

DISCRETIZATION OF THREE DIMENSIONAL NON-UNIFORM GRID: CONDITIONAL MOMENT CLOSURE ELLIPTIC EQUATION USING FINITE DIFFERENCE METHOD

M.M. Noor^{1,2}, Andrew P. Wandel¹ and Talal Yusaf^{2,3}

¹Computational Engineering and Science Research Centre, School of Mechanical and Electrical Engineering, University of Southern Queensland (USQ), Australia

²Faculty of Mechanical Engineering, Universiti Malaysia Pahang (UMP), Malaysia

³National Centre for Engineering in Agriculture, USQ, Australia

Email: muhamad@ump.edu.my

ABSTRACT

In most engineering problems, the solution of meshing grid is non-uniform where fine grid is identified at the sensitive area of the simulation and coarse grid at the normal area. The purpose of the experiment is to ensure the simulation is accurate and utilizes appropriate resources. The discretization of non-uniform grid was done using Taylor expansion series and Finite Difference Method (FDM). Central difference method was used to minimize the error on the effect of truncation. The purpose of discretization is to transform the calculus problem (as continuous equation) to numerical form (as discrete equation). The steps are discretizing the continuous physical domain to discrete finite different grid and then approximate the individual partial derivative in the partial differential equation. This discretization method was used to discretize the Conditional Moment Closure (CMC) equation. The discrete form of CMC equation can be then coded using FORTRAN or MATLAB software.

Keywords: finite difference method, Taylor series, conditional moment closure, non-uniform grid, FORTRAN, MATLAB

INTRODUCTION

The fossil fuel is predicted to be the main energy resources for the next 30 years (IEA, 2009; Maczulak, 2010) Combustion of fossil fuel remains the main source of energy for power generation, transportation, domestic and industrial heating. The demand is increasing but the adequacy of the reserved is still questionable (Shafiee and Topal 2009), Combustion process not only produces heat that convert to useful energy, but also produces pollutant such as oxide of nitrogen (NO_x), soot and unburned hydrocarbon (UHC) and greenhouse gases such as carbon dioxide (CO₂). The unwanted emissions can be reduced by improving the combustion process; thereby, increasing fuel economy. Besides the experimental technique, combustion modeling is becoming more important and cost effective especially in the design and development stage. The basics of the combustion process are fluid flow and chemical reaction process. The continuity equation is very important parameters in the study of fluid flow and chemical reaction. There are various forms of the continuity equations in the Cartesian, cylindrical and spherical forms. The general form in the Cartesian coordinate of continuity equation or the conservation of mass equation is

$$\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho v) = 0 \quad (1)$$

The continuity equation for 2D geometries is given by

$$\frac{\partial \rho}{\partial t} + \frac{\partial(\rho v_x)}{\partial x} + \frac{\partial(\rho v_y)}{\partial y} = 0 \quad (2)$$

where x is axial coordinate, v_x is axial velocity, y is radial coordinate and v_y is radial velocity. For the incompressible fluid flow, density is constant, the first term in the left will be zero and therefore Eq. (2) can be summarized as

$$\frac{\partial(v_x)}{\partial x} + \frac{\partial(v_y)}{\partial y} = 0 \quad (3)$$

The conservation of momentum equation is

$$\frac{\partial(\rho v_i)}{\partial t} + \frac{\partial(\rho v_i v_j)}{\partial x_j} = -\frac{\partial(p)}{\partial x_i} + \frac{\partial(\tau_{ij})}{\partial x_j} + \rho g + F_i \quad (4)$$

where p is the static pressure, ρg is gravitational force and F is other forces. Viscous stress tensor (T_{ij}) is

$$\tau_{ij} = \mu \left(\frac{\partial v_i}{\partial x_j} + \frac{\partial v_j}{\partial x_i} \right) - \frac{2}{3} \delta_{ij} \left(\frac{\partial v_k}{\partial x_k} \right) \quad (5)$$

where μ is molecular viscosity. The momentum equation for 2D geometries is given by

$$\begin{aligned} \frac{\partial(\rho v_x)}{\partial t} + \frac{\partial(y \rho v_x v_x)}{\partial x} + \frac{\partial(y \rho v_y v_x)}{\partial y} + \frac{\partial p}{\partial x} = \frac{\partial}{\partial x} \left[\mu \left(2 \frac{\partial v_x}{\partial x} - \frac{2}{3} \left(\frac{\partial v_x}{\partial x} + \frac{\partial v_y}{\partial y} + \frac{v_x}{x} \right) \right) \right] \\ + \frac{\partial}{\partial y} \left[\mu \left(\frac{\partial v_x}{\partial y} + \frac{\partial v_y}{\partial x} \right) \right] + F_x \end{aligned} \quad (6)$$

And

$$\begin{aligned} \frac{\partial(\rho v_y)}{\partial t} + \frac{\partial(y \rho v_x v_y)}{\partial x} + \frac{\partial(y \rho v_y v_y)}{\partial y} + \frac{\partial p}{\partial y} = \frac{\partial}{\partial y} \left[\mu \left(2 \frac{\partial v_y}{\partial y} - \frac{2}{3} \left(\frac{\partial v_x}{\partial x} + \frac{\partial v_y}{\partial y} + \frac{v_y}{y} \right) \right) \right] \\ + \frac{\partial}{\partial x} \left[\mu \left(\frac{\partial v_y}{\partial x} + \frac{\partial v_x}{\partial y} \right) \right] + F_y \end{aligned} \quad (7)$$

The combustion modeling played a role in the numerical and simulation work before the experimental work is carried out. One of the main modeling in the combustion process is turbulent combustion modeling. For non-premixed combustion, the concept of Conditional Moment Closure (CMC) was independently proposed by Klimenko (1990) and Bilger (1993). The idea is the changes on using normal conventional averages to the concept of condition the reactive scalars on the mixture fraction. Klimenko has found that turbulent diffusion can be modeled much better in mixture fraction space rather than in physical space. Bilger has derived on the observation that the reactive scalars fluctuation can be associated with the mixture fraction fluctuations. By the year 1999, Klimenko and Bilger (1999) reviewed and did the extension of this concept from non-premixed to premixed turbulent combustion. The Conditional Moment Closure (CMC) equation for species a

$$\frac{\partial Q_\alpha}{\partial t} = -\langle u_i | Z \rangle \frac{\partial Q_\alpha}{\partial x_i} + \langle N | Z \rangle \frac{\partial^2 Q_\alpha}{\partial Z^2} - \frac{1}{\bar{\rho}\bar{P}(Z)} \frac{\partial}{\partial x_i} [\langle u_i'' y_\alpha'' | Z \rangle \bar{\rho}\bar{P}(Z)] + \langle w_\alpha | Z \rangle \quad (8)$$

