,j,k}\right)}$, $B'_i=\frac{V_{x_i} m_x}{R\left(C^n_{i,j,k}\right)}$, $C'_j=\frac{D_{y_{ji}} r_y}{R\left(C^n_{i,j,k}\right)}$ and $D'_k=\frac{D_{z_k} r_z}{R\left(C^n_{i,j,k}\right)}$

I=1,2……..,I, j=1,2,……………………J and k=1,2,………………K

In each of the three steps, we have $I+1$ equations for each of (j,k), $J+1$ equations for each of (i,k) and $K+1$ for each of (i,j) value. We also have three unknown values in variables in each step. In all the three cases, the tridiagonal matrix can be solved by use of Thomas algorithm [16]. In numerical algebra, the triadiagonal matrix (TDMA), also known as the Thomas algorithm, which is simplified form of Gaussian elimination that can be used to solve numerical equations like this. The triadiagonal system of one dimension for n unknown may be written as;

$$
a_i x_{i-1}+b_i x_i+c_i x_{i+1}=d_i \quad (1.33)
$$

Where $a_1=0$ and $c_n=0$ This algorithm is only applicable to matrixes that are diagonally dominant, as illustrated below;

$$
\begin{bmatrix}
b_1 & c_1 & & & & & & & 0\\
a_2 & b_2 & c_2 & & & & & & \\
 & a_3 & b_3 & c_3 & & & & & \\
 & & - & - & - & & & & \\
 & & & - & - & - & & & \\
 & & & & - & - & - & & \\
 & & & & & - & - & - & \\
 & & & & & & - & - & - \\
 & & & & & & & - & - & c_{n-1}\\
0 & & & & & & & & a_n & b_n
\end{bmatrix}
\begin{bmatrix} x_1\\ x_2\\ x_3\\ -\\ -\\ -\\ -\\ -\\ x_{n-1}\\ x_n \end{bmatrix}
=
\begin{bmatrix} d_1\\ d_2\\ d_3\\ -\\ -\\ -\\ -\\ -\\ d_{n-1}\\ d_n \end{bmatrix} \quad (1.34)
$$

The first step consists of modifying the coefficients as follows, denoting the new modified coefficients with primes

$$
c'=\begin{cases}\frac{c_i}{b_i};i=1\\ \frac{c_i}{b_i-c'_{i-1}a_i};i=2,3,.......n-1\end{cases} \quad (1.35)
$$

$$
d'_i=\begin{cases}\frac{d_i}{b_i};i=1\\ \frac{d_i-d_{i-1}a_i}{b_i-c'_{i-1}a_i};i=2,3,..........n-1\end{cases} \quad (1.36)
$$

This is a forward sweep. The solution is obtained by back substitution;

$$x_n = d'_n$$

$$x_i = d'_i - c'_i x_{i+1}; i = n-1, n-2, ..., 1 \quad (1.36b)$$

This will be the method that will be applied in find the solution in the equations,

Theorem 1: The ADI Method used in solving the model equation is unconditionally stable.

Proof: -
The three-dimension equation;
Douglas and Gunn [1964] derived an ADI scheme based on ‘’approximating factoring’’ that is unconditionally stable and retains second order accuracy when applied to three dimensions' schemes.
A development of the scheme that highlights the approximate factorization point of view is best carried out making use of a *delta* form of the equation. A delta form expresses the unknown quantity as the change from a known value of the variable of interest. Here we use a time delta and defined $C^{n+1}_{i,j,k} = C^n_{i,j,k} + \Delta C_{i,j,k}$.
(1.37)
In this analysis, the discrete Fourier transform of the non-homogeneous is used so as to establish taking, $C^n_{i,j,k} = \sum_{ijk} \hat{C}^n_{i,j,k} e^{\kappa\theta_x i} e^{\kappa\theta_y j} e^{\kappa\theta_z k}$,
(1.38)
$\kappa = \sqrt{-1}$
$\theta_x = 2\pi\omega_x x_i$, $\theta_y = 2\pi\omega_y y_j$, and $\theta_z = 2\pi\omega_z z_k$.
$i = 0,1,................, I-1$, $j = 0,1,...........J-1$, and $k = 0,1,..........., K-1$,
$-\pi \le \theta_x, \theta_y, \theta_z \le \pi$, and $\omega = (\omega_x, \omega_y, \omega_z)$
using the discretization and Fourier transform for equations (1.37) to (1.38) the to the equations below

Stage 1

$$\left(1 - A'_i\partial_x^2 + \frac{1}{2}B'_i\partial_x\right)C^{n+\frac{1}{3}} = \left(1 + A'_i\partial_x^2 - \frac{1}{2}B'_i\partial_x + \frac{1}{2}C'_j\partial_y^2 + \frac{1}{2}D'_k\partial_z^2\right)C^n \quad (1.39)$$

Equation (5.39) becomes;

$$C^{n+\frac{1}{3}}_{i,j,k} - A'_i\left(C^{n+\frac{1}{3}}_{i+1,j,k} - 2C^{n+\frac{1}{3}}_{i,j,k} + C^{n+\frac{1}{3}}_{i-1,j,k}\right) + \frac{B'_i}{2}\left(C^{n+\frac{1}{3}}_{i+1,j,k} - C^{n+\frac{1}{3}}_{i-1,j,k}\right) = \begin{bmatrix} C^n_{i,j,k} + A'_i\left(C^n_{i+1,j,k} - 2C^n_{i,j,k} + C_{i-1,j,k}\right) \\ -\frac{B'_i}{2}\left(C^n_{i+1,j,k} - C^n_{i-1,j,k}\right) \\ +\frac{1}{2}C'_j\left(C^n_{i,j+1,k} - 2C^n_{i,j,k} + C^n_{i,j-1,k}\right) \\ +\frac{1}{2}D'_k\left(C^n_{i,j,k+1} - 2C^n_{i,j,k} + C^n_{i,j,k}\right) \end{bmatrix} (1.40)$$

