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A Review analysis on Combustion Modelling and implementation of CFD

[1]Shad Husain & [2]Bhuvan Bhasker Srivastava
[1]*Associate professor Department of Physics Shia PG College Lucknow*
[2]*Associcte Professor Department of Physics Shia PG College Lucknow*
[2]*Corresponding Author Email: bbshrivastava1@gmail.com*

Abstract
The study of the CFD in various sectors is becoming very efficient day by day. In this paper, a review on combustion modelling is presented in detail and the future scope is also discussed. Combustion modelling has become popular because of its advanced technology and easy computational work in a wide area of application. This review helps us to model the combustion process that is used for the prediction of flow temperature and emission from the various combustion systems. This study also focused on the numerical approaches used in combustion modelling. The paper includes the discussion of turbulent reacting flows' effect on the different combustion modellings.

Keywords: *Direct numerical simulation, large eddy simulation, RANS approach, EDM, modelling*

I. Introduction

Combustion modelling is the process that is applied in industry from many years. For this, many commercial software like ANSYS fluent 18.0 and 15.0 CFX provide different models for different combustion modellingswhich enable us to understand and describe the reactor and fluid flow in different time scales. Different types of combustion chambers are used in industry like swirl combustion chamber, low NOx burner, biomass furnace, combustion chamber of a gas turbine, evaporated diesel for an ATR, mixing chamber andautomobile heater etc. Basically, the study of combustion includes stoichiometry, chemical transfer, turbulence chemistry interaction and particle transport.

The phenomenon of combustion decides which model should be applied on combustion process.This phenomenon is based on the feed of fuel or oxides in the furnaces or whether it is premixed, non-premixed and partially premixed combustion.

The other factor on which combustion model applicability depends is the numerical reaction rate that can be defined by finding out the Damkohler Number;the fast chemical reaction rates are defined by a Damkholar number which is more than 1and for DA<1,it is slow.

The computational fluid dynamics study includes the pre-processing, solver and post processing.Turbulent combustion requiresa model for turbulent chemistry interaction for predicting turbulent reacting flows.The study of combustion based on the fast chemistry is done by using EDM model provided in ANSYS fluent with finite rate chemistry model. Combustion modelling introduced the model for turbulent diffusion flame that is assumed PDF used for turbulence chemistry interaction solution. Most of the researchers worked on the different combustors and used different approaches in their research that will be reviewed in this paper**.**

REVIEWED STUDY ON COMBUSTION MODELLING

Combustion modelling defines some new models for modelling of turbulent reactive flows. This modelling is done for CFD simulation of gas explosion in complex geometries such as offshore modules. The chemical reaction is also the major consideration for the study of computational fluid dynamics of combustion process. The reduction of chemical reaction mechanism is very important for reducing the computational efforts [1]. Turbulent flow shows complex instability because of high Reynolds Number that requires more efficiency for the computation [2]. Mostly, for representing the turbulence and combustion, models like Eddy Break up model type and k-ε turbulence model are used. For the calculation, these types of models strongly depend on grid size and initial value for turbulence field. Combustion modelling required the flame models to show the flame propagation. The flame models exhibit the criteria to find the burning velocity such as burning velocity model [3].The three numerical approaches are used for simulation of combustion process. Direct numerical simulation is a research tool. The flow variables such as velocity and pressure that show the complete description of turbulent flows are solved numerically as a function of space and time. This type of simulation

shows that the turbulent of the flows increases with the increase of Reynolds Number. DNS is time trusted methodology [4].

Fru *et al.* analyzed the DNS approach in his research work. The response of laminar spherical premixed CH_4- air flame kernel was done in this study. They used mechanism of methane oxidation and multi component molecular transport model. The approach was used for the investigation of effect of turbulence on consumption speed and flame speed. The equivalence ratio was taken for increasing the integral Reynolds Number and it reached up to 4513 [5].Wall bounded flows occurred in the turbulent flows unable to solve by DNS. LES was used to compute such type of flow. The literature reviewed that DNS has some limitations, that it is not suitable for flow having high Reynolds number [6]. This is because of the wide range of scale in turbulent flow. If the Reynolds number of turbulent flow is 10^4 that it is impossible to simulate even with good supercomputer. It becomes less efficient to its large computing time [7].

$N_t=\frac{T}{t_s}=\frac{L}{U}\frac{\varepsilon^{1/2}}{\vartheta}=(\frac{UL}{\vartheta})^{1/2}=Re^{1/2}$

Large eddy simulation was introduced in 1970 by Deardorff who used this approach for the simulation of the turbulent flow in a channel at infinite Reynolds Number [8,9]. Large eddy simulation is a tool for the simulation of turbulence flow in which small scale motions are modelled whereas large scale motion is explicitly resolved. Large eddy simulation approach is used for the resolution of sub-grid models[10].

Baudoin studied the LES approach for time resolved numerical simulation. LES motion defined the fluid motion. The simulation of density was done by using mixture fraction. The main aim of his study was to investigate the sensitivity of the low dynamics and mixing conditions [11].Wu and Chan used the LES approach to simulate the slot Bunsen Flame in 2D. This combination of progress variable and mixture fraction was used to describe the turbulent premixed flame with different values of equivalence ratio. The changes in equivalence ratio were described by progress variable equation applied in flame front and mixture fraction equation. The computational result was compared with experimental data. The result showed that LES approach reasonably simulates the turbulent premixed flames [12].