2D elliptic CMC equation for species α need to use the cylindrical coordinate for the term $\langle u_i | Z \rangle \frac{\partial Q_\alpha}{\partial x_i}$ since the combustion chamber used is cylindrical in shape. The comparison for the Cartesian $(x, y, 0)$ and cylindrical coordinate (x, r, θ) is as below

$$\frac{\partial \phi}{\partial t} + \frac{\partial(\phi u)}{\partial x} + \frac{\partial(\phi v)}{\partial y} + \frac{\partial(\phi w)}{\partial z} = 0 \quad (9)$$

$$\frac{\partial \phi}{\partial t} + \frac{\partial(\phi u_x)}{\partial x} + \frac{\partial(\phi u_r)}{\partial r} + \frac{1}{r} \frac{\partial(\phi u_\theta)}{\partial \theta} = 0 \quad (10)$$

where for the cylindrical coordinate, x is for axial, r is for radial and θ is for azimuthal direction. The 2D elliptic CMC equation need axial and radial direction flow and becomes

$$\frac{\partial Q_\alpha}{\partial t} = -\langle u_x | Z \rangle \frac{\partial Q_\alpha}{\partial x} - \langle u_r | Z \rangle \frac{\partial Q_\alpha}{\partial r} + \langle N | Z \rangle \frac{\partial^2 Q_\alpha}{\partial Z^2} + \langle w_\alpha | Z \rangle - \frac{1}{\bar{\rho}\bar{P}(Z)} \frac{\partial}{\partial x} [\langle u_x'' y_\alpha'' | Z \rangle \bar{\rho}\bar{P}(Z)] - \frac{1}{\bar{\rho}\bar{P}(Z)} \frac{\partial}{\partial r} [\langle u_r'' y_\alpha'' | Z \rangle \bar{\rho}\bar{P}(Z)] \quad (11)$$

for the term $\langle u_i | Z \rangle \frac{\partial Q_\alpha}{\partial x_i}$ the conditional velocity $\langle u_i | Z \rangle$ which can be considered as “ u_i ” is a function of “ Z ”. For the term $\frac{1}{\bar{\rho}\bar{P}(Z)} \frac{\partial}{\partial x_i} [\langle u_i'' y_\alpha'' | Z \rangle \bar{\rho}\bar{P}(Z)]$ the modelling can be done using the Eq. (12) and (13). The conditional turbulent fluxes for any quantity of y_α'' , h'' or T'' (in general use ϕ) can be modeled with "gradient-diffusion" or "Boussinesq" approximation as below,

$$\rho \langle u'' \phi'' | Z \rangle = -D_t \frac{\partial \phi_\alpha}{\partial x} \quad (12)$$

where turbulent diffusivity (D_t) can be calculate by the relation of turbulent viscosity (μ_t) and Schmidt number (Sc_t) as below,

$$D_t = -\frac{\mu_t}{Sc_t} \quad (13)$$

Turbulent viscosity (μ_t) and Schmidt number (Sc_t) are constant. For non-premixed bluff-body flame, Schmidt number used is 1.0 (Giacomazzi et al., 2000, 2004) then the equation is summarised as below. For many cases Schmidt number is varied from 0.45 to 1.0 depending on the flow characteristics. In auto-ignition CMC simulation, $Sc_t = 0.9$ was used (Wright, 2005). For the axial direction

$$\frac{1}{\bar{\rho}\bar{P}(Z)} \frac{\partial}{\partial x} [\langle u_i'' y_\alpha'' | Z \rangle \bar{\rho}\bar{P}(Z)] = \frac{1}{\bar{\rho}\bar{P}(Z)} \frac{\partial}{\partial x} \left[-\frac{\mu_t}{Sc_t} \frac{\partial Q_\alpha}{\partial x} (\bar{P}(Z)) \right] \quad (14)$$

$$= -\frac{\mu_t}{\bar{\rho}Sc_t\bar{P}(Z)} \left[\bar{P}(Z) \frac{\partial^2 Q_\alpha}{\partial x^2} + \frac{\partial Q_\alpha}{\partial x} \frac{\partial \bar{P}(Z)}{\partial x} \right] \quad (15)$$

For the radial direction

$$\frac{1}{\bar{\rho}\tilde{P}(Z)} \frac{\partial}{\partial r} [\langle u_i'' y_\alpha'' | Z \rangle \bar{\rho}\tilde{P}(Z)] = \frac{1}{\bar{\rho}\tilde{P}(Z)} \frac{\partial}{\partial r} \left[-\frac{\mu_t}{Sc_t} \frac{\partial Q_\alpha}{\partial r} (\tilde{P}(Z)) \right] \quad (16)$$

$$= -\frac{\mu_t}{\bar{\rho}Sc_t\tilde{P}(Z)} \left[\tilde{P}(Z) \frac{\partial^2 Q_\alpha}{\partial r^2} + \frac{\partial Q_\alpha}{\partial r} \frac{\partial \tilde{P}(Z)}{\partial r} \right] \quad (17)$$

This paper discusses the discretization of the CMC combustion turbulent model using finite difference central method and Taylor expansion series. The discretization for 2D CMC elliptic equation is presented for uniform and non-uniform meshing grids.

TAYLOR EXPANSION

The implicit formulae can be derived from a Taylor series expansion. Implicit finite difference relations have been derived by many mathematicians and physicists with various way and methods (Chapra and Canale, 2006; Adam, 1975; Adam, 1977; Collatz, 1966; Rubin and Graves, 1975; Rubin and Khosla, 1977; Peyret, 1978; Peyret and Taylor, 1982; Krause, 1971; Leventhal, 1980; Hirsh, 1975; Lele, 1992; Ciment, and Leventhal, 1975;). Taylor series is a good tool to study and discretized the numerical equation since the theory provides a means to predict a function value at one point in term of the function value and its derivatives at another point. In particular, the theorem states that any smooth function can be approximated as a polynomial (Chapra and Canale, 2006). There are many different types of numerical differentiation formulation, depending on the number of point, direction of the formula and the required derivative order (Griffiths and Smith, 2006). Taylor Expansion is a useful method to reduce the error term. To calculate the value for $\phi(x + \Delta x_{+1})$ and $\phi(x + \Delta x_{-1})$ until 7th order are as below,

$$\begin{aligned} \phi(x + \Delta x_{+1}) = & \phi(x) + (\Delta x_{+1}) \frac{d\phi}{dx} \Big|_{x_0} + \frac{(\Delta x_{+1})^2}{2!} \frac{d^2\phi}{dx^2} \Big|_{x_0} + \frac{(\Delta x_{+1})^3}{3!} \frac{d^3\phi}{dx^3} \Big|_{x_0} + \frac{(\Delta x_{+1})^4}{4!} \frac{d^4\phi}{dx^4} \Big|_{x_0} + \\ & \frac{(\Delta x_{+1})^5}{5!} \frac{d^5\phi}{dx^5} \Big|_{x_0} + \frac{(\Delta x_{+1})^6}{6!} \frac{d^6\phi}{dx^6} \Big|_{x_0} + \frac{(\Delta x_{+1})^7}{7!} \frac{d^7\phi}{dx^7} \Big|_{x_0} \end{aligned} \quad (18)$$

$$\begin{aligned} \phi(x - \Delta x_{-1}) = & \phi(x) - (\Delta x_{-1}) \frac{d\phi}{dx} \Big|_{x_0} + \frac{(\Delta x_{-1})^2}{2!} \frac{d^2\phi}{dx^2} \Big|_{x_0} - \frac{(\Delta x_{-1})^3}{3!} \frac{d^3\phi}{dx^3} \Big|_{x_0} + \frac{(\Delta x_{-1})^4}{4!} \frac{d^4\phi}{dx^4} \Big|_{x_0} - \\ & \frac{(\Delta x_{-1})^5}{5!} \frac{d^5\phi}{dx^5} \Big|_{x_0} + \frac{(\Delta x_{-1})^6}{6!} \frac{d^6\phi}{dx^6} \Big|_{x_0} - \frac{(\Delta x_{-1})^7}{7!} \frac{d^7\phi}{dx^7} \Big|_{x_0} \end{aligned} \quad (19)$$

