Simulation of In Cylinder Processes Accounting SDR Fluctuations for Better Predictions Using Hemispherical Piston

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Abstract: The research pertaining to modeling of engine processes is growing day by day where the important information about Incylinder fluid motion, turbulence, temperature distribution, species concentration and many other characteristics are predicted. The Incylinder gas flow is complex three dimensional, unsteady and turbulent and hence poses many problems and uncertainties in the theoretical predictions. The computational Fluid Dynamic models have gained momentum with the advent of high end computers for analysis of IC engine combustion process. The Computational Fluid Dynamic code considered at present is FLUENT. It is found that ignoring the effect of Scalar Dissipation Rate Fluctuations may cause inconsistency in predictions. Hence it is aimed to adopt Scalar Dissipation Rate Fluctuations by writing the User Defined Function (UDF) and appending it to existing code. The validation of the modified computer code is done by comparing the measured available data. It is a known fact that piston bowl configuration plays a vital role on the air motion and performance of the engine. In order to understand and demonstrate this effect, computations for spherical bowl configurations have been carried out. The results predicted with and without scalar dissipation rate fluctuations are compared to ascertain the need of inclusion of scalar dissipation rate fluctuations.

Keywords: SDRF, CFD, Flamelet equation, PDF

1.Introduction

Compression ignition combustion process is extremely complex. The details of the process depend on the characteristics of the fuel, on the design of the engine combustion chamber and fuel-injection system and on the engine operating conditions. It is unsteady, heterogeneous and three dimensional combustion process. While adequate conceptual understanding of diesel engine combustion process has been developed, to date an ability to describe many of the critical individual processes in a quantitative manner is lacking. A better understanding of the in-cylinder fluid motion will help in simplifying the above problem to a great extent.

2. Problem Definition

It is not agreed that the codes using multidimensional modeling are consistent for all operating conditions and for a wide variety of engines. When the inconsistency of the predictions being questioned the reasons are attributed to the restrictions and assumptions imposed on the codes. The assumptions are justified particularly while dealing with the problems on in-cylinder flows which involves complex equations and also in view of simplicity of the code. One such important restriction that is ignoring the effect of scalar dissipation rate fluctuations henceforth called as SDRF is accounted. Hence it is proposed to look into this gap and come out with possible inclusion of SDRF in multidimensional modeling. For this purpose, the fluid dynamic code FLUENT is selected in the present work, because the code has greater flexibility to write user defined functions (UDF) suitable to different applications.

Initially it is planned to check the validity of the predictions when SDRF is accounted and compared using available experimental data in the literature. The bowl configuration considered for analyses is Hemispherical Bowl (HSB). For the injection timing of 28° bTDC and the injection duration of 23.5° and the swirl ratios 2.

3. Theory of Computation

In technical process, combustion always takes place within a turbulent rather than a laminar flow field. The reason for this is twofold: First, turbulence increases the mixing processes and thereby enhances combustion. Second, combustion releases heat and thereby generates flow instability by buoyancy and gas expansion, which then enhances the transition to turbulence.[1]

The turbulence combustion models rely on the modeling procedures which are highly disputed because they rely on empiricism and some kind of intuition supplemented by physical arguments [2]. It is clear that with combustion, empiricism and the number of necessary simplifications increase. This is reflected by the large variety of different combustion models that have been formulated and that are pursued and continuously improved by different groups in the combustion community.

FLUENT have the inbuilt models such as turbulence models, spray models, combustion models etc. More attention is paid on the turbulent combustion models which are responsible for non premixed combustion and the emphasis is more focused on introducing the flamelet equations responsible for accounting the effect of SDRF. The non premixed modeling approach involves the solution of transport equations for one or two conserved scalar (mixture fraction). Equations for individual species are not solved. Instead species concentrations are derived from the predicted mixture fraction fields. The thermochemistry calculations are processed and then tabulated for look-up in FLUENT.