Using equation (5.38), we find the following expression;

$$\left[1 - A'_i\left(\frac{e^{\kappa\theta_x} + e^{-\kappa\theta_x}}{2} - 1\right) + B'_i\kappa\left(\frac{e^{\kappa\theta_x} - e^{-\kappa\theta_x}}{2}\right)\right]\hat{C}^{n+\frac{1}{3}}_{i,j,k} = \begin{bmatrix} 1 + 2A'_i\left(\frac{e^{\kappa\theta_x} + e^{-\kappa\theta_x}}{2} - 1\right) - B'_i\kappa\left(\frac{e^{\kappa\theta_x} - e^{\kappa\theta_x}}{2\kappa}\right) \\ 2C'_j\left(\frac{e^{\kappa\theta_y} + e^{-\kappa\theta_y}}{2} - 1\right) + 2D'_k\left(\frac{e^{\kappa\theta_z} + e^{-\kappa\theta_z}}{2} - 1\right) \end{bmatrix}\hat{C}^n_{i,j,k}$$

(1.41)

From basic trigonometry, $Sin\theta = \frac{e^{\kappa\theta} - e^{-\kappa\theta}}{2i}$ and $Cos\theta = \frac{e^{\kappa\theta} + e^{-\kappa\theta}}{2}$. Therefore;

$$\left[1 - 2A'_i(Cos\theta_x - 1) + B_i\kappa Sin\theta_x\right]\hat{C}^{n+\frac{1}{3}}_{i,j,k} = \left[1 + 2A'_i(Cos\theta_x - 1) - B'_i\kappa Sin\theta_x + 2C'_j(Cos\theta_y - 1) + 2D'_k(Cos\theta_z - 1)\right]\hat{C}^n_{i,j,k} \quad (1.42)$$

$$Cos\theta = Cos^2\frac{\theta}{2} - Sin^2\frac{\theta}{2}, \; Sin^2\frac{\theta}{2} + Cos^2\frac{\theta}{2} = 1 \text{ and } Sin\theta = 2Sin\frac{\theta}{2}Cos\frac{\theta}{2},$$

Therefore,

$$\left[1 + 4A'_i Sin^2\frac{\theta_x}{2} + 2\kappa B'_i Sin\frac{\theta_x}{2}Cos\frac{\theta_x}{2}\right]\hat{C}^{n+\frac{1}{3}}_{i,j,k} = \begin{bmatrix} 1 - 4A'_i Sin^2\frac{\theta_x}{2} - 2B'_i\kappa Sin\frac{\theta_x}{2}Cos\frac{\theta_x}{2} \\ -4C'_j Sin\frac{\theta_y}{2} - 4D'_k Sin\frac{\theta_z}{2} \end{bmatrix}\hat{C}^n_{i,j,k} \quad (1.43)$$

The amplification factor $\xi^{\frac{1}{3}}$ is given as;

$$\left[1+4A_i'Sin^2\frac{\theta_x}{2}+2\kappa B_i'Sin\frac{\theta_x}{2}Cos\frac{\theta_x}{2}\right]\xi^{\frac{1}{3}}=\left[1-4A_i'Sin^2\frac{\theta_x}{2}-2B_i'\kappa Sin\frac{\theta_x}{2}Cos\frac{\theta_x}{2}-4C_j'Sin^2\frac{\theta_y}{2}-4D_k'Sin^2\frac{\theta_z}{2}\right] \quad (1.44)$$

Where $\theta_x=\theta_y=\theta_z=\theta=m\Pi; m\in I,J,K$, and let $\xi^{\frac{1}{3}}=G_x$

$$|G_x|=\left[\frac{\left|\left(1-4A_i'Sin^2\frac{\theta_x}{2}-4C_j'Sin^2\frac{\theta_y}{2}-4D_k'Sin^2\frac{\theta_z}{2}\right)^2+\left(-2B_i'Sin\frac{\theta_x}{2}Cos\frac{\theta_x}{2}\right)^2\right|}{\left|\left(1+4A_i'Sin^2\frac{\theta_x}{2}\right)^2+\left(2B_i'Sin\frac{\theta_x}{2}Cos\frac{\theta_x}{2}\right)^2\right|}\right]\le 1 \quad (1.45)$$

Stage 2

$$C^{n+\frac{2}{3}}-\frac{1}{2}C_j'\partial_y^2C^{n+\frac{2}{3}}=C^n+A_i'\partial_x^2C^{n+\frac{1}{3}}-\frac{1}{2}B_i'\partial_xC^{n+\frac{1}{3}}+A_i'\partial_x^2C^n-\frac{1}{2}B_i'\partial_xC^n+\frac{1}{2}C_j'\partial_y^2C^n+D_k'\partial_z^2\left(C^n\right)$$

(1.46)