CENTRAL DIFFERENCE METHOD FOR UNIFORM GRID

Assuming Δx is constant, $\phi(x + \Delta x_{+1})$ will be $\phi(x + \Delta x)$ and $\phi(x - \Delta x_{-1})$ will be $\phi(x - \Delta x)$ as below,

$$\begin{aligned} \phi(x + \Delta x) = & \phi(x) + \Delta x \frac{d\phi}{dx} \Big|_{x_0} + \frac{\Delta x^2}{2} \frac{d^2\phi}{dx^2} \Big|_{x_0} + \frac{\Delta x^3}{6} \frac{d^3\phi}{dx^3} \Big|_{x_0} + \frac{\Delta x^4}{24} \frac{d^4\phi}{dx^4} \Big|_{x_0} + \frac{\Delta x^5}{120} \frac{d^5\phi}{dx^5} \Big|_{x_0} + \\ & \frac{\Delta x^6}{720} \frac{d^6\phi}{dx^6} \Big|_{x_0} + \frac{\Delta x^7}{5040} \frac{d^7\phi}{dx^7} \Big|_{x_0} \end{aligned} \quad (20)$$

$$\begin{aligned} \phi(x - \Delta x) = & \phi(x) - \Delta x \frac{d\phi}{dx} \Big|_{x_0} + \frac{\Delta x^2}{2} \frac{d^2\phi}{dx^2} \Big|_{x_0} - \frac{\Delta x^3}{6} \frac{d^3\phi}{dx^3} \Big|_{x_0} + \frac{\Delta x^4}{24} \frac{d^4\phi}{dx^4} \Big|_{x_0} - \frac{\Delta x^5}{120} \frac{d^5\phi}{dx^5} \Big|_{x_0} + \\ & \frac{\Delta x^6}{720} \frac{d^6\phi}{dx^6} \Big|_{x_0} - \frac{\Delta x^7}{5040} \frac{d^7\phi}{dx^7} \Big|_{x_0} \end{aligned} \quad (21)$$

Rearranging both Eq. (20) and (21) will result in the first order derivative equation. This is finite forward difference method which is calculating $\frac{d\phi}{dx}$ on the basis of forward movement from $\phi(x)$ and $\phi(x + \Delta x)$.

$$\frac{d\phi}{dx} = \frac{\phi(x+\Delta x)-\phi(x)}{\Delta x} - \frac{\Delta x}{2} \frac{d^2\phi}{dx^2} + \frac{\Delta x^2}{6} \frac{d^3\phi}{dx^3} - \frac{\Delta x^3}{24} \frac{d^4\phi}{dx^4} + \frac{\Delta x^4}{120} \frac{d^5\phi}{dx^5} - \frac{\Delta x^5}{720} \frac{d^6\phi}{dx^6} + \frac{\Delta x^6}{5040} \frac{d^7\phi}{dx^7} \quad (22)$$

This is finite backward difference method which is calculating $\frac{d\phi}{dx}$ based on backward movement from $\phi(x)$ and $\phi(x - \Delta x)$.

$$\frac{d\phi}{dx} = \frac{\phi(x)-\phi(x-\Delta x)}{\Delta x} + \frac{\Delta x}{2} \frac{d^2\phi}{dx^2} - \frac{\Delta x^2}{6} \frac{d^3\phi}{dx^3} + \frac{\Delta x^3}{24} \frac{d^4\phi}{dx^4} - \frac{\Delta x^4}{120} \frac{d^5\phi}{dx^5} + \frac{\Delta x^5}{720} \frac{d^6\phi}{dx^6} - \frac{\Delta x^6}{5040} \frac{d^7\phi}{dx^7} \quad (23)$$

This is finite central difference method which is calculating $\frac{d\phi}{dx}$ base on central movement from $\phi(x - \Delta x)$ and $\phi(x + \Delta x)$ obtained from the difference between 20 and 21.

$$\frac{d\phi}{dx} = \frac{\phi(x+\Delta x)-\phi(x-\Delta x)}{2\Delta x} - \frac{\Delta x^2}{6} \frac{d^3\phi}{dx^3} + \frac{\Delta x^4}{120} \frac{d^5\phi}{dx^5} - \frac{\Delta x^6}{5040} \frac{d^7\phi}{dx^7} \quad (24)$$

with leading error term of $O(\Delta x^2)$. Higher order finite difference method is necessary to ensure the simulations is more accurate and more error term is cancelled off by higher derivative. Using central different derivative, the addition of Eq. (20) and (21), can summarized as

$$\frac{d^2\phi}{dx^2} = \frac{\phi(x+\Delta x)-2\phi(x)+\phi(x-\Delta x)}{\Delta x^2} - \frac{\Delta x^2}{12} \frac{d^4\phi}{dx^4} + \frac{\Delta x^4}{360} \frac{d^6\phi}{dx^6} \quad (25)$$

with leading error term of $O(\Delta x^2)$. First order derivative for fifth order Taylor expansion scheme are summarized as below, for the derivative between $\phi(x + 2\Delta x)$ to $\phi(x - 2\Delta x)$

$$\frac{d\phi}{dx} = \frac{\phi(x-2\Delta x)-8\phi(x-\Delta x)+8\phi(x+\Delta x)-\phi(x+2\Delta x)}{12\Delta x} + \frac{\Delta x^4}{30} \frac{d^5\phi}{dx^5} \quad (26)$$

with leading error term of $O(\Delta x^4)$. Second order derivative for fifth order Taylor expansion scheme are summarized as below, for the derivative between $\phi(x + 3\Delta x)$ to $\phi(x - 3\Delta x)$:

$$\frac{d^2\phi}{dx^2} = \frac{-\phi(x-2\Delta x)+16\phi(x-\Delta x)-30\phi(x)+16\phi(x+\Delta x)-\phi(x+2\Delta x)}{12\Delta x^2} + \frac{\Delta x^4}{90} \frac{d^6\phi}{dx^6} \quad (27)$$

with leading error term of $O(\Delta x^4)$. Third order derivative for fifth order Taylor expansion scheme are summarized as below, for the derivative between $\phi(x + 3\Delta x)$ to $\phi(x - 3\Delta x)$:

$$\frac{d^3\phi}{dx^3} = \frac{-\phi(x-2\Delta x)+2\phi(x-\Delta x)-2\phi(x+\Delta x)+\phi(x+2\Delta x)}{2\Delta x^2} - \frac{\Delta x^2}{4} \frac{d^5\phi}{dx^5} \quad (28)$$

with leading error term of $O(\Delta x^2)$. Assuming that there is a uniform spacing of Δx , using notation that is $\phi^k = \frac{d^k y}{dx^k}$, for the Taylor series expansion, central difference derivatives can be summarized as Eq. (29):

$$\phi^k = \sum_{i=-\frac{(n-1)}{2}}^{\frac{(n-1)}{2}} z_i \phi_i + ET \quad (29)$$

Forward difference derivatives can be summarized as:

$$\phi^k = \sum_{i=0}^{n-1} z_i \phi_i + ET \quad (30)$$

Backward difference derivatives can be summarized as:

$$\phi^k = \sum_{i=-(n-1)}^0 z_i \phi_i + ET \quad (31)$$

where n is the number of points ($\phi_{-2}, \phi_{-1}, \phi_0, \phi_1, \phi_2$ is equal to five points), ET is the leading error term and z_i is the coefficient of ϕ for each point i .