Volume 3 Issue 3, March 2014 www.ijsr.net

3.1 Flamelet equations

Assuming an irreversible one-step reaction of the form $V_{F}F + V_{0}D - > Pv$

Where F,O and D denote the feel, oxidizer and reaction product respectively, the flamelet equations for the mass fractions of fuel y_F , oxidizer y_0 reaction product y_p and temperature T

$$\frac{\partial y_i}{\partial t} - \frac{x}{2} \frac{\partial^2 y_i}{\partial Z^2} + v_i W_i \omega = 0.0 \dots 1 \text{ i} = \text{F}, 0, \text{F}$$
$$\frac{\partial T}{\partial t} - \frac{x}{2} \frac{\partial^2 T}{\partial Z^2} - \frac{Q}{cp} \omega = 0.0 \dots 2$$
Where $Q = -\sum_{i=1}^N v_i W_i h_i \dots 3$

3.2 Non-dimensionalization

In order to investigate the flamelet equations with respect to the relevant non-dimensional parameters it is convenient to introduce the non-dimensional temperature θ and mass fractions of fuel y_F , oxidizer y_0 and reaction product y_P [3]as

$$\theta = \left(\frac{T - T_{st,u}}{T_{st,b} - T_{st,u}}\right) \quad \dots \dots 4$$

By non-dimensional we can yet multi information at a time θ

including various parameters ex:Re= $\frac{\rho l V}{V}$

$$y_{F} = \frac{y_{F}}{y_{F,st,u}} \dots 5$$

$$y_{0} = \frac{y_{0}}{y_{D,st,u}} \dots 6$$

$$y_{P} = (\nu + 1) \frac{\nu_{F} W_{F} \nu_{P}}{\nu_{P} W_{P} \nu_{F,1}} \dots 7$$

The mixture fraction equation can be expressed as

$$Z = \left(\frac{\nu y_F - y_0 + 1}{\nu + 1}\right).....8$$

Where the reference value for the scalar dissipation rate $X_{st,0}$ and the parameter Δz will be introduced. The nondimensional scalar dissipation rate x, the Damkohler's number D_a and the zeldovich number Z_e are defined as

$$x = \frac{X}{X_{st,0}} \dots 9$$

$$D_{a} = \frac{VV_{F} a P_{st,u} y_{0}}{(1+v)W_{0}} \frac{A}{X_{st,D}} \exp(-\beta_{ref}) \dots 10$$

Where the non-dimensional chemical source term is given by

$$\omega = D_a \frac{(1+\nu)^2 (1-\alpha) \exp(\beta_{ref} - \beta)}{1-\alpha(1-\theta)} y_F y_0 \exp\left(-\frac{Z_e(1-\theta)}{1-\alpha(1-\theta)}\right) \dots \dots 11$$

$$\omega = D_a \frac{(1-\alpha)\exp(\beta_{ref} - \beta)}{1-\alpha(1-\theta)} \left(\frac{z}{z_{st}} - \theta\right) \exp\left(-\frac{z_e(1-\theta)}{1-\alpha(1-\theta)}\right) \dots 12$$

with equation 12 the flamelet equation for the nondimensional temperature depends only on temperature itself and can be integrated without solving the equations for the mass fractions of fuel oxidizer and product.

3.3 Stochastic differential equations

Here a joint pdf of the temperature and the scalar dissipation rate are derived. To complete above equation we need a stochastic differential equation (SDE) that governs the evolution of the scalar dissipation rate.

We consider strantonovich SDE given by

$$dX_{st} = f(X_{st})dt + \sigma\phi(X_{st})dW(t).....13$$

Where W(t) denotes Wiener process. The stationary probability density function corresponding to strantonovich SDE can be found

$$P_{s}(X_{st}) = \frac{N}{\sigma\phi(X_{st})} \exp\left(\int_{0}^{X_{st}} \frac{2f(z)dz}{\sigma^{2}\phi^{2}(z)}\right) \dots \dots 14$$

A good approximation for a stationary P.D.F [4] of $X_{st}(t)$ is a log normal distribution given as

$$P_{s}(X_{st}) = \frac{1}{X_{st}} \frac{1}{\sqrt{2\pi\sigma^{2}}} \exp\left(-\frac{\left(\ln X_{st} - \ln X_{st,0}\right)^{2}}{2\sigma^{2}}\right) \dots \dots \dots 15$$

The diffusion term evaluated at stoichiometric conditions can be written using Taylor series of approximation.

Substituting above equation in flamelet equation

$$\frac{d\theta_{st}}{d\tau} + x(\tau)\theta_{st} - \omega(\theta_{st}) = 0.0 \dots 17$$

with
$$D_a(1-\alpha)\exp(\beta_{ref} - \beta)(1-\alpha)^2 \exp(-\frac{Z_e(1-\theta_{st})}{2}) = 18$$

 $\frac{1-\alpha(1-\theta_{st})}{1-\alpha(1-\theta_{st})}(1-\theta_{st})^2 \exp\left(-\frac{2\epsilon(1-\theta_{st})}{1-\alpha(1-\theta_{st})}\right)$ This equation analyzes how random fluctuations of the scalar dissipation rate can influence the non-premixed combustion process.