Following the same process as in stage 1;

$$\left(1+2C_j'Sin^2\frac{\theta_y}{2}\right)\hat{C}_{i,j,k}^{n+\frac{2}{3}}=\left[1-4A_i'Sin^2\frac{\theta_x}{2}-2C_j'Sin^2\frac{\theta_y}{2}-4D_k'Sin^2\frac{\theta_z}{2}-2B_i'\kappa Sin\frac{\theta_x}{2}Cos\frac{\theta_x}{2}\right]\hat{C}_{i,j,k}^{n}-\left[4A_i'Sin^2\frac{\theta_x}{2}+2B_i'\kappa Sin\frac{\theta_x}{2}Cos\frac{\theta_x}{2}\right]\hat{C}_{i,j,k}^{n+\frac{1}{3}} \quad (1.47)$$

$$\hat{C}_{i,j,k}^{n+\frac{1}{3}}=\left[\frac{1-4A_i'Sin^2\frac{\theta_x}{2}-4C_j'Sin^2\frac{\theta_y}{2}-4D_k'Sin^2\frac{\theta_z}{2}-2\kappa B_i'Sin\frac{\theta_x}{2}Cos\frac{\theta_x}{2}}{1+4A_i'Sin^2\frac{\theta_x}{2}+2\kappa B_i'Sin\frac{\theta_x}{2}Cos\frac{\theta_x}{2}}\right]\hat{C}_{i,j,k}^{n}$$

Making the denominator real numbers gives us;

$$\hat{C}_{i,j,k}^{n+\frac{1}{3}}=\left(\frac{\left(1-4A_i'Sin^2\frac{\theta_x}{2}-4C_j'Sin^2\frac{\theta_y}{2}-4D_k'Sin^2\frac{\theta_z}{2}\right)\left(\left(1+4A_i'Sin^2\frac{\theta_x}{2}\right)-\left(2B_i'Sin\frac{\theta_x}{2}Cos\frac{\theta_x}{2}\right)^2\right)-\kappa\left(\left(1-4A_i'Sin^2\frac{\theta_x}{2}-4C_j'Sin^2\frac{\theta_y}{2}-4D_z'Sin^2\frac{\theta_z}{2}\right)\left(2B_i'Sin\frac{\theta_x}{2}Cos\frac{\theta_x}{2}\right)+\left(2B_j'Sin\frac{\theta_x}{2}Cos\frac{\theta_x}{2}\right)\left(1+4A_i'Sin^2\frac{\theta_x}{2}\right)\right)}{\left(1+4A_i'Sin^2\frac{\theta_x}{2}\right)^2+\left(2B_i'Sin\frac{\theta_x}{2}Cos\frac{\theta_x}{2}\right)^2}\right)$$

(5.48)

$$\xi_{i,j,k}^{n+\frac{2}{3}} = \left[\frac{\begin{array}{l}\left(1-4A_i'Sin^2\frac{\theta_x}{2}-2C_j'Sin^2\frac{\theta_y}{2}-4D_k'Sin^2\frac{\theta_z}{2}\right)\left(\left(1+4A_i'Sin^2\frac{\theta_x}{2}\right)^2+\left(\begin{array}{l}2B_i'Sin\frac{\theta_x}{2}\\ Cos\frac{\theta_x}{2}\end{array}\right)^2\right)\\ -\left[\left(1-4A_i'Sin^2\frac{\theta_x}{2}-4C_j'Sin^2\frac{\theta_y}{2}-4D_k'Sin^2\frac{\theta_z}{2}\right)\left(1+4A_i'Sin^2\frac{\theta_x}{2}\right)\right]\left(4A_i'Sin^2\frac{\theta_x}{2}\right)\\ +\left[\left(2B_i'Sin\frac{\theta_x}{2}Cos\frac{\theta_x}{2}\right)^2\left(4A_i'Sin^2\frac{\theta_x}{2}\right)\right]\\ -\kappa\left[\begin{array}{l}\left[\begin{array}{l}\left(1-4A_i'Sin^2\frac{\theta_x}{2}-4C_j'Sin^2\frac{\theta_y}{2}-4D_k'Sin^2\frac{\theta_z}{2}\right)\left(1+4A_i'Sin^2\frac{\theta_x}{2}\right)\\ +\left(2B_i'Sin\frac{\theta_x}{2}Cos\frac{\theta_x}{2}\right)^2\end{array}\right]\left(2B_i'Sin\frac{\theta_x}{2}Cos\frac{\theta_x}{2}\right)\\ +\left(4A_i'Sin^2\frac{\theta_x}{2}\right)\left(1-4A_i'Sin^2\frac{\theta_x}{2}-4C_j'Sin^2\frac{\theta_x}{2}-4D_k'Sin^2\frac{\theta_z}{2}\right)\left(2B_i'Sin\frac{\theta_x}{2}Cos\frac{\theta_x}{2}\right)\\ +\left(1+4A_i'Sin^2\frac{\theta_x}{2}\right)\left(2B_i'Sin\frac{\theta_x}{2}Cos\frac{\theta_x}{2}\right)\\ +\left(2B_i'Sin\frac{\theta_x}{2}Cos\frac{\theta_x}{2}\right)\left(\left(1+4A_i'\sin^2\frac{\theta_x}{2}\right)^2+\left(2B_i'Sin\frac{\theta_x}{2}Cos\frac{\theta_x}{2}\right)^2\right)\end{array}\right]\end{array}}{\left(1+2C_j'Sin^2\frac{\theta_y}{2}\right)\left(\left(1+4A_i'Sin^2\frac{\theta_x}{2}\right)^2+\left(2B_i'Sin\frac{\theta_x}{2}Cos\frac{\theta_x}{2}\right)^2\right)}\right]$$

$$\hat{C}_{i,jk}^{n}$$

The amplification factor $\xi^{\frac{2}{3}}$ is given above;