CENTRAL DIFFERENCE METHOD FOR NON-UNIFORM GRID

Equation (18) multiply by $(\Delta x_{-1})^2$ and Eq. (19) multiply by $(\Delta x_{+1})^2$

$$\begin{aligned} \phi(x + \Delta x_{+1})(\Delta x_{-1})^2 &= \phi(x)(\Delta x_{-1})^2 + (\Delta x_{+1})(\Delta x_{-1})^2 \left. \frac{d\phi}{dx} \right|_{x_0} + \frac{(\Delta x_{+1})^2(\Delta x_{-1})^2}{2!} \left. \frac{d^2\phi}{dx^2} \right|_{x_0} + \\ &\frac{(\Delta x_{+1})^3(\Delta x_{-1})^2}{3!} \left. \frac{d^3\phi}{dx^3} \right|_{x_0} + \frac{(\Delta x_{+1})^4(\Delta x_{-1})^2}{4!} \left. \frac{d^4\phi}{dx^4} \right|_{x_0} + \frac{(\Delta x_{+1})^5(\Delta x_{-1})^2}{5!} \left. \frac{d^5\phi}{dx^5} \right|_{x_0} + \\ &\frac{(\Delta x_{+1})^6(\Delta x_{-1})^2}{6!} \left. \frac{d^6\phi}{dx^6} \right|_{x_0} + \frac{(\Delta x_{+1})^7(\Delta x_{-1})^2}{7!} \left. \frac{d^7\phi}{dx^7} \right|_{x_0} \end{aligned} \quad (32)$$

$$\begin{aligned} \phi(x - \Delta x_{-1})(\Delta x_{+1})^2 &= \phi(x)(\Delta x_{+1})^2 - (\Delta x_{-1})(\Delta x_{+1})^2 \left. \frac{d\phi}{dx} \right|_{x_0} + \frac{(\Delta x_{-1})^2(\Delta x_{+1})^2}{2!} \left. \frac{d^2\phi}{dx^2} \right|_{x_0} - \\ &\frac{(\Delta x_{-1})^3(\Delta x_{+1})^2}{3!} \left. \frac{d^3\phi}{dx^3} \right|_{x_0} + \frac{(\Delta x_{-1})^4(\Delta x_{+1})^2}{4!} \left. \frac{d^4\phi}{dx^4} \right|_{x_0} - \frac{(\Delta x_{-1})^5(\Delta x_{+1})^2}{5!} \left. \frac{d^5\phi}{dx^5} \right|_{x_0} + \\ &\frac{(\Delta x_{-1})^6(\Delta x_{+1})^2}{6!} \left. \frac{d^6\phi}{dx^6} \right|_{x_0} - \frac{(\Delta x_{-1})^7(\Delta x_{+1})^2}{7!} \left. \frac{d^7\phi}{dx^7} \right|_{x_0} \end{aligned} \quad (33)$$

Take the difference between Eq. (32) and (33), The $\frac{d\phi}{dx}$ is

$$\begin{aligned} \phi(x + \Delta x_{+1})(\Delta x_{-1})^2 - \phi(x - \Delta x_{-1})(\Delta x_{+1})^2 &= \phi(x)(\Delta x_{-1})^2 - \phi(x)(\Delta x_{+1})^2 + \\ &(\Delta x_{+1})(\Delta x_{-1})^2 \left. \frac{d\phi}{dx} \right|_{x_0} + (\Delta x_{-1})(\Delta x_{+1})^2 \left. \frac{d\phi}{dx} \right|_{x_0} + \frac{(\Delta x_{+1})^3(\Delta x_{-1})^2}{3!} \left. \frac{d^3\phi}{dx^3} \right|_{x_0} + \\ &\frac{(\Delta x_{-1})^3(\Delta x_{+1})^2}{3!} \left. \frac{d^3\phi}{dx^3} \right|_{x_0} + \frac{(\Delta x_{+1})^4(\Delta x_{-1})^2}{4!} \left. \frac{d^4\phi}{dx^4} \right|_{x_0} + \frac{(\Delta x_{-1})^4(\Delta x_{+1})^2}{4!} \left. \frac{d^4\phi}{dx^4} \right|_{x_0} + \\ &\frac{(\Delta x_{+1})^5(\Delta x_{-1})^2}{5!} \left. \frac{d^5\phi}{dx^5} \right|_{x_0} + \frac{(\Delta x_{-1})^5(\Delta x_{+1})^2}{5!} \left. \frac{d^5\phi}{dx^5} \right|_{x_0} + \frac{(\Delta x_{+1})^6(\Delta x_{-1})^2}{6!} \left. \frac{d^6\phi}{dx^6} \right|_{x_0} + \\ &\frac{(\Delta x_{-1})^6(\Delta x_{+1})^2}{6!} \left. \frac{d^6\phi}{dx^6} \right|_{x_0} + \frac{(\Delta x_{+1})^7(\Delta x_{-1})^2}{7!} \left. \frac{d^7\phi}{dx^7} \right|_{x_0} + \frac{(\Delta x_{-1})^7(\Delta x_{+1})^2}{7!} \left. \frac{d^7\phi}{dx^7} \right|_{x_0} \end{aligned} \quad (34)$$

The error becomes smaller and the equation will be truncated with leading error term of $O(\Delta x^2)$

$$\begin{aligned} \phi(x + \Delta x_{+1})(\Delta x_{-1})^2 - \phi(x - \Delta x_{-1})(\Delta x_{+1})^2 &= \phi(x)(\Delta x_{-1})^2 - \phi(x)(\Delta x_{+1})^2 + \\ (\Delta x_{+1})(\Delta x_{-1})^2 \frac{d\phi}{dx} + (\Delta x_{-1})(\Delta x_{+1})^2 \frac{d\phi}{dx} &+ \frac{(\Delta x_{+1})^3(\Delta x_{-1})^2}{3!} \frac{d^3\phi}{dx^3} + \frac{(\Delta x_{-1})^3(\Delta x_{+1})^2}{3!} \frac{d^3\phi}{dx^3} \end{aligned} \quad (35)$$

$$\begin{aligned} [(\Delta x_{+1})(\Delta x_{-1})^2 + (\Delta x_{-1})(\Delta x_{+1})^2] \frac{d\phi}{dx} &= \phi(x + \Delta x_{+1})(\Delta x_{-1})^2 - \phi(x - \Delta x_{-1})(\Delta x_{+1})^2 - \phi(x)[(\Delta x_{-1})^2 - (\Delta x_{+1})^2] + \\ \frac{1}{6} [(\Delta x_{+1})^3(\Delta x_{-1})^2 + (\Delta x_{-1})^3(\Delta x_{+1})^2] \frac{d^3\phi}{dx^3} \end{aligned} \quad (36)$$

$$\begin{aligned} \frac{d\phi}{dx} &= \frac{\phi(x + \Delta x_{+1})(\Delta x_{-1})^2 - \phi(x)[(\Delta x_{-1})^2 - \Delta x_{+1}^2] - \phi(x - \Delta x_{-1})(\Delta x_{+1})^2}{(\Delta x_{+1})(\Delta x_{-1})[(\Delta x_{-1}) + (\Delta x_{+1})]} \\ &+ \frac{1}{6} \frac{[(\Delta x_{+1})^3(\Delta x_{-1})^2 + (\Delta x_{-1})^3(\Delta x_{+1})^2] \frac{d^3\phi}{dx^3}}{(\Delta x_{-1})(\Delta x_{-1})[(\Delta x_{-1})(\Delta x_{-1})]} \end{aligned} \quad (37)$$