4. Results and Discussion

By till date number of works is attempted by using the fluid dynamic codes which are commercially available. But lot of inconsistency in results is noticed. The results are presented accounting the effect of SDRF. The results obtained with and without SDRF inclusion are compared. Also the results are validated with the available experimental data and good agreement is noticed. The consistency and reduction in the error percentage in results are observed taking into account the scalar dissipation rate fluctuations. The tangential velocity vectors at selected planes within the piston bowl are presented which depict the true information of the flow field.

Volume 3 Issue 3, March 2014 www.ijsr.net

Paper ID: 020131030

4.1 Modeling, Meshing and post processing of results

Model is created using GAMBIT. For Hemispherical bowl the meshing is done using hexahedral elements. The number of cells considered for meshing is around 654400. FLUENT 6.3 Version [5] is used for solving and for post processing the results.

4.2 Presentation of results

The results pertaining to test computations for an engine fitted with a hemispherical bowl-in-piston is discussed.

4.3 Test Computations

These computations pertain to the test engine fitted with hemi-spherical bowl-in-piston. Fig 4.1 shows the view of typical mesh which represents the in-cylinder flow field. The computed pressure histories considering the effect of SDRF and ignoring SDRF is compared with the available measured pressure histories.

4.3.1 Comparison of experimental and predicted pressure histories

Figure 4.2 gives the comparison of the predicted and experimental pressure histories. A good agreement is obtained during compression. The predicted pressures are slightly higher during the combustion and the small deviation between the two goes hand in hand during the later part of expansion stroke. In the normal engine operation, the incylinder charge prior to the combustion contains some portion of residual gases which could not be exhausted completely in the previous cycle. But only pure air without any residual gas is assumed to be compressed, in the present modeling. Hence higher predicted combustion pressures are resulted. The predicted peak pressures without SDRF, experimental [6] and with SDRF are 7.147 MPa, 6.829 MPa and 7.01Mpa respectively. The %error in the predicted peak pressure without SDRF and experimental value is 4.449% and the %error in the predicted peak pressure with SDRF and experimental value is 2.58%.

4.3.2 Variation of temperature with crank angle

Temperature inside the engine cylinder is almost the lowest at the end of the suction stroke. During combustion, there is a rapid rise in temperature to a peak value which again drops during the expansion. Fig 4.3 gives the comparison between predicted without SDRF, experimental and predicted with SDRF values for cylinder temperatures. The maximum cylinder temperature attained is 2620.61 k, 2601.9 k and 2610 for without SDRF, experimental and with SDRF values respectively. The problem with the attainment of high temperatures in the engine cylinder is that the high temperatures are responsible for the formation of NO_x at high temperature.

4.3.3 Variation of total energy with crank angle

Figure 4.4 shows the variation of total energy with crank angle. The peak energy reached during the operating cycle is 449 KJ\kg without SDRF, 429 KJ\kg for experimental and 442 KJ\kg for with SDRF. Generally it is more difficult to determine the start of combustion precisely. It is normally identified from the change in slope of the heat release rate.

The pressure rate alone may indicate this, when the pressure change first occurs due to combustion. The cumulative energy only increases when there is start of combustion and prior to that no substantial growth in energy is noticed.

4.3.4 Variation of turbulent kinetic with crank angle

In turbulent flows, local fluctuations in the flow field results in molecular diffusions. It leads to increased rates of momentum and heat and mass transfers, which is essential for the rapid mixing of the fuel and air in CI engines. Turbulent flows are always dissipative [7]. Viscous shear stresses perform deformation work on the fluid which increases its internal energy at the expense of its turbulent kinetic energy (TKE). So energy is required to generate turbulence. If no energy is supplied turbulence decays. A common source of energy for turbulent velocity fluctuations is shear in the mean flow. Fig 4.5 shows the variation of TKE with crank angle. Increased TKE can be observed near TDC. The peak values of TKE with and without SDRF are 93.96 m²/s² and 93.11 m²/s² respectively.

4.3.5 Emissions

Computed NO, HC, CO, and CO_2 characteristics are presented. Available experimental results for HC and CO are compared with those of computed values with and without considering the effect of SDRF.