Pitsch *et al.*, in their paper formulated for large eddy simulation, the G equation of premixed turbulent combustion. The sub-grid burning velocity model was developed to show Damkohler's limit from large and small scale turbulence. Regime diagram for turbulent premixed combustion shows that the changes in LES filter width with changes along constant Karlovitz number lines. One thing that was also considered was the choice of filter width that changes the sub-grid burning velocity from Reynolds averaged turbulent to the laminar burning velocity, the dependence was shown to be weak[13].

Bardina *et al.* explained the rotation effect on turbulence and determined that turbulence model used an additional term to find out the effect of rotation correctly [14].The third approach RANS approach focused on mean flow and the effect of turbulence on mean flow properties. NS-equation is time averaged flow equation because of the interaction of turbulent fluctuations. To compute turbulence models, Reynolds stress scalar transport term and the system of mean flow equation is required [15]. Application of URANS was used to investigate the flow in a continuous casting tundish and of a jet in a cross flow. The author concluded that URANS and LES can be complex flow turbulence and structures [16].

DIFFERENT MODELS USED IN MODELLING COMBUSTION PROCESS

The EBU model was first revised by Spalding (1971).Eddy break up model is the model used for the study of turbulence chemistry interaction. Eddy breakup model assumes that the chemical reaction rates are limited by mixing. This approach is valid for Da>>1. Reaction between fuel and oxidizer occurs quickly, but do not take place until the separate eddies in which the reactants are found dissipate and allow the reactants to mix. Also, in premixed systems, reaction does not takes place until the eddies of hot product and cold reactants fluid mix. The eddy life time is represented by k/epsilon, where k is the turbulent kinetic energy and ε is its rate of dissipation [17–25]. Some approaches also compare the turbulent mixing limited rate with a chemical reaction rate and use the slower of the two. This algorithm is simple to code and computationally efficient [26].Liakos with his colleagues described the work on non-premixed natural gas diffusion flames. The flame producedand increased the layer of burnt gases while decreased fuel and oxidizer layer [27].

Kotochouko *et al.* introduced the use of extended EBU model to simulate the turbulent hydrogen-air combustion and compared the computational data with experimental data [28]. The aim of his study was to determine accelerated flame and space of mixture and study the environmental parameters. The extension EBU model was applicable for the chemistry and K-epsilon model for turbulence that results to be the very least

expensive and simple modeling approach. Lean hydrogen-air mixture is taken to study the behavior of combustion process [29,30]. EBU model was applied on the rectangular grid of equidistance. The mean reaction rate is defined by the ratio of turbulent kinetic energy to laminar flame velocity. As a result of this study, the researchers concluded that the model remains valid for very small domain and the validity of the model is due to less Damkohler number condition[31]. Basically, EBU model now becomes more advanced after being further introduced by Magnussen and Hjertager. It was previously used for non-premixed combustion but now also for premixed combustion [32].

Holkar *et al.* used Eddy Dissipation Model to simulate the data of boiler furnace. The coal combustion case studied computationally; was very expensive if it was to be simulated by Eddy Break up Model. The governing equations are discretized by finite volume method and simulation was run on ANSYS by k-epsilon model[33–35].

Findings of Lewis *et al.*in their paper resemble the study of modelling of compartment fires done by incorporating the complex representations of the physical and chemical processes. The introduction of a flamelet based combustion model was also studied to show the detailed chemistry. The geometrical dimension of compartment fire experiments having square shaped plane of the length 2.8 m and height 2.18 m in which ceramic fiber board insulation and a circular gas burners were also incorporated, fueled by commercial grade methane and having a diameter of 0.3 m. Numerical simulation was done by using finite volume discretization. Eddy break-up model for combustion was used for studying the mixing rate and turbulent timescales. The SOFIE simulations demonstrated that the detailed qualitative predictions of the velocity and temperature fields in compartment fires can be performed accurately [36].

PDF Flamelet Model

Generally this model is used for non-premixed combustion. The combustionprocess in which flame is turbulent and Damkohler number is greater than one, PDF flamelet model is used.

Da=$\frac{\tau_t}{\tau_c}$

Here,

τ_t=turbulent time scale,

τ_c = chemical time scale.

Whenever fast chemistry case occurs, presumed PDF approach is widely used. Mixture fraction is presented as a function of profiles and reactive species concentration for non-premixed combustion. PDF flamelet model uses the modeling equation for mixture fraction[37]. The mixture fraction is computed as:

$$\frac{\partial(\rho Z)}{\partial t}+\frac{\partial(\rho Z)}{\partial x_j}=\frac{\partial}{\partial x_j}(\rho D\frac{\partial Z}{\partial x_j})$$

Where; Z= mixture fraction.