Then for three dimensional elliptic equations, first derivative is

$$\frac{d\phi}{dx} = \frac{\phi(x + \Delta x_{+1}, y, z)(\Delta x_{-1})^2 - \phi(x, y, z)[(\Delta x_{-1})^2 - (\Delta x_{+1})^2] - \phi(x - \Delta x_{-1}, y, z)(\Delta x_{+1})^2}{(\Delta x_{+1})(\Delta x_{-1})[(\Delta x_{-1}) + (\Delta x_{+1})]} \quad (38)$$

$$\frac{d\phi}{dy} = \frac{\phi(x, y + \Delta y_{+1}, z)(\Delta y_{-1})^2 - \phi(x, y, z)[(\Delta y_{-1})^2 - (\Delta y_{+1})^2] - \phi(x, y - \Delta y_{-1}, z)(\Delta y_{+1})^2}{(\Delta y_{+1})(\Delta y_{-1})[(\Delta y_{-1}) + (\Delta y_{+1})]} \quad (39)$$

$$\frac{d\phi}{dz} = \frac{\phi(x, y, z + \Delta z_{+1})(\Delta z_{-1})^2 - \phi(x, y, z)[(\Delta z_{-1})^2 - (\Delta z_{+1})^2] - \phi(x, y, z - \Delta z_{-1})(\Delta z_{+1})^2}{(\Delta z_{+1})(\Delta z_{-1})[(\Delta z_{-1}) + (\Delta z_{+1})]} \quad (40)$$

For the term $\frac{d^2\phi}{dx^2}$, the term must $\frac{d\phi}{dx}$ be cancel off. Equation (18) multiply by Δx_{-1} and Eq. (19) multiply by Δx_{+1}

$$\begin{aligned} \phi(x + \Delta x_{+1})(\Delta x_{-1}) &= \phi(x)(\Delta x_{-1}) + (\Delta x_{+1})(\Delta x_{-1}) \frac{d\phi}{dx} \Big|_{x_0} + \frac{(\Delta x_{+1})^2(\Delta x_{-1})}{2!} \frac{d^2\phi}{dx^2} \Big|_{x_0} + \\ \frac{(\Delta x_{+1})^3(\Delta x_{-1})}{3!} \frac{d^3\phi}{dx^3} \Big|_{x_0} &+ \frac{(\Delta x_{+1})^4(\Delta x_{-1})}{4!} \frac{d^4\phi}{dx^4} \Big|_{x_0} + \frac{(\Delta x_{+1})^5(\Delta x_{-1})}{5!} \frac{d^5\phi}{dx^5} \Big|_{x_0} + \frac{(\Delta x_{+1})^6(\Delta x_{-1})}{6!} \frac{d^6\phi}{dx^6} \Big|_{x_0} + \\ &\frac{(\Delta x_{+1})^7(\Delta x_{-1})}{7!} \frac{d^7\phi}{dx^7} \Big|_{x_0} \end{aligned} \quad (41)$$

$$\begin{aligned} \phi(x - \Delta x_{-1})(\Delta x_{+1}) &= \phi(x)(\Delta x_{+1}) - (\Delta x_{-1})(\Delta x_{+1}) \frac{d\phi}{dx} \Big|_{x_0} + \frac{(\Delta x_{-1})^2(\Delta x_{+1})}{2!} \frac{d^2\phi}{dx^2} \Big|_{x_0} - \\ \frac{(\Delta x_{-1})^3(\Delta x_{+1})}{3!} \frac{d^3\phi}{dx^3} \Big|_{x_0} &+ \frac{(\Delta x_{-1})^4(\Delta x_{+1})}{4!} \frac{d^4\phi}{dx^4} \Big|_{x_0} - \frac{(\Delta x_{-1})^5(\Delta x_{+1})}{5!} \frac{d^5\phi}{dx^5} \Big|_{x_0} + \frac{(\Delta x_{-1})^6(\Delta x_{+1})}{6!} \frac{d^6\phi}{dx^6} \Big|_{x_0} - \\ &\frac{(\Delta x_{-1})^7(\Delta x_{+1})}{7!} \frac{d^7\phi}{dx^7} \Big|_{x_0} \end{aligned} \quad (42)$$

Take the summation of the Eq. (41) and (42), Then $\frac{d^2\phi}{dx^2}$ is

$$\begin{aligned} \phi(x + \Delta x_{+1})(\Delta x_{-1}) + \phi(x - \Delta x_{-1})(\Delta x_{+1}) &= \phi(x)(\Delta x_{-1}) + \phi(x)(\Delta x_{+1}) + \\ \frac{(\Delta x_{+1})^2(\Delta x_{-1})}{2!} \frac{d^2\phi}{dx^2} \Big|_{x_0} &+ \frac{(\Delta x_{-1})^2(\Delta x_{+1})}{2!} \frac{d^2\phi}{dx^2} \Big|_{x_0} + \frac{(\Delta x_{+1})^3(\Delta x_{-1})}{3!} \frac{d^3\phi}{dx^3} \Big|_{x_0} - \frac{(\Delta x_{-1})^3(\Delta x_{+1})}{3!} \frac{d^3\phi}{dx^3} \Big|_{x_0} + \\ \frac{(\Delta x_{+1})^4(\Delta x_{-1})}{4!} \frac{d^4\phi}{dx^4} \Big|_{x_0} &+ \frac{(\Delta x_{-1})^4(\Delta x_{+1})}{4!} \frac{d^4\phi}{dx^4} \Big|_{x_0} + \frac{(\Delta x_{+1})^5(\Delta x_{-1})}{5!} \frac{d^5\phi}{dx^5} \Big|_{x_0} - \frac{(\Delta x_{-1})^5(\Delta x_{+1})}{5!} \frac{d^5\phi}{dx^5} \Big|_{x_0} + \end{aligned}$$

$$\frac{(\Delta x_{+1})^6(\Delta x_{-1})}{6!} \frac{d^6 \phi}{dx^6} \Big|_{x_0} + \frac{(\Delta x_{-1})^6(\Delta x_{+1})}{6!} \frac{d^6 \phi}{dx^6} \Big|_{x_0} + \frac{(\Delta x_{+1})^7(\Delta x_{-1})}{7!} \frac{d^7 \phi}{dx^7} \Big|_{x_0} - \frac{(\Delta x_{-1})^7(\Delta x_{+1})}{7!} \frac{d^7 \phi}{dx^7} \Big|_{x_0} \quad (43)$$