Where $\theta_x = \theta_y = \theta_z = \theta = m\Pi; m \in I, J, K$, and let $\xi^{\frac{2}{3}} = G_y$

$$\left|G_y\right| = \frac{\left|\begin{bmatrix} \left(1-4A_i'Sin^2\frac{\theta_x}{2}-2C_j'Sin^2\frac{\theta_y}{2}-4D_k'Sin^2\frac{\theta_z}{2}\right)\left(\left(1+4A_i'Sin^2\frac{\theta_x}{2}\right)^2+\left(2B_i'Sin\frac{\theta_x}{2}Cos\frac{\theta_x}{2}\right)^2\right) \\ -\left(1-4A_i'Sin^2\frac{\theta_x}{2}-4C_j'Sin^2\frac{\theta_y}{2}-4D_k'Sin^2\frac{\theta_z}{2}\right)\left(\left(1+4A_i'Sin^2\frac{\theta_x}{2}\right)\left(4A_i'Sin^2\frac{\theta_x}{2}\right)\right) \\ -\left(4A_i'Sin^2\frac{\theta_x}{2}\right)\left(2B_i'Sin\frac{\theta_x}{2}Cos\frac{\theta_x}{2}\right)^2 \end{bmatrix}^2 + \begin{bmatrix} \left(-\left(1-4A_i'Sin^2\frac{\theta_x}{2}-4C_j'Sin^2\frac{\theta_y}{2}-4D_k'Sin^2\frac{\theta_z}{2}\right)\right)\left(2B_i'Sin\frac{\theta_x}{2}Cos\frac{\theta_x}{2}\right) \\ -\begin{pmatrix} \left(1+4A_i'Sin^2\frac{\theta_x}{2}\right)\left(2B_i'Sin\frac{\theta_x}{2}Cos\frac{\theta_x}{2}\right)\left(1-4A_i'Sin^2\frac{\theta_x}{2}-4C_j'Sin^2\frac{\theta_y}{2}-4D_k'Sin^2\frac{\theta_z}{2}\right) \\ +\left(2B_i'Sin\frac{\theta_x}{2}Cos\frac{\theta_x}{2}\right)^3 \end{pmatrix} \\ -\left(1+4A_i'Sin^2\frac{\theta_x}{2}\right)\left(2B_i'Sin\frac{\theta_x}{2}Cos\frac{\theta_x}{2}\right) \\ -\left(2B_i'Sin\frac{\theta_x}{2}Cos\frac{\theta_x}{2}\right)\left(\left(1+4A_i'Sin^2\frac{\theta_x}{2}\right)^2+\left(2Sin\frac{\theta_x}{2}Cos\frac{\theta_x}{2}\right)^2\right) \end{bmatrix}^2\right|}{\left|\left[\left(1+2C_j'Sin^2\frac{\theta_y}{2}\right)\left(\left(1+4A_i'Sin^2\frac{\theta_x}{2}\right)^2+\left(2B_i'Sin\frac{\theta_x}{2}Cos\frac{\theta_x}{2}\right)^2\right)\right]^2\right|} \tag{1.49}$$

Stage 3

$$R(C)\left(C^{n+1}-C^n\right) = D_x r_x \partial_x^2\left(C^{n+\frac{1}{3}}+C^n\right) - \frac{v_x m_x}{2}\partial_x\left(C^{n+\frac{1}{3}}+C^n\right) + \frac{D_y r_y}{2}\partial_y^2\left(C^{n+\frac{2}{3}}+C^n\right) + \frac{D_z r_z}{2}\partial_z^2\left(C^{n+1}+C^n\right) \tag{1.50}$$

Following the process in Stage 3;

$$\left(1+2D_k'Sin^2\frac{\theta_z}{2}\right)\hat{C}_{i,j,k}^{n+1} = \left[1-4A_i'Sin^2\frac{\theta_x}{2}-2C_j'Sin^2\frac{\theta_y}{2}-2D_k'Sin^2\frac{\theta_z}{2}-2B_i'\kappa Sin\frac{\theta_x}{2}Cos\frac{\theta_x}{2}\right]\hat{C}_{i,j,k}^{n} - \left[4A_i'Sin^2\frac{\theta_x}{2}+2B_i'\kappa Sin\frac{\theta_x}{2}Cos\frac{\theta_x}{2}\right]\hat{C}_{i,j,k}^{n+\frac{1}{3}} - 2C_j'Sin^2\frac{\theta_y}{2}\hat{C}_{i,j,k}^{n+\frac{2}{3}} \tag{1.51}$$