As per modified research, presumed PDF approach was introduced for modelling the premixed turbulent flames. Lipatnico and his colleague's research explained the modified presumed PDF approaches for progress variable to averaging reaction rate in premixed and partial premixed turbulent flames [38]. The modification was done because of failure of presumed PDF for the modified presumed approaches which consisted of presumed progress value P(c) based on the mean rate. The conclusion was dictated that DNS condition applied to study the presumed PDF approaches has been failed in predicting mean more rate of produces So to resolve this problem modified resumed PDF problem, modified resumed PDF was used that showed reasonably good result.

Turbulent Premixed Combustion Model based on Zimont Theory [39]

Reaction progress variable required the solution of transport equation based on the turbulent flame speed. Progress variable defines the use of mass fraction of major species [40]. The progress variable is defined as:

$$c=\frac{\sum_{i=1}^{n}Y_i}{\sum_{i=1}^{n}Y_{i,ad}}$$

Where, n=number of products,

Y_i = mass fraction of species i,

$Y_{i,ad}$ = mass fraction of species i after complete adiabatic combustion,

If c=0 mixture is unburnt, c=1 mixture is burnt.

Pierce *et al.* described the simulation of reacting flow for Large Eddy Simulation. The indirect mapping approach was used to reduce system of tracking scalars. The only two scalars were considered for this study.

One was a mixture fraction variable and other was a progress variable. The mixture fraction variable was used for tracking the mixing of fuel and oxidizer. The progress variable was used for tracking the global extent of reaction of the local mixture. The performance was compared with the fast chemistry and steady flamelet models for predicting the concentration of species, temperature and velocity profile in a coaxial jet combustor with methane fuel. That approach was able to capture the unsteady lifted flame dynamics observed in the experiment and obtained good profile with the experimental data [41].

Hegetschweiler *et al.* explained the combustion modeling approach for premixed, non-premixed and partially premixed combustion. As already described the laminar flamelet models have valuable applicability in non-premixed flame simulation but this approach is also applicable in partially premixed regime. So, in this paper laminar flamelet concept is used for the simulation of non-premixed turbulent combustion. The joint PDF method is used to find statistics of a progress variable, mixture fraction and scalar dissipation rate. Numerical study of turbulent lifted diffusion flame and a premixed Bunsen Flame was evolved to make it applicable for various industries. The results shows that 2D model of premixed Bunsen Flame is good in premixed combustion and in partially premixed combustion[42].

Jianwen *et al.* used PDF approaches for the turbulent chemistry interaction.They used two different PDF approaches first is Pope's evolution approaches, and the assumed PDF method. Laminar flamelet model was used to simulate interaction of turbulent and combustion was scramjet. Modified CFD code AHL3D was applied to simulate DLR scramjet and compared the result with previous studies [43].

Baudoin *et al.* explained the CFD approach used for the studyof turbulent premixed and partially premixed combustion. In this study the modeling based on flamelet concept is used in which G equation is applied to study high density ratio flames. The application of model for premixed and partially premixed combustion process validate and modelling used lean premixed bluff body stabilized by flames and partially premixed flames stabilized in a conical burner[44].Traditionally DNS data and experimental was used by burning velocity model for determining the series of coefficients [45].Burning velocity model for the simulation of flows in which combustion reactions occur. It is also known as turbulent flame closure. This model used to close the combustion source term for reaction progress. The reaction progress is computed in burning velocity model [46]:

$$\frac{\partial(\tilde{\rho}\tilde{c})}{\partial t}+\frac{\partial(\tilde{u_j}\tilde{c})}{\partial t}=\frac{\partial}{\partial x_j}\left[\left(\overline{\rho D}+\frac{\mu_t}{\sigma_c}\right)\frac{\partial\tilde{c}}{\partial x_j}\right]+\overline{w_c}$$

$$\overline{w_c}=\bar{S_c}-\frac{\partial}{\partial x_j}\left[(\overline{\rho D})\frac{\partial\tilde{c}}{\partial x_j}\right]$$

$\bar{S_c}=\overline{\rho_u}S_T\left|\widetilde{\nabla c}\right|$

$\bar{S_c}$=source term,

D=Damkohler Number.

$\mu_t = viscosity,$

$\tilde{c}$=progress variable.

Peters applied level set approach for the study of premixed turbulent combustion. The study was based on Kolmogorav number scale that is used define the reaction zone regime. The Kolmogorav scale is smaller than flame thickness, in this problem due to this; thin reaction zone investigation was used [47].

II. Conclusion

The reviewed study of combustion modeling concluded that the three approaches DNS, LES, RANS have many advantageous features. Many models and sub-models are developed for the simulation of combustion system. But still there is lot of scope in their application. The defined equation can be further modified for the new models. DNS approach as compared to LES and RANS are less efficient. This review makes us understand the basic requirement of simulation. LES approach has many applicable features and less time consuming approach. RANS on the other hand, is an effective approach but conclusively very expensive.Eddy Dissipation Model is very efficient for the simulation of one step combustion reaction. But for the simulation of multistep combustion reaction, finite rate chemistry and EDM approach are combined together to get efficient results. PDF approach is one of the best approaches for turbulence chemistry interaction study in premixed combustion.The approaches and combustion make the simulation of complex geometries easier and less time consuming.

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