The error becomes smaller and the equation will be truncated with leading error term of $O(\Delta x^2)$

$$\phi(x + \Delta x_{+1})(\Delta x_{-1}) + \phi(x - \Delta x_{-1})(\Delta x_{+1}) = \phi(x)(\Delta x_{-1}) + \phi(x)(\Delta x_{+1}) + \frac{(\Delta x_{+1})^2(\Delta x_{-1})}{2!} \frac{d^2 \phi}{dx^2} + \frac{(\Delta x_{-1})^2(\Delta x_{+1})}{2!} \frac{d^2 \phi}{dx^2} + \frac{(\Delta x_{+1})^3(\Delta x_{-1})}{3!} \frac{d^3 \phi}{dx^3} - \frac{(\Delta x_{-1})^3(\Delta x_{+1})}{3!} \frac{d^3 \phi}{dx^3} \quad (44)$$

$$\frac{1}{2} [(\Delta x_{+1})^2(\Delta x_{-1})^2 + (\Delta x_{-1})^2(\Delta x_{+1})^2] \frac{d^2 \phi}{dx^2} = \phi(x + \Delta x_{+1})(\Delta x_{-1}) - \phi(x)[(\Delta x_{-1})(\Delta x_{+1})] + \phi(x - \Delta x_{-1})(\Delta x_{+1}) + \frac{1}{6} [(\Delta x_{+1})^3(\Delta x_{-1})^2 - (\Delta x_{-1})^3(\Delta x_{+1})^2] \frac{d^3 \phi}{dx^3} \quad (45)$$

$$\frac{d^2 \phi}{dx^2} = 2 \frac{\phi(x + \Delta x_{+1})(\Delta x_{-1}) - \phi(x)[(\Delta x_{-1})(\Delta x_{+1})] + \phi(x - \Delta x_{-1})(\Delta x_{+1})}{(\Delta x_{+1})(\Delta x_{-1})[(\Delta x_{+1}\Delta x_{-1})]} + \frac{1}{6} \frac{[(\Delta x_{+1})^3(\Delta x_{-1})^2(\Delta x_{-1})^3(\Delta x_{+1})]^2 \frac{d^3 \phi}{dx^3}}{(\Delta x_{+1})(\Delta x_{-1})[(\Delta x_{+1}\Delta x_{-1})]} \quad (46)$$

The term of $O(\Delta x^2)$ can be truncated and becomes the error term. Then for three dimensional equation, second derivative is

$$\frac{d^2 \phi}{dx^2} = 2 \frac{\phi(x+\Delta x_{+1},y,z)(\Delta x_{-1}) - \phi(x,y,z)[(\Delta x_{-1})+(\Delta x_{+1})] + \phi(x-\Delta x_{-1},y,z)(\Delta x_{+1})}{(\Delta x_{+1})(\Delta x_{-1})[(\Delta x_{+1})+(\Delta x_{-1})]} \quad (47)$$

$$\frac{d^2 \phi}{dy^2} = 2 \frac{\phi(x,y+\Delta y_{+1},z)(\Delta y_{-1}) - \phi(x,y,z)[(\Delta y_{-1})+(\Delta y_{+1})] + \phi(x,y-\Delta y_{-1},z)(\Delta y_{+1})}{(\Delta y_{+1})(\Delta y_{-1})[(\Delta y_{+1})+(\Delta y_{-1})]} \quad (48)$$

$$\frac{d^2 \phi}{dz^2} = 2 \frac{\phi(x,y,z+\Delta z_{+1})(\Delta z_{-1}) - \phi(x,y,z)[(\Delta z_{-1})+(\Delta z_{+1})] + \phi(x,y,z-\Delta z_{-1})(\Delta z_{+1})}{(\Delta z_{+1})(\Delta z_{-1})[(\Delta z_{+1})+(\Delta z_{-1})]} \quad (49)$$

NUMERICAL METHOD: FINITE DIFFERENCE METHOD

When the complex engineering problem comes with many dimensions and parameters, the same non-linear partial differential equations (PDEs) are used for all the problems. Solving these types of problems using analytical solutions is extremely difficult and in most cases do not have analytical solutions. Then, to solve this type of problem, numerical solution has been developed, such as finite difference method (FDM), finite element method (FEM) and finite volume method (FVM) (Fletcher, 1991; Hoftman et al., 2000, 2001; Slingerland and Kump, 2011). The FDM is a numerical method for approximating the solutions to partial differential equations by using finite difference equations. FDM uses approximate derivatives based on the properties of Taylor expansions and on the straight forward application of the definition of derivatives (Hirsh, 2007). The objective is to transform the equation from continuous form. The steps are discretizing the continuous physical domain to discrete finite different grid and then approximate the individual partial derivative in the partial differential equation. Using Taylor expansion method, partial differential equation was discretized in order to transform it to FORTRAN code.

Homogeneous CMC

The Homogenous CMC equation is

$$\frac{\partial \langle Y|Z \rangle}{\partial t} = \langle N|Z \rangle \frac{\partial^2 \langle Y|Z \rangle}{\partial Z^2} + \langle W|Z \rangle + \langle S|Z \rangle \quad (50)$$

For a passive, conserved scalar CMC equation:

$$\frac{\partial \langle Y|Z \rangle}{\partial t} = \langle N|Z \rangle \frac{\partial^2 \langle Y|Z \rangle}{\partial Z^2} \quad (51)$$

From the equation, the conditional mass fraction term $\langle Y|Z \rangle$ is mathematically written as Y to the function of Z (written as Y(Z)) and conditional scalar dissipation $\langle N|Z \rangle$ is written as N to the function of Z (written as N(Z)). Then CMC equation becomes:

$$\frac{d\phi}{dt} = N \frac{d^2\phi}{dz^2} \quad (52)$$

From Taylor expansion, equation can be summarized as

$$\frac{d\phi}{dt} = \frac{\phi(z,t+\Delta t) - \phi(z,t)}{(\Delta t)} \quad (53)$$

$$\frac{d^2\phi}{dz^2} = \frac{\phi(z+\Delta z,t) - 2\phi(z,t) + \phi(z-\Delta z,t)}{(\Delta z)^2} \quad (54)$$

The final form of CMC equation after discretize is as

$$\phi(i, j + 1) = (1 - (2 * B)) * \phi(i, j) + B * \phi(i + 1, j) + B * \phi(i - 1, j) \quad (55)$$

where $B = N \frac{\Delta t}{(\Delta z)^2}$. Equation (55) was coded in FORTRAN or MATLAB to simulate the CMC modelling (Noor et al., 2012). The parameter for the code:

dt = changing in time

dz = changing in space

TT = total time for the simulation

Two Dimensional CMC

For 2D modeling, the CMC equation

$$\begin{aligned} \frac{\partial Q_\alpha}{\partial t} = & -\langle u_x|Z \rangle \frac{\partial Q_\alpha}{\partial x} + \langle u_r|Z \rangle \frac{\partial Q_\alpha}{\partial r} + \langle N|Z \rangle \frac{\partial^2 Q_\alpha}{\partial Z^2} + \langle w_\alpha|Z \rangle - \frac{1}{\bar{\rho}\bar{P}(Z)} \frac{\partial}{\partial x} [\langle u_x'' y_\alpha''|Z \rangle \bar{\rho}\bar{P}(Z)] - \\ & \frac{1}{\bar{\rho}\bar{P}(Z)} \frac{\partial}{\partial x} [\langle u_r'' y_\alpha''|Z \rangle \bar{\rho}\bar{P}(Z)] \end{aligned} \quad (56)$$

Discretization term by term

$$\frac{d\phi}{dt} = \frac{\phi_{i,j,k}^{p+1} - \phi_{i,j,k}^p}{\Delta t} \quad (57)$$