$$+\kappa\left[\frac{\begin{array}{l}-\left(2B_i'Sin\frac{\theta_x}{2}Cos\frac{\theta_x}{2}\right)\left(1+2C_j'Sin^2\frac{\theta_y}{2}\right)\left(\left(1+4A_i'Sin^2\frac{\theta_x}{2}\right)^2+\left(2B_i'Sin\frac{\theta_x}{2}Cos\frac{\theta_x}{2}\right)^2\right)\\
-\left(2B_i'Sin\frac{\theta_x}{2}Cos\frac{\theta_x}{2}\right)\left(1+2C_j'Sin^2\frac{\theta_z}{2}\right)\left(\begin{array}{l}\left(1-4A_i'Sin^2\frac{\theta_x}{2}-4C_j'Sin^2\frac{\theta_y}{2}-4D_k'Sin^2\frac{\theta_z}{2}\right)\left(1+4A_i'Sin^2\frac{\theta_x}{2}\right)\\-\left(2B_i'Sin\frac{\theta_x}{2}Cos\frac{\theta_x}{2}\right)^2\end{array}\right)\\
-4A_i'Sin^2\frac{\theta_x}{2}\left(\begin{array}{l}\left(1-4A_i'Sin^2\frac{\theta_x}{2}-4C_j'Sin^2\frac{\theta_y}{2}-4D_k'Sin^2\frac{\theta}{2}\right)\left(2B_i'Sin\frac{\theta_x}{2}Cos\frac{\theta_x}{2}\right)\\-\left(2B_i'Sin^2\frac{\theta_x}{2}Cos\frac{\theta_x}{2}\right)\left(1+4A_i'Sin^2\frac{\theta_x}{2}\right)\end{array}\right)\\
-\left(\left(1+4A_i'Sin^2\frac{\theta_x}{2}\right)^2+\left(2B_i'Sin\frac{\theta_x}{2}Cos\frac{\theta_x}{2}\right)\right)\left(2B_i'Sin\frac{\theta_x}{2}Cos\frac{\theta_x}{2}\right)\left(2C_j'Sin^2\frac{\theta_x}{2}\right)\\
-\left(2C_j'Sin^2\frac{\theta_y}{2}\right)\left(\left(1+4A_i'Sin^2\frac{\theta_x}{2}\right)\left(2B_i'Sin\frac{\theta_x}{2}Cos\frac{\theta}{2}\right)\left(1-4A_i'Sin^2\frac{\theta_x}{2}-4C_j'Sin^2\frac{\theta_y}{2}-4D_k'Sin^2\frac{\theta_z}{2}\right)\right)\\
-\left(2C_j'Sin^2\frac{\theta}{2}\right)\left(2B_i'Sin\frac{\theta_x}{2}Cos\frac{\theta_x}{2}\right)\left(1-4A_i'Sin^2\frac{\theta}{2}-4C_j'Sin^2\frac{\theta_y}{2}-4D_k'Sin^2\frac{\theta_z}{2}\right)\\
-\left(2B_i'Sin\frac{\theta_x}{2}Cos\frac{\theta_x}{2}\right)\left(1+4A_i'Sin^2\frac{\theta_x}{2}\right)\left(2C_j'Sin^2\frac{\theta_y}{2}\right)\end{array}}{}\right]$$

$$
\hat{C}_{i,j,k}^{n+1}\left[\left(\frac{\begin{aligned}
&\left(\left(1-4A_i'Sin^2\frac{\theta_x}{2}-2C_j'Sin^2\frac{\theta_y}{2}-2D_k'Sin^2\frac{\theta_z}{2}\right)\left(1+2C_j'Sin^2\frac{\theta_y}{2}\right)\right.\\
&\left.\left(\left(1+4A_i'Sin^2\frac{\theta_x}{2}\right)^2+\left(2B_i'Sin\frac{\theta_x}{2}Cos\frac{\theta_x}{2}\right)^2\right)\right)\\
&-\left(\left(4A_i'Sin^2\frac{\theta_x}{2}\right)\left(1+4A_i'Sin^2\frac{\theta_x}{2}\right)\left(1-4A_i'Sin^2\frac{\theta_x}{2}4C_j'Sin^2\frac{\theta_y}{2}-4D_k'Sin^2\frac{\theta_z}{2}\right)\right)\\
&-\left(2B_i'Sin\frac{\theta_x}{2}Cos\frac{\theta_x}{2}\right)^2\left(1+2C_j'Sin^2\frac{\theta_x}{2}\right)\\
&-\left(2C_j'Sin^2\frac{\theta_y}{2}\right)\left(\begin{aligned}
&\left(1-4A_i'Sin^2\frac{\theta_x}{2}-2C_j'Sin^2\frac{\theta_y}{2}-4D_k'Sin^2\frac{\theta_z}{2}\right)\\
&\left(\left(1+4A_i'Sin^2\frac{\theta_x}{2}\right)^2+\left(2B_i'Sin\frac{\theta_x}{2}Cos\frac{\theta_x}{2}\right)\right)\\
&-\left(1-4A_i'Sin^2\frac{\theta_x}{2}-4C_j'Sin^2\frac{\theta_y}{2}-4D_k'Sin^2\frac{\theta_z}{2}\right)\left(4A_i'Sin^2\frac{\theta_x}{2}\right)\left(1+4A_i'Sin^2\frac{\theta_x}{2}\right)\\
&+\left(4A_i'Sin^2\frac{\theta_x}{2}\right)\left(2B_i'Sin\frac{\theta_x}{2}Cos\frac{\theta_x}{2}\right)^2
\end{aligned}\right)\\
&-\left[\begin{aligned}
&\left(1-4A_i'Sin^2\frac{\theta_x}{2}-4C_j'Sin^2\frac{\theta_y}{2}-4D_k'Sin^2\frac{\theta_z}{2}\right)2B_i'Sin\frac{\theta_x}{2}Cos\frac{\theta_x}{2}\\
&-\left(1+4A_i'Sin^2\frac{\theta_x}{2}\right)\left(2B_i'Sin\frac{\theta_x}{2}Cos\frac{\theta_x}{2}\right)
\end{aligned}\right]\left(2B_i'Sin\frac{\theta_x}{2}Cos\frac{\theta_x}{2}\right)
\end{aligned}}{\left(1+2D_k'Sin^2\frac{\theta}{2}\right)\left(1+2C_j'Sin^2\frac{\theta_y}{2}\right)\left(\left(1+4A_i'Sin^2\frac{\theta_x}{2}\right)^2+\left(2B_i'Sin\frac{\theta_x}{2}Cos\frac{\theta_x}{2}\right)^2\right)}\right)\right] \quad 1.52)
$$