4.3.5.1 HC emissions:

Hydrocarbons or more appropriately organic emissions are the consequence of incomplete combustion of the hydrocarbon fuel. The total hydrocarbon emission is a useful measure of combustion efficiency. There are many processes that could contribute the HC emissions in a diesel engine. The two primary paths by which fuel can escape the normal combustion process without burning: the fuel-air mixture can become too lean to auto ignite or to support a propagating flame at the conditions prevailing inside the combustion chamber, or, during the primary combustion process, the fuel air mixture may be too rich to ignite or support a flame. This fuel can then be consumed only by slower thermal oxidation reactions later in the expansion process after mixing with additional air. Thus hydrocarbons remained unconsumed due to improper mixing of fuel and air.

Figure 4.6 gives the variation of HC emission with crank angle. It is noticed that the HC mass in the cylinder gradually reduces and remains constant during later part of the expansion stroke. This mass is considered to be exhausted during the exhaust stroke. This measured HC emission is marked on the y-axis. The prediction with and without SDRF and the measured emissions show moderate agreement. The predicted value of HC emission with and without SDRF is 0.003% and 0.0029% where as the measured value is 0.0022%. In actual engine operation the blow-by bypasses some of the unburnt hydrocarbons thus reducing its composition in the exhaust. As already mentioned, this blowby phenomenon is not included in this present model which may be one of the reasons for higher value of predicted emissions.

4.3.5.2 NO Emission

While Nitric oxide (NO) and nitrogen dioxide (N₂O) are usually grouped together as NO_x emission, nitric oxide (NO)

is the predominant oxide of nitrogen produced inside the engine cylinder. The principal source of NO is the oxidation of atmospheric nitrogen. However, if the fuel contains significant nitrogen, the oxidation of the nitrogen in the fuel is an additional source of NO.

Figure 4.7 show the NO emission verses crank angle. The figure shows that NO emission is more pronounced when the in-cylinder gas temperature is very high. Cooling and expansion of gas ceases the No producing reactions. The maximum NO without SDRF is 0.01535% and with SDRF NO is 0.01522%.

4.5.5.3 CO Emission

It is generated in an engine when it is operated with a fuelrich equivalence ratio. When there is not enough oxygen to convert all carbon to CO_2 , some fuel doesn't get burned and some carbon ends up with CO. Not only CO is considered as an undesirable emission, but it also represents lost chemical energy. As diesel engine operates on overall lean side generally they have very low CO emissions. Figure 4.8 gives CO emission versus crank angle. The CO emission with and without SDRF is 0.312% and 0.305% where as the measured value is 0.318% during one cycle of operation. Measured CO emission is more. In the engine, significant fraction of the carbon atoms are involved in soot formation and combustion which give rise to CO formation. This phenomenon is not included in this model and hence may result in agreement with predicted emission.

4.3.5.4 CO₂ Emission

With rich fuel-air there is insufficient oxygen to burn all the carbon in the fuel to form CO_2 . That means carbon dioxide forms due to the burning of carbon in the fuel in the presence of oxygen and hence it can be correlated to the combustion efficiency. Fig 4.9 gives the variation of CO_2 emission with crank angle. During one cycle of operation, CO_2 emission without and with SDRF is 0.1723% and 1688% respectively.

4.3.6 In-Cylinder Flow Predictions

The predicted velocities of the in-cylinder gas are represented by means of velocity vector plots. For better understanding of the results, the results are presented in K-plane. However it may be noted that these plots represent the velocity components at each mesh point in that particular point only but not the velocities in the entire cylinder domain. In total five appropriate locations of the bowl namely K₁, K₂, K₃, K₄ and K₅ are selected for the presentations of results. The velocity contours are presented with respect to various crank angle positions at TDC (without and with SDRF for K₃, K4 and K₅ planes), 5⁰ aTDC (without and with SDRF for K₁, K₂, K₃, K₄ and K₅ planes) and 10⁰ aTDC (without and with SDRF for K₁, K₂, K₃, K₄ and K₅ planes).

4.3.6.1 Velocity vectors in different k-Planes

Plots which are important to be illustrated are chosen carefully for presentation. Five planes namely K_1 , K_2 , K_3 , K_4 and K_5 from the bottom of the piston bowl to top of the piston bowl were chosen. Fig 3.10 gives the velocity plots in K_3 , K_4 and K_5 planes at TDC. It is observed that the velocities in the lower planes are less. From the fig 4.10 K_3 plane, the tangential velocity increases with radius on either direction of the cylinder axis. It is also interesting to observe

the increase in swirl in k_3 plane is less. In fig 4.10 (K₄ plane), the tangential velocity further increases in this plane because within bowl the velocities in the upper planes are higher. It is interesting to note that the angular momentum is decreasing during compression while the angular velocities (swirl velocities) are increasing. This is quite possible in engines with bowl-in-piston. The reason for this is explained below.