Where superscript p represents time, subscript i and j represent the coordinate system for the numerical space and k represents the mixture fraction. For non-uniform grid, Δx is not uniform

$$u \frac{d\phi}{dx} = \begin{cases} 1: \frac{u}{\Delta x_{i,j,k}^-} (\phi_{i,j,k}^p - \phi_{i-1,j,k}^p) \text{ for } u \geq 0 \\ 1: \frac{u}{\Delta x_{i,j,k}^+} (\phi_{i+1,j,k}^p - \phi_{i,j,k}^p) \text{ for } u < 0 \end{cases} \quad (58)$$

where $\Delta x_{i,j,k}^- = x_{i,j,k} - x_{i-1,j,k}$ and $\Delta x_{i,j,k}^+ = x_{i+1,j,k} - x_{i,j,k}$. For the radial direction

$$u \frac{d\phi}{dr} = \begin{cases} 1: \frac{u}{\Delta r_{i,j,k}^-} (\phi_{i,j,k}^p - \phi_{i,j-1,k}^p) \text{ for } u \geq 0 \\ 1: \frac{u}{\Delta r_{i,j,k}^+} (\phi_{i,j+1,k}^p - \phi_{i,j,k}^p) \text{ for } u < 0 \end{cases} \quad (59)$$

where $\Delta r_{i,j,k}^- = r_{i,j,k} - r_{i,j-1,k}$ and $\Delta r_{i,j,k}^+ = r_{i,j+1,k} - r_{i,j,k}$. For the $N \frac{\partial^2 \phi}{dz^2}$ the discretization is

$$N \frac{\partial^2 \phi}{dz^2} = \frac{N}{\Delta z^2} (\phi_{i,j,k+1}^p - 2\phi_{i,j,k}^p + \phi_{i,j,k-1}^p) \quad (60)$$

For three dimensional elliptic equation, from Eq. (38) and (40), the first derivative is

$$\frac{\partial \phi}{\partial x} = \frac{\phi(x+\Delta x_{+1},y,z)(\Delta x_{-1})^2 - \phi(x,y,z)[(\Delta x_{-1})^2 - (\Delta x_{+1})^2] - \phi(x-\Delta x_{-1},y,z)(\Delta x_{+1})^2}{(\Delta x_{+1})(\Delta x_{-1})[(\Delta x_{+1})+(\Delta x_{-1})]} \quad (61)$$

$$= \frac{\phi_{i+1,j,k}^p (\Delta x_{i-1})^2 - \phi_{i,j,k}^p [(\Delta x_{i-1})^2 - (\Delta x_{i+1})^2] - \phi_{i-1,j,k}^p (\Delta x_{i+1})^2}{(\Delta x_{i+1})(\Delta x_{i-1})[(\Delta x_{i+1})+(\Delta x_{i-1})]} \quad (62)$$

$$\frac{\partial \phi}{\partial y} = \frac{\phi(x,y+\Delta y_{+1},z)(\Delta y_{-1})^2 - \phi(x,y,z)[(\Delta y_{-1})^2 + (\Delta y_{+1})^2] - \phi(x,y-\Delta y_{-1},z)(\Delta y_{+1})^2}{(\Delta y_{+1})(\Delta y_{-1})[(\Delta y_{+1})+(\Delta y_{-1})]} \quad (63)$$

$$= \frac{\phi_{i,j+1,k}^p (\Delta y_{j-1})^2 - \phi_{i,j,k}^p [(\Delta y_{j-1})^2 - (\Delta y_{j+1})^2] - \phi_{i,j-1,k}^p (\Delta y_{j+1})^2}{(\Delta y_{j+1})(\Delta y_{j-1})[(\Delta y_{j+1})+(\Delta y_{j-1})]} \quad (64)$$

$$\frac{\partial \phi}{\partial z} = \frac{\phi(x,y,z+\Delta z_{+1})(\Delta z_{-1})^2 - \phi(x,y,z)(\Delta z_{-1})^2 - (\Delta z_{+1})^2 - \phi(x,y,z-\Delta z_{-1})(\Delta z_{+1})^2}{(\Delta z_{+1})(\Delta z_{-1})[(\Delta z_{+1})+(\Delta z_{-1})]} \quad (65)$$

$$= \frac{\phi_{i,j,k+1}^p (\Delta z_{k-1})^2 - \phi_{i,j,k}^p [(\Delta z_{k-1})^2 - (\Delta z_{k+1})^2] - \phi_{i,j,k-1}^p (\Delta z_{k+1})^2}{(\Delta z_{k+1})(\Delta z_{k-1})[(\Delta z_{k+1})+(\Delta z_{k-1})]} \quad (66)$$

For two dimensional elliptic equation, the cylindrical equation needs to be used since the combustion chamber is in the cylindrical shape. From Eq. (38) and (39), the first derivative is

$$\frac{\partial \phi}{\partial x} = \frac{\phi(x+\Delta x_{+1},r,\theta)(\Delta x_{-1})^2 - \phi(x,r,\theta)[(\Delta x_{-1})^2 - (\Delta x_{+1})^2] - \phi(x-\Delta x_{-1},r,\theta)(\Delta x_{+1})^2}{(\Delta x_{+1})(\Delta x_{-1})[(\Delta x_{+1})+(\Delta x_{-1})]} \quad (67)$$

$$= \frac{\phi_{i+1,j,k}^p (\Delta x_{i-1})^2 - \phi_{i,j,k}^p [(\Delta x_{i-1})^2 - (\Delta x_{i+1})^2] - \phi_{i-1,j,k}^p (\Delta x_{i+1})^2}{(\Delta x_{i+1})(\Delta x_{i-1})[(\Delta x_{i+1})+(\Delta x_{i-1})]} \quad (68)$$

$$\frac{\partial \phi}{\partial r} = \frac{\phi(x,r+\Delta r_{+1},\theta)(\Delta r_{-1})^2 - \phi(x,r,\theta)[(\Delta r_{-1})^2 - (\Delta r_{+1})^2] - \phi(x,r-\Delta r_{-1},\theta)(\Delta r_{+1})^2}{(\Delta r_{+1})(\Delta r_{-1})[(\Delta r_{+1})+(\Delta r_{-1})]} \quad (69)$$

$$= \frac{\phi_{i,j+1,k}^p (\Delta r_{j-1})^2 - \phi_{i,j,k}^p [(\Delta r_{j-1})^2 - (\Delta r_{j+1})^2] - \phi_{i,j-1,k}^p (\Delta r_{j+1})^2}{(\Delta r_{j+1})(\Delta r_{j-1})[(\Delta r_{j+1})+(\Delta r_{j-1})]} \quad (70)$$