$$
\xi_{i,j,k}^{n+1}\left[\left(\frac{\begin{array}{l}
\left(\begin{array}{l}\left(1-4A_i'Sin^2\frac{\theta_x}{2}-2C_j'Sin^2\frac{\theta_y}{2}-2D_k'Sin^2\frac{\theta_z}{2}\right)\left(1+2C_j'Sin^2\frac{\theta_y}{2}\right)\\
\left(\left(1+4A_i'Sin^2\frac{\theta_x}{2}\right)^2+\left(2B_i'Sin\frac{\theta_x}{2}Cos\frac{\theta_x}{2}\right)^2\right)\end{array}\right)\\
-\left(\left(4A_i'Sin^2\frac{\theta_x}{2}\right)\left(1+4A_i'Sin^2\frac{\theta_x}{2}\right)\left(1-4A_i'Sin^2\frac{\theta_x}{2}4C_j'Sin^2\frac{\theta_y}{2}-4D_k'Sin^2\frac{\theta_z}{2}\right)\right)\\
-\left(2B_i'Sin\frac{\theta_x}{2}Cos\frac{\theta_x}{2}\right)^2\left(1+2C_j'Sin^2\frac{\theta_x}{2}\right)\\
-\left(2C_j'Sin^2\frac{\theta_y}{2}\right)\left(\begin{array}{l}\left(1-4A_i'Sin^2\frac{\theta_x}{2}-2C_j'Sin^2\frac{\theta_y}{2}-4D_k'Sin^2\frac{\theta_z}{2}\right)\\
\left(\left(1+4A_i'Sin^2\frac{\theta_x}{2}\right)^2+\left(2B_i'Sin\frac{\theta_x}{2}Cos\frac{\theta_x}{2}\right)\right)\\
-\left(1-4A_i'Sin^2\frac{\theta_x}{2}-4C_j'Sin^2\frac{\theta_y}{2}-4D_k'Sin^2\frac{\theta_z}{2}\right)\left(4A_i'Sin^2\frac{\theta_x}{2}\right)\left(1+4A_i'Sin^2\frac{\theta_x}{2}\right)\\
+\left(4A_i'Sin^2\frac{\theta_x}{2}\right)\left(2B_i'Sin\frac{\theta_x}{2}Cos\frac{\theta_x}{2}\right)^2\end{array}\right)\\
-\left[\begin{array}{l}\left(1-4A_i'Sin^2\frac{\theta_x}{2}-4C_j'Sin^2\frac{\theta_y}{2}-4D_k'Sin^2\frac{\theta_z}{2}\right)2B_i'Sin\frac{\theta_x}{2}Cos\frac{\theta_x}{2}\\
-\left(1+4A_i'Sin^2\frac{\theta_x}{2}\right)\left(2B_i'Sin\frac{\theta_x}{2}Cos\frac{\theta_x}{2}\right)\end{array}\right]\left(2B_i'Sin\frac{\theta_x}{2}Cos\frac{\theta_x}{2}\right)
\end{array}}{\left(1+2D_k'Sin^2\frac{\theta}{2}\right)\left(1+2C_j'Sin^2\frac{\theta_y}{2}\right)\left(\left(1+4A_i'Sin^2\frac{\theta_x}{2}\right)^2+\left(2B_i'Sin\frac{\theta_x}{2}Cos\frac{\theta_x}{2}\right)^2\right)}\right)\right]
$$

$$
+\kappa\left[\frac{\begin{array}{l}
-\left(2B_i'Sin\frac{\theta_x}{2}Cos\frac{\theta_x}{2}\right)\left(1+2C_j'Sin^2\frac{\theta_y}{2}\right)\left(\left(1+4A_i'Sin^2\frac{\theta_x}{2}\right)^2+\left(2B_i'Sin\frac{\theta_x}{2}Cos\frac{\theta_x}{2}\right)^2\right)\\
-\left(2B_i'Sin\frac{\theta_x}{2}Cos\frac{\theta_x}{2}\right)\left(1+2C_j'Sin^2\frac{\theta_z}{2}\right)\left(\begin{array}{l}\left(1-4A_i'Sin^2\frac{\theta_x}{2}-4C_j'Sin^2\frac{\theta_y}{2}-4D_k'Sin^2\frac{\theta_z}{2}\right)\left(1+4A_i'Sin^2\frac{\theta_x}{2}\right)\\-\left(2B_i'Sin\frac{\theta_x}{2}Cos\frac{\theta_x}{2}\right)^2\end{array}\right)\\
-4A_i'Sin^2\frac{\theta_x}{2}\left(\begin{array}{l}\left(1-4A_i'Sin^2\frac{\theta_x}{2}-4C_j'Sin^2\frac{\theta_y}{2}-4D_k'Sin^2\frac{\theta}{2}\right)\left(2B_i'Sin\frac{\theta_x}{2}Cos\frac{\theta_x}{2}\right)\\-\left(2B_i'Sin^2\frac{\theta_x}{2}Cos\frac{\theta_x}{2}\right)\left(1+4A_i'Sin^2\frac{\theta_x}{2}\right)\end{array}\right)\\
-\left(\left(1+4A_i'Sin^2\frac{\theta_x}{2}\right)^2+\left(2B_i'Sin\frac{\theta_x}{2}Cos\frac{\theta_x}{2}\right)\right)\left(2B_i'Sin\frac{\theta_x}{2}Cos\frac{\theta_x}{2}\right)\left(2C_j'Sin^2\frac{\theta_x}{2}\right)\\
-\left(2C_j'Sin^2\frac{\theta_y}{2}\right)\left(\left(1+4A_i'Sin^2\frac{\theta_x}{2}\right)\left(2B_i'Sin\frac{\theta_x}{2}Cos\frac{\theta}{2}\right)\left(1-4A_i'Sin^2\frac{\theta_x}{2}-4C_j'Sin^2\frac{\theta_y}{2}-4D_k'Sin^2\frac{\theta_z}{2}\right)\right)\\
-\left(2C_j'Sin^2\frac{\theta}{2}\right)\left(2B_i'Sin\frac{\theta_x}{2}Cos\frac{\theta_x}{2}\right)\left(1-4A_i'Sin^2\frac{\theta}{2}-4C_j'Sin^2\frac{\theta_y}{2}-4D_k'Sin^2\frac{\theta_z}{2}\right)\\
-\left(2B_i'Sin\frac{\theta_x}{2}Cos\frac{\theta_x}{2}\right)\left(1+4A_i'Sin^2\frac{\theta_x}{2}\right)\left(2C_j'Sin^2\frac{\theta_y}{2}\right)
\end{array}}{\quad}\right]
$$