The total angular momentum of the charge within the cylinder does decay due to friction and turbulent dissipation [8]. However the computer generated vector plots show swirling velocities of the charge increasing substantially. The total angular momentum is a product of moment of inertia of the gas about the cylinder axis and angular velocity. With a bowl in piston the moment of inertia of the gas reduces gradually as the piston moves upward, being minimum at TDC. Neglecting the effects of friction, angular momentum is conserved and with the decrease of moment of inertia, the swirl velocity must increase.

In figure 4.10 (refer K_5 plane), as the plane is selected away from the top of the bowl, substantial reduction in the swirl velocities can be witnessed. The vectors appear to be in an organized manner with the reduced swirls. From fig 4.11 when the crank angle is 5^o aTDC, in all the planes weak swirl is observed owing to the fact that the combustion inside the cylinder is completed. The disturbed swirl, when the piston is at TDC now appeared to be reestablished.

Simultaneous representation of all the velocity vectors considering the effect of SDRF is presented in figures. In general, the dominant physical processes are those of non linear amplification by scalar dissipation rate fluctuations and destruction by molecular diffusivity [9]. Scalar dissipation tends to form elongated structures in space, with only a limited overlap with zones of intense energy dissipation. Though this overlap is marginal, this is responsible for the reduction in the intensity of velocity vectors that is apparently seen in the velocity vector distribution plots considering the effect of SDRF.



Figure 4.1: Computational mesh of hemispherical bowl

International Journal of Science and Research (IJSR) ISSN (Online): 2319-7064



Figure 4.2: Variation of cylinder pressure with crank angle



Figure 4.3: Variation of temperature with crank angle



Figure 4.4: variation of energy with crank angle



Figure 4.5: variation of turbulent kinetic energy with crank angle



Figure 4.6: variation of mass fraction of HC with crank angle







Figure 4.8: variation of mass fraction of CO with crank angle



Figure 4.9: Variation of mass fraction of CO₂ with crank angle

International Journal of Science and Research (IJSR) ISSN (Online): 2319-7064







International Journal of Science and Research (IJSR) ISSN (Online): 2319-7064



(a₂) Top view Two views of velocity vectors in K₅ plane when crank angle is at TDC with SDRF Fig 4.10[b₁]



 (a₂) Top view Fig 3.11(b₁) Two views of velocity vectors in K₁ plane at crank angle 5° aTDC without SDRF

International Journal of Science and Research (IJSR) ISSN (Online): 2319-7064



(a2) Top view Two views of velocity vectors in K2 plane at crank angle 5° aTDC with SDRF Fig 4.11(b₁)





(a2) Top view Two views of velocity vectors in K2 plane at crank angle 5° aTDC with SDRF Fig 4.11(b₁)(contd)

International Journal of Science and Research (IJSR) ISSN (Online): 2319-7064





5. Conclusions

SDRF found to have tremendous impact on the in-cylinder flow processes. The predicted results with and without SDRF are compared with the available experimental data. It is concluded that it is better to rely on accounting the effect of SDRF which is nearer to validated results. The important conclusions from the present paper are presented in the subsequent sections.

5.1 Test Computations

- The validity of the results accounting SDRF is assessed by comparing the predicted and available measured pressure histories. The results are encouraging as very good agreement is noticed for the pressure histories reducing error percentage between predicted and measured histories and also for temperature variations.
- There is larger deviation in case of total energy for experimental and predicted values and predictions with SDRF come as compromise between the two testifying the importance of inclusion of SDRF.

5.2 Effect of piston bowl configuration

- Hemispherical bowl gives optimum values in view of pollutant emissions. In this case CO, NO and HC are very much optimum.
- The gas flow velocities are maximum up to the top of the bowl and outside the bowl portion they are minimum. Swirl velocities increase during the compression stroke and decrease during expansion stroke.

6. Future Scope

There are lot of inconsistencies observed in the predictions and are attributed to the restrictions and assumptions imposed on the codes. Hence the predictive capability of the tool may be increased by possible inclusion of some more restrictions and assumptions.

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