For 2D elliptic equation, from Eq. (47) and (49), the second derivative is:

$$\frac{d^2\phi}{dx^2} = 2 \frac{\phi(x+\Delta x_{+1}, r, \theta)(\Delta x_{-1}) - \phi(x, r, \theta)(\Delta x_{-1}) - \phi(x-\Delta x_{-1}, r, \theta)(\Delta x_{+1})}{(\Delta x_{+1})(\Delta x_{-1})[(\Delta x_{+1})+(\Delta x_{-1})]} \quad (71)$$

$$= 2 \frac{\phi_{i+1,j,k}^p(\Delta x_{i-1}) - \phi_{i,j,k}^p[\Delta x_{i-1} - \Delta x_{i+1}] - \phi_{i-1,j,k}^p(\Delta x_{i+1})}{(\Delta x_{i+1})(\Delta x_{i-1})[(\Delta x_{i+1})+(\Delta x_{i-1})]} \quad (72)$$

$$\frac{d^2\phi}{dr^2} = 2 \frac{\phi(x, r+\Delta r_{+1}, \theta)(\Delta r_{-1}) - \phi(x, r, \theta)[(\Delta r_{-1}) - (\Delta r_{+1})] + \phi(x, r-\Delta r_{-1}, \theta)(\Delta r_{+1})}{(\Delta r_{+1})(\Delta r_{-1})[(\Delta r_{+1})+(\Delta r_{-1})]} \quad (73)$$

$$= 2 \frac{\phi_{i,j+1,k}^p(\Delta r_{j-1}) - \phi_{i,j,k}^p[\Delta z_{j-1} - \Delta x_{j+1}] + \phi_{i,j-1,k}^p \Delta r_{j+1}}{(\Delta r_{j+1})(\Delta r_{j-1})[(\Delta r_{j+1})+(\Delta r_{j-1})]} \quad (74)$$

Two dimensional CMC Eq. (56) can be discretised using Eq. (57), (58), (59), (60), (68), (70), (72) and (74).

CONCLUSIONS

The CMC equation was discretized in order to transform the calculus partial differential equation to algebra discrete equation. The discretization process of elliptic CMC equation was using Taylor expansion. For the small and simple fluid flow problem, uniform grid can be used, but turbulent combustion modeling, which is a very complex process, requiring the application of non-uniform grid meshing. The term by term discretization can be coded into FORTRAN or MATLAB software in order to solve the turbulent combustion modeling using CMC turbulence model.

ACKNOWLEDGMENTS

The authors would like to thank University of Southern Queensland (USQ), Ministry of Education, Malaysia (MOE), Universiti Malaysia Pahang (UMP) and Education Malaysia Australia (EMA) for providing financial support.

REFERENCES

- Adam, Y. 1975 A hermitian finite difference method for the solution of parabolic equations, *Computational Mathematics Application*, 1, 393-406.
- Adam, Y. 1977 Highly accurate compact implicit methods and boundary conditions, *Journal Computational Physics*, 24, 10-22.
- Bilger, R.W. 1993, Conditional moment closure for turbulent reacting flow, *Physics of Fluids A*, 5, 436-444.
- Chapra C.S. and Canale R.P. 2006 *Numerical methods for engineers*, McGraw Hill, 5th ed, Singapore.
- Ciment, M. and Leventhal, S.H. 1975, Higher order compact implicit schemes for the wave equation, *Mathematics Computational*, 29, 885-944
- Collatz, L. 1966 *The numerical treatment of differential equations*, Springer, Berlin.
- Fletcher, C.A.J. 1991 *Computational techniques for fluid dynamics*, Springer, Berlin
- Giacomazzi, E., Battaglia, V. and Bruno, C. 2004 The Coupling of turbulence and chemistry in a premixed bluff-body flame as studied by LES, *Combustion and Flame* 138, 320-335
- Giacomazzi, E., Bruno, C. and Favini, B. 2000 Fractal modeling of turbulent combustion, *Combustion Theory and Modelling* 4(4), 391-412.

- Griffiths D.V. and Smith IM 2006 Numerical methods for engineers, Chapman and Hall/CRC, Second Edition, New York.
- Hirsh, C. 2007 Numerical computation of internal and external flows: fundamentals of computational fluid dynamics, Butterworth-Heinemann, Vol 1, Burlington, USA.
- Hirsh, R.S. 1975, Higher order accurate difference solutions of fluid mechanics problems by a compact differencing scheme, Journal Computational Physics, 19, 20–109.
- Hoffmann, K. A. and S. T. Chiang 2000 Computational fluid dynamics for engineers, Engineering Education System, Wichita, KS,
- Hoffmann, K. A., J.-F. Dietiker, and A. Devahastin 2001 Student guide to CFD Vol. I. Engineering Education System, Wichita, KS,
- IEA. 2009 World Energy Outlook. Paris, International Energy Agency
- Klimenko, A.Y. 1990, multicomponent diffusion of various admixtures in turbulent flow, Fluid Dynamics, 25, No. 3, 327-334.
- Klimenko, A.Y. and Bilger, R.W. 1999 Conditional moment closure for turbulent combustion, Progress in Energy and Combustion Science, 25, 595-687.
- Krause, E. 1971 Mehrstellen verfahren zur integration der Grenzschicht gleichungen, DLR Mitteilungen, 71(13), 109-140.
- Lele, S.K. 1992, Compact finite differences with spectral-like resolution, Journal Computational Physics, 103(1), 16-42.
- Leventhal, S.H. 1980, The operator compact implicit method for reservoir simulation, Journal Society of Petroleum Engineering, 20, 120-128.
- Maczulak, A. 2010. Renewable energy, sources and methods, New York, USA, Facts on File Inc.
- Noor, M.M., Hairuddin, A.A., Wandel, A.P., Yusaf, T., 2012 Modelling of non-premixed turbulent combustion of hydrogen using conditional moment closure method, IOP: Materials Sciences and Engineering, 36, Paper No. 012036, 1-17.
- Peyret, R. 1978 A hermitian finite difference method for the solution of the navier–stokes equations, Proceedings First of the Conference on Numerical Methods in Laminar and Turbulent Flows, Pentech Press, Plymouth, UK 43-54.
- Peyret, R. and Taylor, T.D. 1982 Computational methods for fluid flow, Springer Verlag, NewYork.
- Rubin, S.G. and Graves, R.A. 1975 Viscous flow solutions with a cubic spline Approximation Computational Fluid, 3, 1-36.
- Rubin, S.G. and Khosla, P.K. 1977 Polynomial interpolation method for viscous flow calculations, Journal Computational Physics, 24, 217-246.
- Shafiee S. and Topal E. 2009 When will fossil fuel reserves be diminished, Energy Policy, 37(1):181-189.
- Slingerland, R. and Kump, L. 2011 Mathematical modeling, of earth’s dynamical systems, Princeton University Press, New jersey, US
- Wright, Y.M. 2005 Numerical investigation of turbulent spray combustion with conditional moment closure, PhD thesis, ETH Zurich.

NOMENCLATURE

CMC	Conditional Moment Closure
c_p	specific heat, J/kgK
D	diffusivity

g	gravitational acceleration, m/s^2
k	thermal conductivity, W/mK
N	scalar dissipation rate
P	gas pressure
P, PDF	Probability Density Function
T	temperature, K
u	velocity, m/s
V	volume, m^3
W	chemical source term
w	molecular weight of a gas mixture
Z	mixture fraction (a conserved scalar)
α	thermal diffusivity, m^2/s
μ	dynamic viscosity, $\text{Pa}\cdot\text{s}$, Ns/m
ν	kinematic viscosity, m^2/s
ρ	density or concentration of a gas, kg/m^3
$\langle \cdot \cdot \rangle$	conditional average
$\langle N Z \rangle$	conditional scalar dissipation
$\langle S Z \rangle$	conditional generation due to droplet evaporation
$\langle W Z \rangle$	conditional chemical source term
$\langle Y Z \rangle$	mass fraction of fuel