(1.53)

$$G_z=\xi^{\,n+1}$$

Let $Sin\frac{\theta_x}{2}=S_x, Cos\frac{\theta_x}{2}=C_x, Sin\frac{\theta_y}{2}=S_y, Sin\frac{\theta_z}{2}=S_z$

$$
|G_z| = \left[\left[\frac{
\begin{array}{l}
\left(\begin{array}{l}
(1-4A'_iS_x^2-2C'_jS_y^2-2D'_iS_y^2)(1+2C_j^2S_y^2)\left((1+4A'_iS_x^2)^2+(B'_xS_xC_x)^2\right)\\
-(4A'_iS_x^2)(1+2C'_jS_y^2)\left((1-4A'_iS_x^2-4C'_jS_y^2-D'_kS_z^2)(1+4A'_iS_x^2)-(2B'_iS_xC_x)^2\right)\\
-(2C'_jS_y^2)\left[\begin{array}{l}(1-4A'_iS_x^2-2C'_jS_y^2-4D'_kS_z^2)\left((1+4A'_xS_x^2)^2+(2B'_iS_xC_x)^2\right)\\(1-4A'_iS_x^2-4C'_yS_y^2-4D'_kS_z^2)(4A'_iS_x^2)(1+4A'_iS_x^2)\\+(4A'_iS_x^2)(2B'_iS_xC_x)\end{array}\right]\\
-\left((1-4A'_iS_x^2-4C'_jS_y^2-4D'_kS_z^2)(2B'_iS_xC_x)-(2B'_iS_xS_x)(1-4A'_iS_x^2)\right)
\end{array}\right)^2\\
+\left(\begin{array}{l}
-(2B'_iS_xC_x)(1+2C'_jS_y^2)\left((1+4A'_iS_x^2)^2+(2B'_iS_xC_x)^2\right)\\
-(2B'_iS_xC_x)(1+2C'_jS_y^2)\left((1-4A'_iS_x^2-4C'_jS_y^2-4D'_kS_z^2)(2B'_iS_xC_x)-(2B'_iS_xC_x)^2\right)\\
-(2B'_iS_xC_x)(2C'_jS_y^2)\left((1+4A'_iS_x^2)^2+(2B'_iS_xC_x)^2\right)\\
-(2C'_jS_y^2)\left((1+4A'_iS_x^2)(2B'_iS_xC_x)(1-4A'_iS_x^2-4C'_jS_y^2-4D'_kS_z^2)-(2B'_iS_xC_x)\right)\\
-(2C'_jS_y^2)(2B'_iS_xC_x)(1-4A'_iS_x^2-4C'_jS_y^2-4D'_kS_z^2)\\
-(2B'_iS_xC_x)(1+4A'_iS_x^2)(2C'_jS_y^2)
\end{array}\right)^2
\end{array}
}{\left((1+2D'_kS_z^2)(1+2C'_jS_y^2)\left((1+4A'_iS_x^2)^2+(2B'_iS_xC_x)^2\right)\right)^2}\right]\right]
$$

$$|G_x||G_y||G_z| = |G_xG_yG_z| = |G| \le 1$$

From the details above, the nominator is diminishing and denominator increasing therefore the theorem is right.

(1.54)

2.3.3 Determination of time step using stability criteria

Fourier or Von Neumann Stability analysis

Using Fourier transform,

$$C_{i,j,k}^n = \sum \hat{C}_{i,j,k}^n e^{\kappa\theta_x i} e^{\kappa\theta_y j} e^{\kappa\theta_z k} \text{ and let } \Delta x = \Delta y = \Delta z = h \qquad (1.55)$$

$$C_{i,j,k}^{n+1} = C_{i,j,k}^n + \Delta C_{i,j,k}\,. \quad (1.56)$$

Fitting this in the model equation (5.18);

$$, \quad R(C)\frac{\partial C}{\partial t} = 2D_x\frac{\partial^2 C}{\partial x^2} - 2v_x\frac{\partial C}{\partial x} + D_y\frac{\partial^2 C}{\partial y^2} + D_z\frac{\partial^2 C}{\partial z^2}$$

Using equation (5.55),

Fourier transforms give;

$$R\left(\hat{C}_{i,j,k}^n\right)\frac{\partial \hat{C}_{x,y,z}}{\partial t} = \hat{C}_{i,j,k}^n\left(\frac{4D_x(Cos\theta_x - 1)}{h^2} - \frac{V_x\kappa Sin\theta_x}{h} + \frac{2D_y(Cos\theta_y - 1)}{h^2} + \frac{2D_z(Cos\theta_z - 1)}{h^2}\right)$$

(1.57)

Define;

From equation (1.56)

$$R\left(\hat{C}_{i,j,k}\right)\Delta\hat{C}(\theta_x,\theta_y,\theta_z) = \Delta t\hat{C}_{i,j,k}^n\left(-\frac{8D_x}{h^2}Sin^2\frac{\theta_x}{2} - \frac{4D_y}{h^2}Sin^2\frac{\theta_y}{2} - \frac{4D_z}{h^2}Sin^2\frac{\theta_z}{2} - \frac{V_x}{h}\kappa Sin\theta_x\right)$$

A particular time stepping scheme will be stable provided $\hat{C}$ lies in its stability region. To simplify the discussion suppose that the stability region is contained in an ellipse:

Stability Region: A: $\left(\frac{x}{\alpha_0}\right)^2 + \left(\frac{y}{\beta_0}\right)^2 \le 1$ (1.58)

If real and imaginary parts $\hat{C}$ are;

$$\hat{C} = \Re(\hat{C}) + i\Im(\hat{C}) \quad (1.59)$$

then the scheme is stable provided,

$$\left(\frac{\Re(\hat{C})}{\alpha_0}\right)^2 + \left(\frac{\Im(\hat{C})}{\beta_0}\right)^2 \le 1$$

which implies that;

$$\left[\left(-\frac{4\Delta t}{\alpha_0 h^2}\right)^2 \left(2D_x Sin^2\frac{\theta_x}{2} + D_y Sin^2\frac{\theta_y}{2} + D_z Sin^2\frac{\theta_z}{2}\right)^2 - \left(\frac{-\Delta t}{\beta_0 h}\right)^2 (v_x Sin\theta_x)^2\right] \le 1 \quad (1.60)$$

which can be a sufficient condition, using $\theta_x = \theta_y = \theta_z = \theta = \frac{\pi}{2}$

Maximum value of a sine function is realized at $\frac{\pi}{2}$

$$\left[\left(\frac{-4\Delta t}{\alpha_0 h^2}\right)^2 \left(\frac{D_x}{1} + \frac{D_y}{2} + \frac{D_z}{2}\right)^2 - \left(\frac{-\Delta t}{\beta_0 h}\right)^2 v_x^2\right] \le 1$$

Implying that;

$$\Delta t \le \left|\left[\left(\frac{-4}{\alpha_0 h^2}\right)^2 \left(\frac{D_x}{1} + \frac{D_y}{2} + \frac{D_z}{2}\right)^2 - \left(\frac{-v_x}{\beta_0 h}\right)^2\right]^{-1}\right| \quad (1.61)$$

$\alpha_0 and \beta_0$ are constants which can assumed to be equal to 1.

2.3.4-Determination of fractional step using stability in Multispace dimensions

Model Equation (5.18)

$$R(C)\frac{\partial C}{\partial t} = 2D_x \frac{\partial^2 C}{\partial x^2} - 2v_x \frac{\partial C}{\partial x} + D_y \frac{\partial^2 C}{\partial y^2} + D_z \frac{\partial^2 C}{\partial z^2}$$

$$0 \le x, y, z \le 1$$

$$C(x, y, z, 0) = C_0(x, y, z)$$

$$C \ \ and \ \ C_0 \quad 1 \ \ Period$$

Discretization in space,

$$R(C)\frac{dC}{dt} = \left[2D_{x_i} D_{+x} D_{-x} C_{i,j,k} - 2v_{x_i} D_{+x} C_{i,j,k} + D_{y_j} D_{+y} D_{-y} C_{i,j,k} + D_{z_k} D_{+z} D_{-z} C_{i,j,k}\right] \quad (1.62)$$

$$i = 0,1,2,\ldots\ldots\ldots\ldots\ldots\ldots, N-1$$

$$j = 0,1,2\ldots\ldots\ldots\ldots\ldots\ldots\ldots N-1$$

$$k = 0,1,2\ldots\ldots\ldots\ldots\ldots\ldots\ldots N-1$$

$$\theta_x = 2\pi\omega_x x_i \qquad \theta_y = 2\pi\omega_y y_j \qquad \theta_z = 2\pi\omega_z z_k$$

$$R(C)\frac{dC_w}{dt} = \Delta t\left(-\left(\frac{8D_x Sin^2\frac{\theta_x}{2}}{h_x^2}\right) - \left(\frac{4D_y Sin^2\frac{\theta_y}{2}}{h_y^2}\right) - \left(\frac{4D_z Sin^2\frac{\theta_z}{2}}{h_z^2}\right) - \left(\frac{v_x k Sin\frac{\theta_x}{2} Cos\frac{\theta_x}{2}}{h}\right)\right) \quad (1.63)$$

And the scheme will be stable for,

$$R(C)Q(\theta_x,\theta_y,\theta_z)=\Delta t\left(-\left(\frac{8D_x Sin^2\frac{\theta_x}{2}}{h_x^2}\right)-\left(\frac{4D_y Sin^2\frac{\theta_y}{2}}{h_y^2}\right)-\left(\frac{4D_z Sin^2\frac{\theta_z}{2}}{h_z^2}\right)-\left(\frac{v_x k Sin\frac{\theta_x}{2}Cos\frac{\theta_x}{2}}{h}\right)\right) \quad (1.64)$$

For maximum value $\theta=\frac{\pi}{2}=\theta_x=\theta_y=\theta_z$,

$$\left|(Q)^2\right|=\left|\left[\left(\frac{-4\Delta t}{R(C)}\right)^2\left(\frac{2D_x}{h_x^2}+\frac{D_y}{2h_y^2}+\frac{D_z}{2h_z^2}\right)^2-\left(\frac{v_x}{2hR(C)}\right)^2\right]\right| \quad (1.65)$$

$$\Delta t=\left|(Q)^2\right|\left[\left(\frac{-4}{R(C)}\right)^2\left(\frac{2D_x}{h_x^2}+\frac{D_y}{2h_y^2}+\frac{D_z}{2h_z^2}\right)^2-\left(\frac{v_x}{2hR(C)}\right)^2\right]^{-1} \quad (1.66)$$

For Forward Euler time step, we require, $|1+Q|\le 1$

Or since $Q\in\Re$ we need $-2\le Q\le 0$

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